IMSL
by Perforce

IMSL® Fortran Math Library

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ACKNOWLEDGMENTS

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Introduction

The IMSL Fortran Numerical Library

The IMSL Fortran Numerical Library consists of two separate but coordinated Libraries that allow easy user access. These Libraries are organized as follows:

- MATH/LIBRARY general applied mathematics and special functions

  The User's Guide for IMSL MATH/LIBRARY has two parts:

  - MATH/LIBRARY
  - MATH/LIBRARY Special Functions
- STAT/LIBRARY statistics

Most of the routines are available in both single and double precision versions. Many routines for linear solvers and eigensystems are also available for complex and double -complex precision arithmetic. The same user interface is found on the many hardware versions that span the range from personal computer to supercomputer.

This library is the result of a merging of the products: IMSL Fortran Numerical Libraries and IMSL Fortran 90 Library.

User Background

To use this product you should be familiar with the Fortran 90 language as well as the withdrawn Fortran 77 language, which is, in practice, a subset of Fortran 90. A summary of the ISO and ANSI standard language is found in Metcalf and Reid (1990). A more comprehensive illustration is given in Adams et al. (1992).

Those routines implemented in the IMSL Fortran Numerical Library provide a simpler, more reliable user interface than was possible with Fortran 77. Features of the IMSL Fortran Numerical Library include the use of descriptive names, short required argument lists, packaged user-interface blocks, a suite of testing and benchmark software, and a collection of examples. Source code is provided for the benchmark software and examples.

Some of the routines in the IMSL Fortran Numerical Library can take advantage of a standard (MPI) Message Passing Interface environment but do not require an MPI environment if the user chooses to not take advantage of MPI.

The MPI logo shown below cues the reader when this is the case:

MPI CAPABLE

Routines documented with the MPI Capable logo can be called in a scalar or one computer environment.

Other routines in the IMSL Library take advantage of MPI and require that an MPI environment be present in order to use them. The MPI Required logo shown below clues the reader when this is the case:

MPI REQUIRED

NOTE: It is recommended that users considering using the MPI capabilities of the product read the following sections of the MATH Library documentation:

Introduction: *Using MPI Routines*

Introduction: *Using ScaLAPACK Enhanced Routines*

Chapter 10, "Linear Algebra Operators and Generic Functions" – see *"Dense Matrix Parallelism Using MPI"*.

Vendor Supplied Libraries Usage

The IMSL Fortran Numerical Library contains functions which may take advantage of functions in vendor supplied libraries such as the Intel® Math Kernel Library (MKL) or the Sun™ High Performance Library. Functions in the vendor supplied libraries are finely tuned for performance to take full advantage of the environment for which they are supplied. For these functions, the user of the IMSL Fortran Numerical Library has the option of linking to code which is based on either the IMSL legacy functions or the functions in the vendor supplied library. The following icon in the function documentation alerts the reader when this is the case:

Details on linking to the appropriate IMSL Library and alternate vendor supplied libraries are explained in the online README file of the product distribution.

Getting Started

The IMSL MATH/LIBRARY is a collection of Fortran routines and functions useful in mathematical analysis research and application development. Each routine is designed and documented for use in research activities as well as by technical specialists.

To use any of these routines, you must write a program in Fortran 90 (or possibly some other language) to call the MATH/LIBRARY routine. Each routine conforms to established conventions in programming and documentation. We give first priority in development to efficient algorithms, clear documentation, and accurate results. The uniform design of the routines makes it easy to use more than one routine in a given application. Also, you will find that the design consistency enables you to apply your experience with one MATH/LIBRARY routine to other IMSL routines that you use.

Finding the Right Routine

The MATH/LIBRARY is organized into chapters; each chapter contains routines with similar computational or analytical capabilities. To locate the right routine for a given problem, you may use either the table of contents located in each chapter introduction, or the alphabetical list of routines.

Often the quickest way to use the MATH/LIBRARY is to find an example similar to your problem and then to mimic the example. Each routine document has at least one example demonstrating its application. The example for a routine may be created simply for illustration, it may be from a textbook (with reference to the source), or it may be from the mathematical literature.

Organization of the Documentation

This manual contains a concise description of each routine, with at least one demonstrated example of each routine, including sample input and results. You will find all information pertaining to the MATH/LIBRARY in this manual. Moreover, all information pertaining to a particular routine is in one place within a chapter.

Each chapter begins with an introduction followed by a table of contents that lists the routines included in the chapter. Documentation of the routines consists of the following information:

- IMSL Routine's Generic Name
- Purpose: a statement of the purpose of the routine. If the routine is a function rather than a subroutine the purpose statement will reflect this fact.
- Function Return Value: a description of the return value (for functions only).
- Required Arguments: a description of the required arguments in the order of their occurrence. Input arguments usually occur first, followed by input/output arguments, with output arguments described last. Futhermore, the following terms apply to arguments:
    - **Input** Argument must be initialized; it is not changed by the routine.
    - **Input/Output** Argument must be initialized; the routine returns output through this argument; cannot be a constant or an expression.
    - **Input[/Output]** Argument must be initialized; the routine may return output through this argument based on other optional data the user may choose to pass to this routine; cannot be a constant or an expression.
    - **Input or Output** Select appropriate option to define the argument as either input or output. See individual routines for further instructions.
    - **Output** No initialization is necessary; cannot be a constant or an expression. The routine returns output through this argument.
- Optional Arguments: a description of the optional arguments in the order of their occurrence.
- Fortran 90 Interface: a section that describes the generic and specific interfaces to the routine.
- Fortran 77 Style Interface: an optional section, which describes Fortran 77 style interfaces, is supplied for backwards compatibility with previous versions of the Library.
- ScaLAPACK Interface: an optional section, which describes an interface to a ScaLAPACK-based version of this routine.
- Description: a description of the algorithm and references to detailed information. In many cases, other IMSL routines with similar or complementary functions are noted.

- Comments: details pertaining to code usage.
- Programming notes: an optional section that contains programming details not covered elsewhere.
- Example: at least one application of this routine showing input and required dimension and type statements.
- Output: results from the example(s). **Note** that unique solutions may differ from platform to platform.
- Additional Examples: an optional section with additional applications of this routine showing input and required dimension and type statements.

Naming Conventions

The names of the routines are mnemonic and unique. Most routines are available in both a single precision and a double precision version, with names of the two versions sharing a common root. The root name is also the generic interface name. The name of the double precision specific version begins with a "D_" and the single precision specific version begins with an "S_". For example, the following pairs are precision specific names of routines in the two different precisions: S_GQRUL/D_GQRUL (the root is "GQRUL ," for "Gauss quadrature rule") and S_RECCF/D_RECCF (the root is "RECCF," for "recurrence coefficient"). The precision specific names of the IMSL routines that return or accept the type complex data begin with the letter "C_" or "Z_" for complex or double complex, respectively. Of course, the generic name can be used as an entry point for all precisions supported.

When this convention is not followed the generic and specific interfaces are noted in the documentation. For example, in the case of the BLAS and trigonometric intrinsic functions where standard names are already established, the standard names are used as the precision specific names. There may also be other interfaces supplied to the routine to provide for backwards compatibility with previous versions of the IMSL Fortran Numerical Library. These alternate interfaces are noted in the documentation when they are available.

Except when expressly stated otherwise, the names of the variables in the argument lists follow the Fortran default type for integer and floating point. In other words, a variable whose name begins with one of the letters "I" through "N" is of type INTEGER, and otherwise is of type REAL or DOUBLE PRECISION, depending on the precision of the routine.

An assumed-size array with more than one dimension that is used as a Fortran argument can have an assumed-size declarator for the last dimension only. In the MATH/LIBRARY routines, the information about the first dimension is passed by a variable with the prefix "LD" and with the array name as the root. For example, the argument LDA contains the leading dimension of array *A*. In most cases, information about the dimensions of arrays is obtained from the array through the use of Fortran 90's *size* function. Therefore, arguments carrying this type of information are usually defined as optional arguments.

Where appropriate, the same variable name is used consistently throughout a chapter in the MATH/LIBRARY. For example, in the routines for random number generation, NR denotes the number of random numbers to be generated, and R or IR denotes the array that stores the numbers.

When writing programs accessing the MATH/LIBRARY, the user should choose Fortran names that do not conflict with names of IMSL subroutines, functions, or named common blocks. The careful user can avoid any conflicts with IMSL names if, in choosing names, the following rules are observed:

- Do not choose a name that appears in the Alphabetical Summary of Routines, at the end of the *User's Manual*, nor one of these names preceded by a D, S_, D_, C_, or Z_.

- Do not choose a name consisting of more than three characters with a numeral in the second or third position.

For further details, see the section on *Reserved Names* in the Reference Material.

Using Library Subprograms

The documentation for the routines uses the generic name and omits the prefix, and hence the entire suite of routines for that subject is documented under the generic name.

Examples that appear in the documentation also use the generic name. To further illustrate this principle, note the `LIN_SOL_GEN` documentation (see *Chapter 1, "Linear Systems"*), for solving general systems of linear algebraic equations. A description is provided for just one data type. There are four documented routines in this subject area: `s_lin_sol_gen`, `d_lin_sol_gen`, `c_lin_sol_gen`, and `z_lin_sol_gen`.

These routines constitute single-precision, double-precision, complex, and double-complex precision versions of the code.

The Fortran 90 compiler identifies the appropriate routine. Use of a module is required with the routines. The naming convention for modules joins the suffix "`_int`" to the generic routine name. Thus, the line "use `lin_sol_gen_int`" is inserted near the top of any routine that calls the subprogram "`lin_sol_gen`". More inclusive modules are also available, such as `imsl_libraries` and `numerical libraries`. To avoid name conflicts, Fortran 90 permits re-labeling names defined in modules so they do not conflict with names of routines or variables in the user's program. The user can also restrict access to names defined in IMSL Library modules by use of the "**: ONLY, <list of names>**" qualifier.

When dealing with a complex matrix, all references to the *transpose* of a matrix, A^T, are replaced by the *adjoint* matrix

$$\bar{A}^T \equiv A^* = A^H$$

where the overstrike denotes complex conjugation. IMSL Fortran Numerical Library linear algebra software uses this convention to conserve the utility of generic documentation for that code subject. All references to *orthogonal* matrices are to be replaced by their complex counterparts, *unitary* matrices. Thus, an $n \times n$ orthogonal matrix Q satisfies the condition $Q^T Q = I_n$. An $n \times n$ unitary matrix V satisfies the analogous condition for complex matrices, $V^* V = I_n$.

Programming Conventions

In general, the IMSL MATH/LIBRARY codes are written so that computations are not affected by underflow, provided the system (hardware or software) places a zero value in the register. In this case, system error messages indicating underflow should be ignored.

IMSL codes are also written to avoid overflow. A program that produces system error messages indicating overflow should be examined for programming errors such as incorrect input data, mismatch of argument types, or improper dimensioning.

In many cases, the documentation for a routine points out common pitfalls that can lead to failure of the algorithm.

Library routines detect error conditions, classify them as to severity, and treat them accordingly. This error-handling capability provides automatic protection for the user without requiring the user to make any specific provisions for the treatment of error conditions. See the section on *User Errors* in the Reference Material for further details.

Module Usage

Users are required to incorporate a “use” statement near the top of their program for the IMSL routine being called when writing new code that uses this library. However, legacy code which calls routines in the previous version of the library without the use of a “use” statement will continue to work as before. Also, code that employed the “`use numerical_libraries`” statement from the previous version of the library will continue to work properly with this version of the library.

Users wishing to update existing programs so as to call other routines from this library should incorporate a use statement for the specific new routine being called. (Here, the term “new routine” implies any routine in the library, only “new” to the user’s program.) Use of the more encompassing “`imsl_libraries`” module in this case could result in argument mismatches for the “old” routine(s) being called. (The compiler would catch this.)

Users wishing to update existing programs to call the new generic versions of the routines must change their calls to the existing routines to match the new calling sequences and use either the routine specific interface modules or the all-encompassing “`imsl_libraries`” module.

Using MPI Routines

Users of the IMSL Fortran Numerical Library benefit by having a standard (MPI) Message Passing Interface environment. This is needed to accomplish parallel computing within parts of the Library. *Either of the icons above clues the reader when this is the case*. If parallel computing is not required, then the IMSL Library suite of dummy MPI routines can be substituted for standard MPI routines. All requested MPI routines called by the IMSL Library are in this dummy suite. Warning messages will appear if a code or example requires more than one process to execute. Typically users need not be aware of the parallel codes.

NOTE: A standard MPI environment is not part of the IMSL Fortran Numerical Library. The standard includes a library of MPI Fortran and C routines, MPI “include” files, usage documentation, and other run-time utilities.

Details on linking to the appropriate libraries are explained in the online README file of the product distribution.

There are three situations of MPI usage in the IMSL Fortran Numerical Library:

1. There are some computations that are performed with the ‘box’ data type that benefit from the use of parallel processing. For computations involving a single array or a single problem, there is no IMSL use of parallel processing or MPI codes. The box type data type implies that several problems of the same size and type are to be computed and solved. Each rack of the box is an independent problem. This means that each problem could potentially be solved in parallel. The default for computing a box data type calculation is that a single processor will do all of the problems, one after the other. If this is acceptable there should be no further concern about which version of the libraries is used for linking. If the problems are to be solved in parallel, then the user must link with a working version of an MPI Library and the appropriate IMSL Library. Examples demonstrating the use of box type data may be found in *Chapter 10, “Linear Algebra Operators and Generic Functions”*.

NOTE: Box data type routines are marked with the MPI Capable icon.

2. Various routines in *Chapter 1, "Linear Systems"* allow the user to interface with the ScaLAPACK Library routines. If the user chooses to run on only one processor then these routines will utilize either IMSL Library code or LAPACK Library code based on the libraries the user chooses to use during linking. If the user chooses to run on multiple processors then working versions of MPI, ScaLAPACK, PBLAS, and Blacs will need to be present. These routines are marked with the MPI Capable icon.

3. There are some routines or operators in the Library that require that a working MPI Library be present in order for them to run. Examples are the large-scale parallel solvers and the ScaLAPACK utilities. Routines of this type are marked with the MPI Required icon. For these routines, the user must link with a working version of an MPI Library and the appropriate IMSL Library.

In all cases described above it is the user's responsibility to supply working versions of the aforementioned third party libraries when those libraries are required.

Table 1 below lists the chapters and IMSL routines calling MPI routines or the replacement non-parallel package.

Table 1 — IMSL Routines Calling MPI Routines or Replacement Non-Parallel Package

Chapter Name and Number	**Routine with MPI Utilized**
Linear Systems, 1	`PARALLEL_NONNEGATIVE_LSQ`
Linear Systems, 1	`PARALLEL_BOUNDED_LSQ`
Linear Systems, 1	`Those routines which utilize ScaLAPACK listed in` Table D below.
Linear Algebra and Generic Functions, 10	See entire following Table 2, "Defined Operators and Generic Functions for Dense Arrays."
Utilities, 11	`ScaLAPACK_SETUP`
Utilities, 11	`ScaLAPACK_GETDIM`
Utilities, 11	`ScaLAPACK_READ`
Utilities, 11	`ScaLAPACK_WRITE`
Utilities, 11	`ScaLAPACK_MAP`
Utilities, 11	`ScaLAPACK_UNMAP`
Utilities, 11	`ScaLAPACK_EXIT`
Reference Material	Entire Error Processor Package for IMSL Library, if MPI is utilized

Programming Tips

Each subject routine called or otherwise referenced requires the "use" statement for an interface block designed for that subject routine. The contents of this interface block are the interfaces to the separate routines available for that subject. Packaged descriptive names for option numbers that modify documented optional data or internal parameters might also be provided in the interface block. Although this seems like an additional complication, many errors are avoided at an early stage in development through the use of these interface blocks. The "use" statement is required for each routine called in the user's program. As illustrated in Examples 3 and 4 in routine `lin_geig_gen`, the "use" statement is required for defining the secondary option flags.

The function subprogram for `s_NaN()` or `d_NaN()` does not require an interface block because it has only a single "required" dummy argument. Also, if one is only using the Fortran 77 interfaces supplied for backwards compatibility then the "use" statements are not required.

Optional Subprogram Arguments

IMSL Fortran Numerical Library routines have *required* arguments and may have *optional* arguments. All arguments are documented for each routine. For example, consider the routine `lin_sol_gen` that solves the linear algebraic matrix equation $Ax = b$. The required arguments are three rank-2 Fortran 90 arrays: A, b, and x. The input data for the problem are the A and b arrays; the solution output is the x array. Often there are other arguments for this linear solver that are closely connected with the computation but are not as compelling as the primary problem. The inverse matrix A^{-1} may be needed as part of a larger application. To output this parameter, use the optional argument given by the "`ainv=`" keyword. The rank-2 output array argument used on the right-hand side of the equal sign contains the inverse matrix. See *Example 2 of LIN_SOL_GEN* in *Chapter 1, "Linear Systems"* for an example of computing the inverse matrix.

For compatibility with previous versions of the IMSL Libraries, the `NUMERICAL_LIBRARIES` interface module includes backwards-compatible positional argument interfaces to all routines that existed in the Fortran 77 version of the Library. Note that it is not necessary to include "use" statements when calling these routines by themselves. Existing programs that called these routines will continue to work in the same manner as before.

Some of the primary routines have arguments "`epack=`" and "`iopt=`". As noted the "`epack=`" argument is of derived type `s_error` or `d_error`. The prefix "`s_`" or "`d_`" is chosen depending on the precision of the data type for that routine. These optional arguments are part of the interface to certain routines, and are used to modify internal algorithm choices or other parameters.

Optional Data

This additional optional argument (available for some routines) is further distinguished—a derived type array that contains a number of parameters to modify the internal algorithm of a routine. This derived type has the name `?_options`, where "`?_`" is either "`s_`" or "`d_`". The choice depends on the precision of the data type. The declaration of this derived type is packaged within the modules for these codes.

The definition of the derived types is:

```
type ?_options
integer idummy; real(kind(?)) rdummy
end type
```

where the "`?_`" is either "`s_`" or "`d_`", and the `kind` value matches the desired data type indicated by the choice of "`s`" or "`d`".

Example 3 of LIN_SOL_GEN in *Chapter 1, "Linear Systems"* illustrates the use of iterative refinement to compute a double-precision solution based on a single-precision factorization of the matrix. This is communicated to the routine using an optional argument with optional data. For efficiency of iterative refinement, perform the factorization step once, and then save the factored matrix in the array *A* and the pivoting information in the rank-1 integer array, `ipivots`. By default, the factorization is normally discarded. To enable the routine to be re-entered with a previously computed factorization of the matrix, optional data are used as array entries in the "`iopt=`" optional argument. The packaging of `LIN_SOL_GEN` includes the definitions of the self-documenting integer parameters `lin_sol_gen_save_LU` and `lin_sol_gen_solve_A`. These parameters have the values 2 and 3, but the programmer usually does not need to be aware of it.
The following rules apply to the "`iopt=iopt`" optional argument:

1. Define a relative index, for example `IO`, for placing option numbers and data into the array argument `iopt`. Initially, set `IO` = 1. Before a call to the IMSL Library routine, follow Steps 2 through 4.

2. The data structure for the optional data array has the following form:
   `iopt (IO) = ?_options` (*Option_number*, *Optional_data*)
   [`iopt (IO + 1) =?_options` (*Option_number*, *Optional_data*)]
   The length of the data set is specified by the documentation for an individual routine. (The *Optional_data* is output in some cases and may not be used in other cases.) The square braces `[...]` denote optional items.

   Illustration: *Example 3 of LIN_EIG_SELF* in *Chapter 2, "Singular Value and Eigenvalue Decomposition"*, a new definition for a small diagonal term is passed to `lin_sol_self`. There is one line of code required for the change and the new tolerance:

```
iopt (1) = d_options(d_lin_sol_self_set_small,
epsilon(one) *abs (d(i)))
```

3. The internal processing of option numbers stops when *Option_number* == 0 or when `IO` > `SIZE(iopt)`. This signals each routine having this optional argument that all desired changes to default values of internal parameters have been made. This implies that the last option number is the value zero or the value of `SIZE(iopt)` matches the last optional value changed.

4. To add more options, replace `IO` with `IO` + *n*, where *n* is the number of items required for the previous option. Go to Step 2.

Option numbers can be written in any order, and any selected set of options can be changed from the defaults. They may be repeated. *Example 3 in of LIN_SOL_SELF* in *Chapter 1, "Linear Systems"* uses three and then four option numbers for purposes of computing an eigenvector associated with a known eigenvalue.

Overloaded =, /=, etc., for Derived Types

To assist users in writing compact and readable code, the IMSL Fortran Numerical Library provides overloaded assignment and logical operations for the derived types `s_options`, `d_options`, `s_error`, and `d_error`. Each of these derived types has an individual record consisting of an integer and a floating-point number. The components of the derived types, in all cases, are named `idummy` followed by `rdummy`. In many cases, the item referenced is the component `idummy`. This integer value can be used exactly as any integer by use of the `component selector` character (%). Thus, a program could assign a value and test after calling a routine:

```
     s_epack(1)%idummy = 0
     call lin_sol_gen(A,b,x,epack=s_epack)
     if (s_epack(1)%idummy > 0) call error_post(s_epack)
```

Using the overloaded assignment and logical operations, this code fragment can be written in the equivalent and more readable form:

```
     s_epack(1) = 0
     call lin_sol_gen(A,b,x,epack=s_epack)
     if (s_epack(1) > 0) call error_post(s_epack)
```

Generally the assignments and logical operations refer only to component `idummy`. The assignment "`s_epack(1)=0`" is equivalent to "`s_epack(1)=s_error(0,0E0)`". Thus, the floating-point component `rdummy` is assigned the value `0E0`. The assignment statement "`I=s_epack(1)`", for `I` an integer type, is equivalent to "`I=s_epack(1)%idummy`". The value of component `rdummy` is ignored in this assignment. For the logical operators, a single element of any of the IMSL Fortran Numerical Library derived types can be in either the first or second operand.

Derived Type	**Overloaded Assignments and Tests**						
`s_options`	`I=s_options(1);s_options(1)=I`	= =	/=	<	<=	>	>=
`d_options`	`I=d_options(1);d_options(1)=I`	= =	/=	<	<=	>	>=
`s_epack`	`I=s_epack(1);s_epack(1)=I`	= =	/=	<	<=	>	>=
`d_epack`	`I=d_epack(1);d_epack(1)=I`	= =	/=	<	<=	>	>=

In the examples, `operator_ex01`, … , `_ex37`, the overloaded assignments and tests have been used whenever they improve the readability of the code.

Error Handling

The routines in the IMSL MATH/LIBRARY attempt to detect and report errors and invalid input. Errors are classified and are assigned a code number. By default, errors of moderate or worse severity result in messages being automatically printed by the routine. Moreover, errors of worse severity cause program execution to stop. The severity level and the general nature of the error are designated by an "error type" ranging from 0 to 5. An error type 0 is no error; types 1 through 5 are progressively more severe. In most cases, you need not be concerned with our method of handling errors. For those interested, a complete description of the error-handling system is given in the *Reference Material*, which also describes how you can change the default actions and access the error code numbers.

A separate error handler is provided to allow users to handle errors of differing types being reported from several nodes without danger of "jumbling" or mixing error messages. The design of this error handler is described more fully in Hanson (1992). The primary feature of the design is the use of a separate array for each parallel call to a routine. This allows the user to summarize errors using the routine `error_post` in a non-parallel part of an application. For a more detailed discussion of the use of this error handler in applications which use MPI for distributed computing, see the *Reference Material*.

Printing Results

Most of the routines in the IMSL MATH/LIBRARY (except the line printer routines and special utility routines) do not print any of the results. The output is returned in Fortran variables, and you can print these yourself. See *Chapter 11, "Utilities"* for detailed descriptions of these routines.

A commonly used routine in the examples is the IMSL routine `UMACH` (see the *Reference Material*), which retrieves the Fortran device unit number for printing the results. Because this routine obtains device unit numbers, it can be used to redirect the input or output. The section on *Machine-Dependent Constants* in the Reference Material contains a description of the routine `UMACH`.

Fortran 90 Constructs

The IMSL Fortran Numerical Library contains routines which take advantage of Fortran 90 language constructs, including Fortran 90 array data types. One feature of the design is that the default use may be as simple as the problem statement. Complicated, professional-quality mathematical software is hidden from the casual or beginning user.

In addition, high-level operators and functions are provided in the Library. They are described in *Chapter 10, "Linear Algebra Operators and Generic Functions"*.

Shared-Memory Multiprocessors and Thread Safety

The IMSL Fortran Numerical Library allows users to leverage the high-performance technology of shared memory parallelism (SMP) when their environment supports it. Support for SMP systems within the IMSL Library is delivered through various means, depending upon the availability of technologies such as OpenMP, high performance LAPACK and BLAS, and hardware-specific IMSL algorithms. Use of the IMSL Fortran Numerical Library on SMP systems can be achieved by using the appropriate link environment variable when building your application. Details on the available link environment variables for your installation of the IMSL Fortran Numerical Library can be found in the online README file of the product distribution.

The IMSL Fortran Numerical Library is thread-safe in those environments that support OpenMP. This was achieved by using OpenMP directives that define global variables located in the code so they are private to the individual threads. Thread safety allows users to create instances of routines running on multiple threads and to include any routine in the IMSL Fortran Numerical Library in these threads.

Using Operators and Generic Functions

For users who are primarily interested in easy-to-use software for numerical linear algebra, see *Chapter 10, "Linear Algebra Operators and Generic Functions"*. This compact notation for writing Fortran 90 programs, when it applies, results in code that is easier to read and maintain than traditional subprogram usage.

Users may begin their code development using operators and generic functions. If a more efficient executable code is required, a user may need to switch to equivalent subroutine calls using IMSL Fortran Numerical Library routines.

Table 2 and *Table 3* contain lists of the defined operators and some of their generic functions.

Table 2 — Defined Operators and Generic Functions for Dense Arrays

Defined Array Operation	**Matrix Operation**
`A .x. B`	AB
`.i. A`	A^{-1}
`.t. A`, `.h. A`	A^T, A^*
`A .ix. B`	$A^{-1}B$
`B .xi. A`	BA^{-1}
`A .tx. B`, or `(.t. A) .x. B` `A .hx. B`, or `(.h. A) .x. B`	A^TB, A^*B
`B .xt. A`, or `B .x. (.t. A)` `B .xh. A`, or `B .x. (.h. A)`	BA^T, BA^*
`S=SVD(A [,U=U, V=V])`	$A = USV^T$
`E=EIG(A [[,B=B, D=D], V=V, W=W])`	$(AV = VE), AVD = BVE, (AW = WE), AWD = BWE$
`R=CHOL(A)`	$A = R^TR$
`Q=ORTH(A [,R=R])`	$(A = QR), Q^TQ = I$
`U=UNIT(A)`	$[u_1,\ldots] = [a_1/\|a_1\|,\ldots]$
`F=DET(A)`	$det(A) = determinant$
`K=RANK(A)`	$rank(A) = rank$

Table 2 — Defined Operators and Generic Functions for Dense Arrays

`P=NORM(A[,[type=]i])`	$p = \left\lVert A \right\rVert_1 = \max_j \left(\sum_{i-1}^{m} \lvert a_{ij} \rvert \right)$ $p = \lVert A \rVert_2 = s_1 = \text{largest singular value}$ $p = \left\lVert A \right\rVert_{\infty \leftrightarrow huge(1)} = \max_i \left(\sum_{i-1}^{n} \lvert a_{ij} \rvert \right)$
`C=COND(A)`	$\lVert A^{-1} \rVert \cdot \lVert A \rVert$
`Z=EYE(N)`	$Z = I_N$
`A=DIAG(X)`	$A = diag(x_1, \ldots)$
`X=DIAGONALS(A)`	$x = (x_{11}, \ldots)$
`W=FFT(Z); Z=IFFT(W)`	Discrete Fourier Transform, Inverse
`A=RAND(A)`	random numbers, $0 < A < 1$
`L=isNaN(A)`	test for `NaN`, *if (l) then…*

Table 3 — Defined Operators and Generic Functions for Harwell-Boeing Sparse Matrices

Defined Operation	**Matrix Operation**
`Data Management`	*Define entries of sparse matrices*
`A .x. B`	AB
`.t. A`, `.h. A`	A^T, A^*
`A .ix. B`	$A^{-1}B$
`B .xi. A`	BA^{-1}
`A .tx. B`, or `(.t. A) .x. B` `A .hx. B`, or `(.h. A) .x. B`	$A^T B, A^* B$
`B .xt. A`, or `B .x. (.t. A)` `B .xh. A`, or `B .x. (.h. A)`	BA^T, BA^*
`A+B`	*Sum of two sparse matrices*
`C=COND(A)`	$\lVert A^{-1} \rVert \cdot \lVert A \rVert$

Using ScaLAPACK, LAPACK, LINPACK, and EISPACK

Many of the codes in the IMSL Library are based on LINPACK, Dongarra et al. (1979), and EISPACK, Smith et al. (1976), collections of subroutines designed in the 1970s and early 1980s. LAPACK, Anderson et al. (1999), was designed to make the linear solvers and eigensystem routines run more efficiently on high performance computers. For a number of IMSL routines, the user of the IMSL Fortran Numerical Library has the option of linking to code which is based on either the legacy routines or the more efficient LAPACK routines.

Table 4 below lists the IMSL routines that make use of LAPACK codes. The intent is to obtain improved performance for IMSL codes by using LAPACK codes that have good performance by virtue of using BLAS with good performance. To obtain improved performance we recommend linking with High Performance versions of LAPACK and BLAS, if available. The LAPACK, codes are listed where they are used. Details on linking to the appropriate IMSL Library and alternate libraries for LAPACK and BLAS are explained in the online README file of the product distribution.

Table 4 — IMSL Routines and LAPACK Routines Utilized Within

Generic Name of IMSL Routine	LAPACK Routines used when Linking with High Performance Libraries
LSARG	?GERFS,?GETRF,?GECON, ?=S/D
LSLRG	?GETRF, ?GETRS, ?=S/D
LFCRG	?GETRF,?GECON, ?=S/D
LFTRG	?GETRF, ?=S/D
LFSRG	?GETRS, ?=S/D
LFIRG	?GETRS, ?=S/D
LINRG	?GETRF, ?GETRI, ?=S/D
LSACG	?GETRF, GETRS, ?GECON, ?=C/Z
LSLCG	?GETRF, ?GETRS, ?=C/Z
LFCCG	?GETRF, ?GECON, ?=C/Z
LFTCG	?GETRF, ?=C/Z
LFSCG	?GETRS, ?=C/Z
LFICG	?GERFS,?GETRS, ?=C/Z
LINCG	?GETRF, ?GETRI, ?=C/Z
LSLRT	?TRTRS, ?=S/D

Table 4 — IMSL Routines and LAPACK Routines Utilized Within

LFCRT	?TRCON, ?=S/D
LSLCT	?TRTRS, ?=C/Z
LFCCT	?TRCON, ?=C/Z
LSADS	?PORFS, ?POTRS, ?=S/D
LSLDS	?POTRF, ?POTRS, ?=S/D
LFCDS	?POTRF, ?POCON, ?=S/D
LFTDS	?POTRF, ?=S/D
LFSDS	?POTRS, ?=S/D
LFIDS	?PORFS, ?POTRS, ?=S/D
LINDS	?POTRF, ?=S/D
LSASF	?SYRFS, ?SYTRF, ?SYTRS, ?=S/D
LSLSF	?SYTRF, ?SYTRS, ?=S/D
LFCSF	?SYTRF, ?SYCON, ?=S/D
LFTSF	?SYTRF, ?=S/D
LFSSF	?SYTRF, ?=S/D
LFISF	?SYRFS, ?=S/D
LSADH	?POCON, ?POTRF, ?POTRS, ?=C/Z
LSLDH	?TRTRS, ?POTRF, ?=C/Z
LFCDH	?POTRF, ?POCON, ?=C/Z
LFTDH	?POTRF, ?=C/Z
LFSDH	?TRTRS, ?=C/Z
LFIDH	?PORFS, ?POTRS, ?=C/Z
LSAHF	?HECON, ?HERFS, ?HETRF, ?HETRS, ?=C/Z
LSLHF	?HECON, ?HETRF, ?HETRS, ?=C/Z
LFCHF	?HETRF, ?HECON, ?=C/Z
LFTHF	?HETRF, ?=C/Z
LFSHF	?HETRS, ?=C/Z
LFIHF	?HERFS, ?HETRS, ?=C/Z
LSARB	?GBTRF, ?GBTRS, ?GBRFS, ?=S/D
LSLRB	?GBTRF, ?GBTRS, ?=S/D
LFCRB	?GBTRF, ?GBCON, ?=S/D
LFTRB	?GBTRF, ?=S/D

Table 4 — IMSL Routines and LAPACK Routines Utilized Within

LFSRB	?GBTRS, ?=S/D
LFIRB	?GBTRS, ?GBRFS, ?=S/D
LSQRR	?GEQP3, ?GEQRF, ?ORMQR, ?TRTRS, ?=S/D
LQRRV	?GEQP3, ?GEQRF, ?ORMQR, ?=S/D
LSBRR	?GEQRF, ?=S/D
LQRRR	?GEQRF, ?=S/D
LSVRR	?GESVD, ?=S/D
LSVCR	?GESVD, ?=C/Z
LSGRR	?GESVD, ?=S/D
LQRSL	?TRTRS, ?ORMQR, ?=S/D
LQERR	?ORGQR, ?=S/D
EVLRG	?GEBAL, ?GEHRD, ?HSEQR, ?=S/D
EVCRG	?GEEVX, ?=S/D
EVLCG	?HSEQR, ?GEBAL, ?GEHRD, ?=C/Z
EVCCG	?GEEV, ?=C/Z
EVLSF	?SYEV, ?=S/D
EVCSF	?SYEV, ?=S/D
EVLHF	?HEEV, ?=C/Z
EVCHF	?HEEV, ?=C/Z
GVLRG	?GEQRF, ?ORMQR, ?GGHRD, ?HGEQZ, ?=S/D
GVCRG	?GEQRF, ?ORMQR, ?GGHRD, ?HGEQZ, ?TGEVC, ?=S/D
GVLCG	?GEQRF, ?UMMQR, ?GGHRD, ?HGEQZ,?=C/Z
GVCCG	?GEQRF, ?UMMQR, ?GGHRD, ?HGEQZ,?TGEVC,?=C/Z
GVLSP	?SYGV, ?=S/D
GVCSP	?SYGV, ?=S/D

ScaLAPACK, Blackford et al. (1997), includes a subset of LAPACK codes redesigned for use on distributed memory MIMD parallel computers. A number of IMSL Library routines make use of a subset of the ScaLAPACK library.

Table 5 below lists the IMSL routines that make use of ScaLAPACK codes. The intent is to provide access to the ScaLAPACK codes through the familiar IMSL routine interface. The IMSL routines that utilize ScaLAPACK codes have a ScaLAPACK Interface documented in addition to the FORTRAN 90 Interface. Like the LAPACK codes, access to the ScaLAPACK codes is made by linking to the appropriate library. Details on linking to the appropriate IMSL Library and alternate libraries for ScaLAPACK and BLAS are explained in the online README file of the product distribution.

Table 5 — IMSL Routines and ScaLAPACK Routines Utilized Within

Generic Name of IMSL Routine	ScaLAPACK Routines used when Linking with High Performance Libraries
LSARG	P?GERFS,P?GETRF,P?GETRS, ?=S/D
LSLRG	P?GETRF, P?GETRS, ?=S/D
LFCRG	P?GETRF,P?GECON, ?=S/D
LFTRG	P?GETRF, ?=S/D
LFSRG	P?GETRS, ?=S/D
LFIRG	P?GETRS, P?GERFS, ?=S/D
LINRG	P?GETRF, P?GETRI, ?=S/D
LSACG	P?GETRF, P?GETRS, P?GERFS, ?=C/Z
LSLCG	P?GETRF, P?GETRS, ?=C/Z
LFCCG	P?GETRF, P?GECON, ?=C/Z
LFTCG	P?GETRF, ?=C/Z
LFSCG	P?GETRS, ?=C/Z
LFICG	P?GERFS,P?GETRS, ?=C/Z
LINCG	P?GETRF, P?GETRI, ?=C/Z
LSLRT	P?TRTRS, ?=S/D
LFCRT	P?TRCON, ?=S/D
LSLCT	P?TRTRS, ?=C/Z
LFCCT	P?TRCON, ?=C/Z
LSADS	P?PORFS, P?POTRF, P?POTRS, ?=S/D
LSLDS	P?POTRF, P?POTRS, ?=S/D
LFCDS	P?POTRF, P?POCON, ?=S/D
LFTDS	P?POTRF, ?=S/D
LFSDS	P?POTRS, ?=S/D
LFIDS	P?PORFS, P?POTRS, ?=S/D
LINDS	P?GETRF, P?GETRI, ?=S/D
LSADH	P?POTRF, P?PORFS, P?POTRS, ?=C/Z

Table 5 — IMSL Routines and ScaLAPACK Routines Utilized Within

Generic Name of IMSL Routine	ScaLAPACK Routines used when Linking with High Performance Libraries
LSLDH	P?POTRS, P?POTRF, ?=C/Z
LFCDH	P?POTRF, P?POCON, ?=C/Z
LFTDH	P?POTRF, ?=C/Z
LFSDH	P?POTRS, ?=C/Z
LFIDH	P?PORFS, P?POTRS, ?=C/Z
LSLRB	P?GBTRF, P?GBTRS, ?=S/D
LSQRR	P?GEQPF, P?GEQRF, P?ORMQR, P?TRTRS, ?=S/D
LQRRV	P?TRTRS, P?GEQRF, P?ORMQR, ?=S/D
LQRRR	P?GEQRF, P?GEQPF, P?ORMQR, ?=S/D
LSVRR	P?GESVD, ?=S/D
LSGRR	P?GESVD, ?=S/D
LQRSL	P?TRTRS, P?ORMQR, ?=S/D
LQERR	P?ORGQR, ?=S/D

Using ScaLAPACK Enhanced Routines

General Remarks

Use of the ScaLAPACK enhanced routines allows a user to solve large linear systems of algebraic equations at a performance level that might not be achievable on one computer by performing the work in parallel across multiple computers. One might also use these routines on linear systems that prove to be too large for the address space of the target computer. IMSL has tried to facilitate the use of parallel computing in these situations by providing interfaces to ScaLAPACK routines which accomplish the task. The IMSL Library solver interface has the same look and feel whether one is using the routine on a single computer or across multiple computers.

The basic steps required to utilize the IMSL routines which interface with ScaLAPACK routines are:

1. Initialize MPI
2. Initialize the processor grid
3. Define any necessary array descriptors
4. Allocate space for the local arrays
5. Set up local matrices across the processor grid
6. Call the IMSL routine which interfaces with ScaLAPACK
7. Gather the results from across the processor grid
8. Release the processor grid
9. Exit MPI

Utilities are provided in the IMSL Library that facilitate these steps for the user. Each of these utilities is documented in *Chapter 11, "Utilities"*. We visit the steps briefly here:

1. Initialize MPI

The user should call `MP_SETUP()` in this step. This function is described in detail in *"Getting Started with Modules MPI_setup_int and MPI_node_int"* in *Chapter 10, "Linear Algebra Operators and Generic Functions"*. For ScaLAPACK usage, suffice it to say that following a call to the function `MP_SETUP()`, the module `MPI_node_int` will contain information about the number of processors, the rank of a processor, and the communicator for the application. A call to this function will return the number of processors available to the program. Since the module `MPI_node_int` is used by `MPI_setup_int`, it is not necessary to explicitly use the module `MPI_node_int`. If `MP_SETUP()` is not called, the program computes entirely on one node. No routine from MPI is called.

2. Initialize the processor grid

`SCALAPACK_SETUP` (see *Chapter 11, "Utilities"*) is called at this step. This call will set up the processor grid for the user, define the context ID variable, `MP_ICTXT`, for the processor grid, and place `MP_ICTXT` into the module `GRIDINFO_INT`. Use of `SCALAPACK_SUPPORT` will make the information in `MPI_NODE_INT` and `GRIDINFO_INT` available to the user's program.

3. Define any necessary array descriptors

Consider the generic matrix A which is to be carved up and distributed across the processors in the processor grid. In ScaLAPACK parlance, we refer to `A` as being the "*global*" array `A` which is to be distributed across the processor grid in 2D block cyclic fashion (see *Chapter 11, "Utilities"*). Each processor in the grid will then have access to a subset of the global array `A`. We refer to the subset array to which the individual processor has access as the "*local*" array `A0`. Just as it is sometimes necessary for a program to be aware of the leading dimension of the global array `A`, it is also necessary for the program to be aware of other critical information about the local array `A0`. This information can be obtained by calling the IMSL utility `SCALAPACK_GETDIM`. The ScaLAPACK Library utility `DESCINIT` is then used to store this information in a vector. (For more information, see the *Usage Notes* section of *Chapter 11, "Utilities"*.)

4. Allocate space for the local arrays

The array dimensions, obtained in the previous step, are used at this point to allocate space for any local arrays that will be used in the call to the IMSL routine.

5. Set up local matrices across the processor grid

If the matrices to be used by the solvers have not been distributed across the processor grid, IMSL provides utility routines `SCALAPACK_READ` and `SCALAPACK_MAP` to help in the distribution of global arrays across processors. `SCALAPACK_READ` will read data from a file while `SCALAPACK_MAP` will map a global array to the processor grid. Users may choose to distribute the arrays themselves as long as they distribute the arrays in 2D block cyclic fashion consistent with the array descriptors that have been defined.

6. Call the IMSL routine which interfaces with ScaLAPACK

The IMSL routines which interface with ScaLAPACK are listed in *Table 5*.

7. Gather the results from across the processor grid

IMSL provides utility routines SCALAPACK_WRITE and SCALAPACK_UNMAP to help in the gathering of results from across processors to a global array or file. SCALAPACK_WRITE will write data to a file while SCALAPACK_UNMAP will map local arrays from the processor grid to a global array.

8. Release the processor grid

This is accomplished by a call to SCALAPACK_EXIT.

9. Exit MPI

A call to MP_SETUP with the argument 'FINAL' will shut down MPI and set the value of MP_NPROCS = 0. This flags that MPI has been initialized and terminated. It cannot be initialized again in the same program unit execution. No MPI routine is defined when MP_NPROCS has this value.

Linear Systems

Routines

Usage Notes

Section 1.1 describes routines for solving systems of linear algebraic equations by direct matrix factorization methods, for computing only the matrix factorizations, and for computing linear least-squares solutions.

Section 1.2 describes routines for solving systems of parallel constrained least-squares.

Many of the routines described in sections 1.3 and 1.4 are for matrices with special properties or structure. Computer time and storage requirements for solving systems with coefficient matrices of these types can often be drastically reduced, using the appropriate routine, compared with using a routine for solving a general complex system.

The appropriate matrix property and corresponding routine can be located in the "Routines" section. Many of the linear equation solver routines in this chapter are derived from subroutines from LINPACK, Dongarra et al. (1979). Other routines have been developed by Visual Numerics, derived from draft versions of LAPACK subprograms, Bischof et al. (1988), or were obtained from alternate sources.

A system of linear equations is represented by $Ax = b$ where A is the $n \times n$ coefficient data matrix, b is the known right-hand-side n-vector, and x is the unknown or solution n-vector. Figure 1-1 summarizes the relationships among the subroutines. Routine names are in boxes and input/output data are in ovals. The suffix `**` in the subroutine names depend on the matrix type. For example, to compute the determinant of A use `LFC**` or `LFT**` followed by `LFD**`.

The paths using `LSA**` or `LFI**` use iterative refinement for a more accurate solution. The path using `LSA**` is the same as using `LFC**` followed by `LFI**`. The path using `LSL**` is the same as the path using `LFC**` followed by `LFS**`. The matrix inversion routines `LIN**` are available only for certain matrix types.

Matrix Types

The two letter codes for the form of coefficient matrix, indicated by `**` in *Figure 1*, are as follows:

RG	Real general (square) matrix.
CG	Complex general (square) matrix.
TR or CR	Real tridiagonal matrix.
RB	Real band matrix.
TQ or CQ	Complex tridiagonal matrix.
CB	Complex band matrix.
SF	Real symmetric matrix stored in the upper half of a square matrix.

DS	Real symmetric positive definite matrix stored in the upper half of a square matrix.
DH	Complex Hermitian positive definite matrix stored in the upper half of a complex square matrix.
HF	Complex Hermitian matrix stored in the upper half of a complex square matrix.
QS or PB	Real symmetric positive definite band matrix.
QH or QB	Complex Hermitian positive definite band matrix.
XG	Real general sparse matrix.
ZG	Complex general sparse matrix.
XD	Real symmetric positive definite sparse matrix.
ZD	Complex Hermitian positive definite sparse matrix.

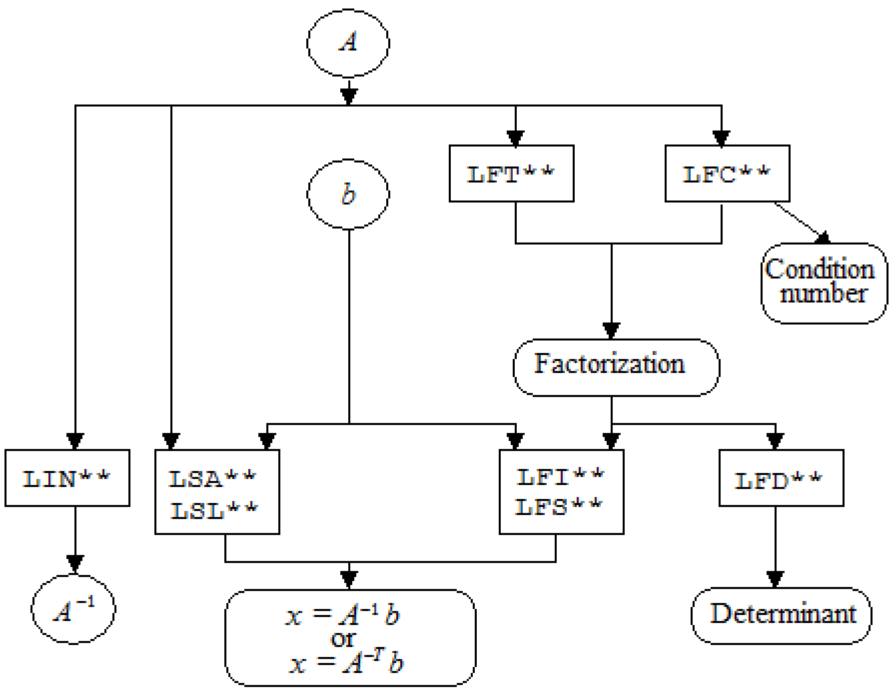

Figure 1, Solution and Factorization of Linear Systems

Solution of Linear Systems

The simplest routines to use for solving linear equations are LSL** and LSA**. For example, the mnemonic for matrices of real general form is RG. So, the routines LSARG and LSLRG are appropriate to use for solving linear systems when the coefficient matrix is of real general form. The routine LSARG uses iterative refinement, and more time than LSLRG, to determine a high accuracy solution.

The high accuracy solvers provide maximum protection against extraneous computational errors. They do not protect the results from instability in the mathematical approximation. For a more complete discussion of this and other important topics about solving linear equations, see Rice (1983), Stewart (1973), or Golub and van Loan (1989).

Multiple Right Sides

There are situations where the LSL** and LSA** routines are not appropriate. For example, if the linear system has more than one right-hand-side vector, it is most economical to solve the system by first calling a factoring routine and then calling a solver routine that uses the factors. After the coefficient matrix has been factored, the routine LFS** or LFI** can be used to solve for one right-hand side at a time. Routines LFI** uses iterative refinement to determine a high accuracy solution but requires more computer time and storage than routines LFS**.

Determinants

The routines for evaluating determinants are named LFD**. As indicated in Figure 1-1, these routines require the factors of the matrix as input. The values of determinants are often badly scaled. Additional complications in structures for evaluating them result from this fact. See Rice (1983) for comments on determinant evaluation.

Iterative Refinement

Iterative refinement can often improve the accuracy of a well-posed numerical solution. The iterative refinement algorithm used is as follows:

$x_0 = A^{-1} b$

For $i = 1, 50$

$r_i = Ax_{i-1} - b$ computed in higher precision

$p_i = A^{-1} r_i$

$x_i = x_{i-1} - p_i$

if $(\|p_i\|_\infty \le \varepsilon \|x_i\|_\infty)$ Exit

End for

Error — Matrix is too ill-conditioned

If the matrix A is in single precision, then the residual $r_i = Ax_{i-1} - b$ is computed in double precision. If A is in double precision, then quadruple-precision arithmetic routines are used.

The use of the value 50 is arbitrary. In fact a single correction is usually sufficient. It is also helpful even when r_i is computed in the same precision as the data.

Matrix Inversion

An inverse of the coefficient matrix can be computed directly by one of the routines named `LIN**`. These routines are provided for general matrix forms and some special matrix forms. When they do not exist, or when it is desirable to compute a high accuracy inverse, the two-step technique of calling the factoring routine followed by the solver routine can be used. The inverse is the solution of the matrix system $AX = I$ where I denotes the $n \times n$ identity matrix, and the solution is $X = A^{-1}$.

Singularity

The numerical and mathematical notions of singularity are not the same. A matrix is considered numerically singular if it is sufficiently close to a mathematically singular matrix. If error messages are issued regarding an exact singularity then specific error message level reset actions must be taken to handle the error condition. By default, the routines in this chapter stop. The solvers require that the coefficient matrix be numerically nonsingular. There are some tests to determine if this condition is met. When the matrix is factored, using routines `LFC**`, the condition number is computed. If the condition number is large compared to the working precision, a warning message is issued and the computations are continued. In this case, the user needs to verify the usability of the output. If the matrix is determined to be mathematically singular, or ill-conditioned, a least-squares routine or the singular value decomposition routine may be used for further analysis.

Special Linear Systems

Toeplitz matrices have entries which are constant along each diagonal, for example:

$$A = \begin{bmatrix} p_0 & p_1 & p_2 & p_3 \\ p_{-1} & p_0 & p_1 & p_2 \\ p_{-2} & p_{-1} & p_0 & p_1 \\ p_{-3} & p_{-2} & p_{-1} & p_0 \end{bmatrix}$$

Real Toeplitz systems can be solved using `LSLTO`. Complex Toeplitz systems can be solved using `LSLTC`.

Circulant matrices have the property that each row is obtained by shifting the row above it one place to the right. Entries that are shifted off at the right reenter at the left. For example:

$$A = \begin{bmatrix} p_1 & p_2 & p_3 & p_4 \\ p_4 & p_1 & p_2 & p_3 \\ p_3 & p_4 & p_1 & p_2 \\ p_2 & p_3 & p_4 & p_1 \end{bmatrix}$$

Complex circulant systems can be solved using LSLCC.

Iterative Solution of Linear Systems

The preconditioned conjugate gradient routines PCGRC and JCGRC can be used to solve symmetric positive definite systems. The routines are particularly useful if the system is large and sparse. These routines use reverse communication, so *A* can be in any storage scheme. For general linear systems, use GMRES.

QR Decomposition

The *QR* decomposition of a matrix *A* consists of finding an orthogonal matrix *Q*, a permutation matrix *P*, and an upper trapezoidal matrix *R* with diagonal elements of nonincreasing magnitude, such that $AP = QR$. This decomposition is determined by the routines LQRRR or LQRRV. It returns *R* and the information needed to compute *Q*. To actually compute *Q* use LQERR. *Figure 2* summarizes the relationships among the subroutines.

The *QR* decomposition can be used to solve the linear system $Ax = b$. This is equivalent to $Rx = Q^T Pb$. The routine LQRSL, can be used to find $Q^T Pb$ from the information computed by LQRRR. Then *x* can be computed by solving a triangular system using LSLRT. If the system $Ax = b$ is overdetermined, then this procedure solves the least-squares problem, i.e., it finds an *x* for which

$$\|Ax - b\|_2^2$$

is a minimum.

If the matrix *A* is changed by a rank-1 update, $A \rightarrow A + \alpha xy^T$, the QR decomposition of *A* can be updated/down-dated using the routine LUPQR. In some applications a series of linear systems which differ by rank-1 updates must be solved. Computing the QR decomposition once and then updating or down-dating it usually faster than newly solving each system.

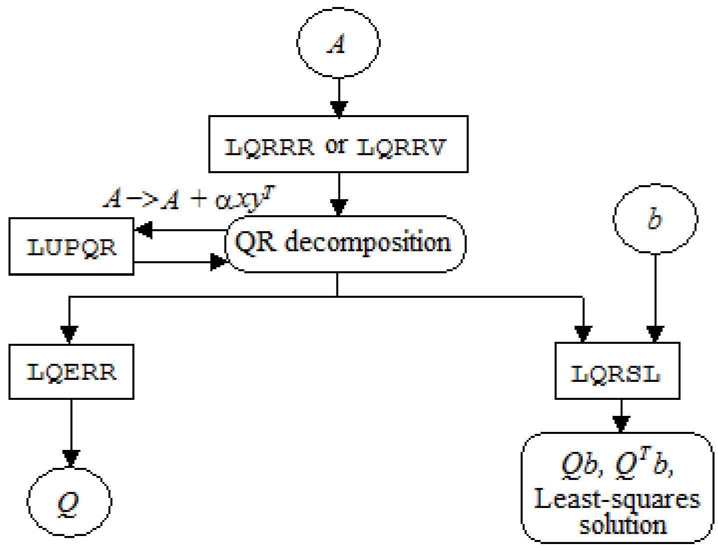

Figure 2, Least-Squares Routine

LIN_SOL_GEN

more...

Solves a general system of linear equations $Ax = b$. Using optional arguments, any of several related computations can be performed. These extra tasks include computing the *LU* factorization of *A* using partial pivoting, representing the determinant of *A*, computing the inverse matrix A^{-1}, and solving $A^T x = b$ or $Ax = b$ given the *LU* factorization of *A*.

Required Arguments

A — Array of size $n \times n$ containing the matrix. (Input [/Output])
If the packaged option `lin_sol_gen_save_LU` is used then the *LU* factorization of `A` is saved in `A`. For solving efficiency, the diagonal reciprocals of the matrix *U* are saved in the diagonal entries of `A`.

B — Array of size $n \times nb$ containing the right-hand side matrix. (Input [/Output])
If the packaged option `lin_sol_gen_save_LU` is used then input *B* is used as work storage and is not saved.

X — Array of size $n \times nb$ containing the solution matrix.(Output)

Optional Arguments

NROWS = `n` (Input)
Uses array `A`(1`:`n, 1`:`n) for the input matrix.
Default: `n` = size (`A`, 1)

NRHS = `nb` (Input)
Uses array `b`(1`:`n, 1`:`nb) for the input right-hand side matrix.
Default: `nb` = size(`b`, 2)
Note that `b` must be a rank-2 array.

pivots = `pivots(:)` (Output [/Input])
Integer array of size `n` that contains the individual row interchanges. To construct the permuted order so that no pivoting is required, define an integer array `ip`(`n`). Initialize `ip`(*i*) = *i*, *i* = 1, `n` and then

execute the loop, after calling `lin_sol_gen`,

```
k=pivots(i)
```
interchange `ip(i)` and `ip(k)`, `i=1,n`

The matrix defined by the array assignment that permutes the rows, A(1:n, 1:n) = A(ip(1:n), 1:n), requires no pivoting for maintaining numerical stability. Now, the optional argument "`iopt=`" and the packaged option number `?_lin_sol_gen_no_pivoting` can be safely used for increased efficiency during the *LU* factorization of *A*.

det = `det(1:2)` (Output)
Array of size 2 of the same type and kind as `A` for representing the determinant of the input matrix. The determinant is represented by two numbers. The first is the base with the sign or complex angle of the result. The second is the exponent. When `det`(2) is within exponent range, the value of this expression is given by abs(`det`(1))`**det`(2) * (`det`(1))/abs(`det`(1)). If the matrix is not singular, abs(`det`(1)) = radix(`det`); otherwise, `det`(1) = 0, and `det`(2) = – huge(abs(`det`(1))).

ainv = `ainv(:,:)` (Output)
Array of the same type and kind as A(1:n, 1:n). It contains the inverse matrix, A^{-1}, when the input matrix is nonsingular.

iopt = `iopt(:)` (Input)
Derived type array with the same precision as the input matrix; used for passing optional data to the routine. The options are as follows:

Packaged Options for **lin_sol_gen**		
Option Prefix = ?	Option Name	Option Value
s_, d_, c_, z_	lin_sol_gen_set_small	1
s_, d_, c_, z_	lin_sol_gen_save_LU	2
s_, d_, c_, z_	lin_sol_gen_solve_A	3
s_, d_, c_, z_	lin_sol_gen_solve_ADJ	4
s_, d_, c_, z_	lin_sol_gen_no_pivoting	5
s_, d_, c_, z_	lin_sol_gen_scan_for_NaN	6
s_, d_, c_, z_	lin_sol_gen_no_sing_mess	7
s_, d_, c_, z_	lin_sol_gen_A_is_sparse	8

iopt(IO) = `?_options(?_lin_sol_gen_set_small`, *Small*)

Replaces a diagonal term of the matrix *U* if it is smaller in magnitude than the value *Small* using the same sign or complex direction as the diagonal. The system is declared singular. A solution is approximated based on this replacement if no overflow results.

Default: the smallest number that can be reciprocated safely

iopt(IO) = `?_options(?_lin_sol_gen_save_LU`, `?_dummy)`

Saves the *LU* factorization of `A`. Requires the optional argument "`pivots=`" if the routine will be used later for solving systems with the same matrix. This is the only case where the input arrays `A` and `b` are not saved. For solving efficiency, the diagonal reciprocals of the matrix *U* are saved in the diagonal entries of `A`.

iopt(IO) = `?_options(?_lin_sol_gen_solve_A`, `?_dummy)`

Uses the *LU* factorization of `A` computed and saved to solve $Ax = b$.

iopt(IO) = `?_options(?_lin_sol_gen_solve_ADJ`, `?_dummy)`

Uses the *LU* factorization of *A* computed and saved to solve $A^T x = b$.

iopt(IO) = ?_options(?_lin_sol_gen_no_pivoting, `?_dummy`)

Does no row pivoting. The array `pivots(:)`, if present, are output as `pivots`$(i) = i$, for $i = 1, \ldots,$ `n`.

iopt(IO) = `?_options(?_lin_sol_gen_scan_for_NaN`, `?_dummy`)

Examines each input array entry to find the first value such that

```
isNaN(a(i,j)) .or. isNan(b(i,j)) == .true.
```

See the `isNaN`() `function`, *Chapter 10*.

Default: Does not scan for NaNs.

iopt(IO) = `?_options(?_lin_sol_gen_no_sing_mess`, `?_dummy`)

Do not output an error message when the matrix *A* is singular.

iopt(IO) = `?_options(?_lin_sol_gen_A_is_sparse`, `?_dummy`)

Uses an indirect updating loop for the LU factorization that is efficient for sparse matrices where all matrix entries are stored.

FORTRAN 90 Interface

Generic:`CALL LIN_SOL_GEN` (A, B, `X [`, …`])`

Specific:The specific interface names are `S_LIN_SOL_GEN`, `D_LIN_SOL_GEN`, `C_LIN_SOL_GEN`, and `Z_LIN_SOL_GEN`.

Description

Routine LIN_SOL_GEN solves a system of linear algebraic equations with a nonsingular coefficient matrix *A*. It first computes the *LU* factorization of *A* with partial pivoting such that *LU* = *A*. The matrix *U* is upper triangular, while the following is true:

$$L^{-1}A \equiv L_n P_n L_{n-1} P_{n-1} \cdots L_1 P_1 A \equiv U$$

The factors P_i and L_i are defined by the partial pivoting. Each P_i is an interchange of row *i* with row $j \geq i$. Thus, P_i is defined by that value of *j*. Every

$$L_i = I + m_i e_i^T$$

is an elementary elimination matrix. The vector m_i is zero in entries 1, …, *i*. This vector is stored as column *i* in the strictly lower-triangular part of the working array containing the decomposition information. The reciprocals of the diagonals of the matrix *U* are saved in the diagonal of the working array. The solution of the linear system $Ax = b$ is found by solving two simpler systems,

$$y = L^{-1}b \text{ and } x = U^{-1}y$$

More mathematical details are found in Golub and Van Loan (1989, Chapter 3).

Fatal and Terminal Error Messages

See the *messages.gls* file for error messages for LIN_SOL_GEN. The messages are numbered 161–175; 181–195; 201–215; 221–235.

Examples

Example 1: Solving a Linear System of Equations

This example solves a linear system of equations. This is the simplest use of lin_sol_gen. The equations are generated using a matrix of random numbers, and a solution is obtained corresponding to a random right-hand side matrix. Also, see operator_ex01, supplied with the product examples, for this example using the operator notation.

```
      use lin_sol_gen_int
      use rand_gen_int
      use error_option_packet

      implicit none

! This is Example 1 for LIN_SOL_GEN.
```

```
      integer, parameter :: n=32
      real(kind(1e0)), parameter :: one=1e0
      real(kind(1e0)) err
      real(kind(1e0)) A(n,n), b(n,n), x(n,n), res(n,n), y(n**2)

! Generate a random matrix.
      call rand_gen(y)


! Generate random right-hand sides.
      call rand_gen(y)
      b = reshape(y,(/n,n/))

! Compute the solution matrix of Ax=b.
      call lin_sol_gen(A, b, x)

! Check the results for small residuals.
      res = b - matmul(A,x)
      err = maxval(abs(res))/sum(abs(A)+abs(b))
      if (err <= sqrt(epsilon(one))) then
         write (*,*) 'Example 1 for LIN_SOL_GEN is correct.'
      end if

      end
```

Output

```
Example 1 for LIN_SOL_GEN is correct.
```

Example 2: Matrix Inversion and Determinant

This example computes the inverse and determinant of *A*, a random matrix. Tests are made on the conditions

$$AA^{-1} = I$$

and

$$\det\left(A^{-1}\right) = \det(A)^{-1}$$

Also, see `operator_ex02`.

```
      use lin_sol_gen_int
      use rand_gen_int

      implicit none

! This is Example 2 for LIN_SOL_GEN.

      integer i
      integer, parameter :: n=32
      real(kind(1e0)), parameter :: one=1.0e0, zero=0.0e0
      real(kind(1e0)) err
      real(kind(1e0)) A(n,n), b(n,0), inv(n,n), x(n,0), res(n,n), &
           y(n**2), determinant(2), inv_determinant(2)

! Generate a random matrix.

      call rand_gen(y)
      A = reshape(y,(/n,n/))
```

```
! Compute the matrix inverse and its determinant.

      call lin_sol_gen(A, b, x, nrhs=0, &
                 ainv=inv, det=determinant)

! Compute the determinant for the inverse matrix.

      call lin_sol_gen(inv, b, x, nrhs=0, &
                 det=inv_determinant)

! Check residuals, A times inverse = Identity.

      res = matmul(A,inv)
      do i=1, n
         res(i,i) = res(i,i) - one
      end do

      err = sum(abs(res)) / sum(abs(a))
      if (err <= sqrt(epsilon(one))) then
         if (determinant(1) == inv_determinant(1) .and. &
            (abs(determinant(2)+inv_determinant(2)) &
            <= abs(determinant(2))*sqrt(epsilon(one)))) then
            write (*,*) 'Example 2 for LIN_SOL_GEN is correct.'
         end if
      end if

      end
```

Output

```
Example 2 for LIN_SOL_GEN is correct.
```

Example 3: Solving a System with Iterative Refinement

This example computes a factorization of a random matrix using single-precision arithmetic. The double-precision solution is corrected using iterative refinement. The corrections are added to the developing solution until they are no longer decreasing in size. The initialization of the derived type array `iopti(1:2) = s_option(0,0.0e0)` leaves the integer part of the second element of `iopti(:)` at the value zero. This stops the internal processing of options inside `lin_sol_gen`. It results in the *LU* factorization being saved after exit. The next time the routine is entered the integer entry of the second element of `iopt(:)` results in a solve step only. Since the *LU* factorization is saved in arrays `A(:,:)` and `ipivots(:)`, at the final step, solve only steps can occur in subsequent entries to `lin_sol_gen`. Also, see `operator_ex03`, *Chapter 10*.

```
      use lin_sol_gen_int
      use rand_gen_int

      implicit none

! This is Example 3 for LIN_SOL_GEN.

      integer, parameter :: n=32
      real(kind(1e0)), parameter :: one=1.0e0, zero=0.0e0
      real(kind(1d0)), parameter :: d_zero=0.0d0
      integer ipivots(n)
      real(kind(1e0)) a(n,n), b(n,1), x(n,1), w(n**2)
```

```
      real(kind(1e0)) change_new, change_old
      real(kind(1d0)) c(n,1), d(n,n), y(n,1)
      type(s_options) ::  iopti(2)=s_options(0,zero)


! Generate a random matrix.

      call rand_gen(w)
      a = reshape(w, (/n,n/))

! Generate a random right hand side.

      call rand_gen(b(1:n,1))

! Save double precision copies of the matrix and right hand side.

      d = a
      c = b

! Start solution at zero.

      y = d_zero
      change_old = huge(one)

! Use packaged option to save the factorization.

      iopti(1) = s_options(s_lin_sol_gen_save_LU,zero)

      iterative_refinement: do
         b = c - matmul(d,y)
         call lin_sol_gen(a, b, x, &
                   pivots=ipivots, iopt=iopti)
         y = x + y
         change_new = sum(abs(x))

! Exit when changes are no longer decreasing.

         if (change_new >= change_old) &
             exit iterative_refinement
         change_old = change_new

! Use option to re-enter code with factorization saved; solve only.
         iopti(2) = s_options(s_lin_sol_gen_solve_A,zero)
      end do iterative_refinement
      write (*,*) 'Example 3 for LIN_SOL_GEN is correct.'
      end
```

Output

```
Example 3 for LIN_SOL_GEN is correct.
```

Example 4: Evaluating the Matrix Exponential

This example computes the solution of the ordinary differential equation problem

$$\frac{dy}{dt} = Ay$$

with initial values $y(0) = y_0$. For this example, the matrix A is real and constant with respect to t. The unique solution is given by the matrix exponential:

$$y(t) = e^{At}y_0$$

This method of solution uses an eigenvalue-eigenvector decomposition of the matrix

$$A = XDX^{-1}$$

to evaluate the solution with the equivalent formula

$$y(t) = Xe^{Dt}z_0$$

where

$$z_0 = X^{-1}y_0$$

is computed using the complex arithmetic version of `lin_sol_gen`. The results for *y*(*t*) are real quantities, but the evaluation uses intermediate complex-valued calculations. Note that the computation of the complex matrix *X* and the diagonal matrix *D* is performed using the IMSL MATH/LIBRARY FORTRAN 77 interface to routine `EVCRG`. This is an illustration of intermixing interfaces of FORTRAN 77 and Fortran 90 code. The information is made available to the Fortran 90 compiler by using the FORTRAN 77 interface for `EVCRG`. Also, see `operator_ex04`, supplied with the product examples, where the Fortran 90 function `EIG()` has replaced the call to `EVCRG`.

```
      use lin_sol_gen_int
      use rand_gen_int
      use Numerical_Libraries

      implicit none

! This is Example 4 for LIN_SOL_GEN.

      integer, parameter :: n=32, k=128
      real(kind(1e0)), parameter :: one=1.0e0, t_max=1, delta_t=t_max/(k-1)
      real(kind(1e0)) err, A(n,n), atemp(n,n), ytemp(n**2)
      real(kind(1e0)) t(k), y(n,k), y_prime(n,k)
      complex(kind(1e0)) EVAL(n), EVEC(n,n)
      complex(kind(1e0)) x(n,n), z_0(n,1), y_0(n,1), d(n)
      integer i

! Generate a random matrix in an F90 array.

      call rand_gen(ytemp)
      atemp = reshape(ytemp,(/n,n/))

! Assign data to an F77 array.
      A = atemp

! Use IMSL Numerical Libraries F77 subroutine for the
! eigenvalue-eigenvector calculation.
      CALL EVCRG(N, A, N, EVAL, EVEC, N)

! Generate a random initial value for the ODE system.
      call rand_gen(ytemp(1:n))
      y_0(1:n,1) = ytemp(1:n)

! Assign the eigenvalue-eigenvector data to F90 arrays.
      d = EVAL; x = EVEC
```

```
! Solve complex data system that transforms the initial values, Xz_0=y_0.
      call lin_sol_gen(x, y_0, z_0)
      t = (/(i*delta_t,i=0,k-1

! Compute y and y' at the values t(1:k).
      y = matmul(x, exp(spread(d,2,k)*spread(t,1,n))* &
                   spread(z_0(1:n,1),2,k))
      y_prime  = matmul(x, spread(d,2,k)* &
                        exp(spread(d,2,k)*spread(t,1,n))* &
                        spread(z_0(1:n,1),2,k))

! Check results. Is  y' - Ay = 0?
      err = sum(abs(y_prime-matmul(atemp,y))) / &
           (sum(abs(atemp))*sum(abs(y)))
      if (err <= sqrt(epsilon(one))) then
         write (*,*) 'Example 4 for LIN_SOL_GEN is correct.'
      end if

      end
```

Output

```
Example 4 for LIN_SOL_GEN is c orrect.
```

LIN_SOL_SELF

more...

Solves a system of linear equations $Ax = b$, where A is a self-adjoint matrix. Using optional arguments, any of several related computations can be performed. These extra tasks include computing and saving the factorization of A using symmetric pivoting, representing the determinant of A, computing the inverse matrix A^{-1}, or computing the solution of $Ax = b$ given the factorization of A. An optional argument is provided indicating that A is positive definite so that the Cholesky decomposition can be used.

Required Arguments

A — Array of size $n \times n$ containing the self-adjoint matrix. (Input [/Output])
If the packaged option `lin_sol_self_save_factors` is used then the factorization of `A` is saved in `A`. For solving efficiency, the diagonal reciprocals of the matrix R are saved in the diagonal entries of `A` when the Cholesky method is used.

B — Array of size $n \times nb$ containing the right-hand side matrix. (Input [/Output])
If the packaged option `lin_sol_self_save_factors` is used then input B is used as work storage and is not saved.

X — Array of size $n \times nb$ containing the solution matrix. (Output)

Optional Arguments

NROWS = `n` (Input)
Uses array `A`(1`:`n, 1`:`n) for the input matrix.
Default: `n` = size(`A`, 1)

NRHS = `nb` (Input)
Uses the array `b`(1`:`n, 1`:`nb) for the input right-hand side matrix.
Default: `nb` = size(`b`, 2)
Note that `b` must be a rank-2 array.

pivots = `pivots(:)` (Output [/Input])

Integer array of size n + 1 that contains the individual row interchanges in the first n locations. Applied in order, these yield the permutation matrix *P*. Location n + 1 contains the number of the first diagonal term no larger than *Small*, which is defined on the next page of this chapter.

det = `det(1:2)` (Output)

Array of size 2 of the same type and kind as A for representing the determinant of the input matrix. The determinant is represented by two numbers. The first is the base with the sign or complex angle of the result. The second is the exponent. When det(2) is within exponent range, the value of the determinant is given by the expression abs(det(1))**det(2) * (det(1))/abs(det(1)). If the matrix is not singular, abs(det(1)) = radix(det); otherwise, det(1) = 0, and det(2) = -huge(abs(det(1))).

ainv = ainv(:,:) (Output)

Array of the same type and kind as A(1:n, 1:n). It contains the inverse matrix, A^{-1} when the input matrix is nonsingular.

iopt = `iopt(:)` (Input)

Derived type array with the same precision as the input matrix; used for passing optional data to the routine. The options are as follows:

Packaged Options for **lin_sol_self**		
Option Prefix = ?	Option Name	Option Value
s_, d_, c_, z_	lin_sol_self_set_small	1
s_, d_, c_, z_	lin_sol_self_save_factors	2
s_, d_, c_, z_	lin_sol_self_no_pivoting	3
s_, d_, c_, z_	lin_sol_self_use_Cholesky	4
s_, d_, c_, z_	lin_sol_self_solve_A	5
s_, d_, c_, z_	lin_sol_self_scan_for_NaN	6
s_, d_, c_, z_	lin_sol_self_no_sing_mess	7

iopt(IO) = `?_options(?_lin_sol_self_set_small`, *Small*)

When Aasen's method is used, the tridiagonal system *Tu* = *v* is solved using *LU* factorization with partial pivoting. If a diagonal term of the matrix *U* is smaller in magnitude than the value *Small*, it is replaced by *Small*. The system is declared singular. When the Cholesky method is used, the upper-triangular matrix *R*, (see *Description*), is obtained. If a diagonal term of the matrix *R* is smaller in magnitude than the value *Small*, it is replaced by *Small*. A solution is approximated based on this replacement in either case.
Default: the smallest number that can be reciprocated safely

iopt(IO) = `?_options(?_lin_sol_self_save_factors, ?_dummy)`

Saves the factorization of `A`. Requires the optional argument "`pivots=`" if the routine will be used for solving further systems with the same matrix. This is the only case where the input arrays `A` and `b` are not saved. For solving efficiency, the diagonal reciprocals of the matrix *R* are saved in the diagonal entries of `A` when the Cholesky method is used.

iopt(IO) = `?_options(?_lin_sol_self_no_pivoting, ?_dummy)`

Does no row pivoting. The array `pivots`(:), if present, satisfies `pivots`(i) = i + 1 for i = 1, …, `n` - 1 when using Aasen's method. When using the Cholesky method, `pivots`(i) = i for i = 1, …, `n`.

iopt(IO) = `?_options(?_lin_sol_self_use_Cholesky, ?_dummy)`

The Cholesky decomposition $PAP^T = R^TR$ is used instead of the Aasen method.

iopt(IO) = `?_options(?_lin_sol_self_solve_A, ?_dummy)`

Uses the factorization of `A` computed and saved to solve $Ax = b$.

iopt(IO) = `?_options(?_lin_sol_self_scan_for_NaN, ?_dummy)`

Examines each input array entry to find the first value such that

```
isNaN(a(i,j)) .or. isNan(b(i,j)) == .true.
```

See the `isNaN`() function, *Chapter 10*.

Default: Does not scan for NaNs

iopt(IO) = `?_options(?_lin_sol_self_no_sing_mess, ?_dummy)`

Do not print an error message when the matrix *A* is singular.

FORTRAN 90 Interface

Generic:`CALL LIN_SOL_SELF (A, B, X [, …])`

Specific:The specific interface names are `S_LIN_SOL_SELF`, `D_LIN_SOL_SELF`, `C_LIN_SOL_SELF`, and `Z_LIN_SOL_SELF`.

Description

Routine `LIN_SOL_SELF` routine solves a system of linear algebraic equations with a nonsingular coefficient matrix *A*. By default, the routine computes the factorization of *A* using Aasen's method. This decomposition has the form

$$PAP^T = LTL^T$$

where *P* is a permutation matrix, *L* is a unit lower-triangular matrix, and *T* is a tridiagonal self-adjoint matrix. The solution of the linear system $Ax = b$ is found by solving simpler systems,

$$u = L^{-1}Pb$$

$$Tv = u$$

and

$$x = P^T L^{-T} v$$

More mathematical details for real matrices are found in Golub and Van Loan (1989, Chapter 4).

When the optional Cholesky algorithm is used with a positive definite, self-adjoint matrix, the factorization has the alternate form

$$PAP^T = R^T R$$

where P is a permutation matrix and R is an upper-triangular matrix. The solution of the linear system $Ax = b$ is computed by solving the systems

$$u = R^{-T}Pb$$

and

$$x = P^T R^{-1} u$$

The permutation is chosen so that the diagonal term is maximized at each step of the decomposition. The individual interchanges are optionally available in the argument "`pivots`".

Fatal and Terminal Error Messages

`See the` *messages.gls* file for error messages for `LIN_SOL_SELF`. These error messages are numbered 321–336; 341–356; 361–376; 381–396.

Examples

Example 1: Solving a Linear Least-squares System

This example solves a linear least-squares system $Cx \cong d$, where C_{mxn} is a real matrix with $m \geq n$. The least-squares solution is computed using the self-adjoint matrix

$$A = C^T C$$

and the right-hand side

$$b = A^T d$$

The $n \times n$ self-adjoint system $Ax = b$ is solved for x. This solution method is not as satisfactory, in terms of numerical accuracy, as solving the system $Cx \cong d$ directly by using the routine `lin_sol_lsq`. Also, see `operator_ex05`, *Chapter 10*.

```
      use lin_sol_self_int
      use rand_gen_int

      implicit none

! This is Example 1 for LIN_SOL_SELF.

      integer, parameter :: m=64, n=32
      real(kind(1e0)), parameter :: one=1e0
      real(kind(1e0)) err
      real(kind(1e0)), dimension(n,n) :: A, b, x, res, y(m*n),&
             C(m,n), d(m,n)

! Generate two rectangular random matrices.
      call rand_gen(y)
      C = reshape(y,(/m,n/))

      call rand_gen(y)
      d = reshape(y,(/m,n/))

! Form the normal equations for the rectangular system.
      A = matmul(transpose(C),C)
      b = matmul(transpose(C),d)

! Compute the solution for Ax = b.
      call lin_sol_self(A, b, x)

! Check the results for small residuals.
      res = b - matmul(A,x)
      err = maxval(abs(res))/sum(abs(A)+abs(b))
      if (err <= sqrt(epsilon(one))) then
         write (*,*) 'Example 1 for LIN_SOL_SELF is correct.'
      end if

      end
```

Output

```
Example 1 for LIN_SOL_SELF is correct.
```

Example 2: System Solving with Cholesky Method

This example solves the same form of the system as Example 1. The optional argument "`iopt=`" is used to note that the Cholesky algorithm is used since the matrix A is positive definite and self-adjoint. In addition, the sample covariance matrix

$$\Gamma = \sigma^2 A^{-1}$$

is computed, where

$$\sigma^2 = \frac{\|d - Cx\|^2}{m - n}$$

the inverse matrix is returned as the "`ainv=`" optional argument. The scale factor σ^2 and Γ are computed after returning from the routine. Also, see `operator_ex06`, *Chapter 10*.

```
      use lin_sol_self_int
      use rand_gen_int
      use error_option_packet

      implicit none

! This is Example 2 for LIN_SOL_SELF.

      integer, parameter :: m=64, n=32
      real(kind(1e0)), parameter :: one=1.0e0, zero=0.0e0
      real(kind(1e0)) err
      real(kind(1e0)) a(n,n), b(n,1), c(m,n), d(m,1), cov(n,n), x(n,1), &
           res(n,1), y(m*n)
      type(s_options) :: iopti(1)=s_options(0,zero)


! Generate a random rectangular matrix and a random right hand side.

      call rand_gen(y)
      c = reshape(y,(/m,n/))

      call rand_gen(d(1:n,1))

! Form the normal equations for the rectangular system.

      a = matmul(transpose(c),c)
      b = matmul(transpose(c),d)

! Use packaged option to use Cholesky decomposition.

      iopti(1) = s_options(s_lin_sol_self_Use_Cholesky,zero)

! Compute the solution of Ax=b with optional inverse obtained.

      call lin_sol_self(a, b, x, ainv=cov, &
                         iopt=iopti)

! Compute residuals, x - (inverse)*b, for consistency check.

      res = x - matmul(cov,b)

! Scale the inverse to obtain the covariance matrix.

      cov = (sum((d-matmul(c,x))**2)/(m-n)) * cov

! Check the results.

      err = sum(abs(res))/sum(abs(cov))
      if (err <= sqrt(epsilon(one))) then
         write (*,*) 'Example 2 for LIN_SOL_SELF is correct.'
      end if

      end
```

Output

```
Example 2 for LIN_SOL_SELF is correct.
```

Example 3: Using Inverse Iteration for an Eigenvector

This example illustrates the use of the optional argument "iopt=" to reset the value of a *Small* diagonal term encountered during the factorization. Eigenvalues of the self-adjoint matrix

$$A = C^T C$$

are computed using the routine lin_eig_self. An eigenvector, corresponding to one of these eigenvalues, λ, is computed using inverse iteration. This solves the near singular system $(A - \lambda I)x = b$ for an eigenvector, x. Following the computation of a normalized eigenvector

$$y = \frac{x}{\|x\|}$$

the consistency condition

$$\lambda = y^T A y$$

is checked. Since a singular system is expected, suppress the fatal error message that normally prints when the error post-processor routine error_post is called within the routine lin_sol_self. Also, see operator_ex07, *Chapter 10*.

```
      use lin_sol_self_int
      use lin_eig_self_int
      use rand_gen_int
      use error_option_packet

      implicit none

! This is Example 3 for LIN_SOL_SELF.

      integer i, tries
      integer, parameter :: m=8, n=4, k=2
      integer ipivots(n+1)
      real(kind(1d0)), parameter :: one=1.0d0, zero=0.0d0
      real(kind(1d0)) err
      real(kind(1d0)) a(n,n), b(n,1), c(m,n), x(n,1), y(m*n), &
             e(n), atemp(n,n)
      type(d_options) :: iopti(4)


! Generate a random rectangular matrix.

      call rand_gen(y)
      c = reshape(y,(/m,n/))

! Generate a random right hand side for use in the inverse
! iteration.

      call rand_gen(y(1:n))
      b = reshape(y,(/n,1/))

! Compute the positive definite matrix.

      a = matmul(transpose(c),c)

! Obtain just the eigenvalues.
```

```
      call lin_eig_self(a, e)

! Use packaged option to reset the value of a small diagonal.
      iopti =    d_options(0,zero)
      iopti(1) = d_options(d_lin_sol_self_set_small,&
                 epsilon(one) * abs(e(1)))
! Use packaged option to save the factorization.
      iopti(2) = d_options(d_lin_sol_self_save_factors,zero)
! Suppress error messages and stopping due to singularity
! of the matrix, which is expected.
      iopti(3) = d_options(d_lin_sol_self_no_sing_mess,zero)
      atemp = a
      do i=1, n
         a(i,i) = a(i,i) - e(k)
      end do

! Compute A-eigenvalue*I as the coefficient matrix.
      do tries=1, 2
         call lin_sol_self(a, b, x, &
                     pivots=ipivots, iopt=iopti)
! When code is re-entered, the already computed factorization
! is used.
         iopti(4) = d_options(d_lin_sol_self_solve_A,zero)
! Reset right-hand side nearly in the direction of the eigenvector.
         b = x/sqrt(sum(x**2))
      end do

! Normalize the eigenvector.
      x = x/sqrt(sum(x**2))

! Check the results.
      err =  dot_product(x(1:n,1),matmul(atemp(1:n,1:n),x(1:n,1))) - &
              e(k)

! If any result is not accurate, quit with no summary printing.
      if (abs(err) <= sqrt(epsilon(one))*e(1)) then
        write (*,*) 'Example 3 for LIN_SOL_SELF is correct.'
      end if

      end
```

Output

```
Example 3 for LIN_SOL_SELF is correct.
```

Example 4: Accurate Least-squares Solution with Iterative Refinement

This example illustrates the accurate solution of the self-adjoint linear system

$$\begin{bmatrix} I & A \\ A^T & 0 \end{bmatrix} \begin{bmatrix} r \\ x \end{bmatrix} = \begin{bmatrix} b \\ 0 \end{bmatrix}$$

computed using iterative refinement. This solution method is appropriate for least-squares problems when an accurate solution is required. The solution and residuals are accumulated in double precision, while the decomposition is computed in single precision. Also, see `operator_ex08`, supplied with the product examples.

```
      use lin_sol_self_int
      use rand_gen_int
```

```
      implicit none

! This is Example 4 for LIN_SOL_SELF.

      integer i
      integer, parameter :: m=8, n=4
      real(kind(1e0)), parameter :: one=1.0e0, zero=0.0e0
      real(kind(1d0)), parameter :: d_zero=0.0d0
      integer ipivots((n+m)+1)
      real(kind(1e0)) a(m,n), b(m,1), w(m*n), f(n+m,n+m), &
            g(n+m,1), h(n+m,1)
      real(kind(1e0)) change_new, change_old
      real(kind(1d0)) c(m,1), d(m,n), y(n+m,1)
      type(s_options) ::  iopti(2)=s_options(0,zero)

! Generate a random matrix.

      call rand_gen(w)

      a = reshape(w, (/m,n/))

! Generate a random right hand side.

      call rand_gen(b(1:m,1))

! Save double precision copies of the matrix and right hand side.

      d = a
      c = b

! Fill in augmented system for accurately solving the least-squares
! problem.

      f = zero
      do i=1, m
         f(i,i) = one
      end do
      f(1:m,m+1:) = a
      f(m+1:,1:m) = transpose(a)

! Start solution at zero.

      y = d_zero
      change_old = huge(one)

! Use packaged option to save the factorization.

      iopti(1) = s_options(s_lin_sol_self_save_factors,zero)

      iterative_refinement: do
         g(1:m,1) = c(1:m,1) - y(1:m,1) - matmul(d,y(m+1:m+n,1))
         g(m+1:m+n,1) = - matmul(transpose(d),y(1:m,1))
         call lin_sol_self(f, g, h, &
                    pivots=ipivots, iopt=iopti)
         y = h + y
         change_new = sum(abs(h))

! Exit when changes are no longer decreasing.

         if (change_new >= change_old) &
             exit iterative_refinement
         change_old = change_new

! Use option to re-enter code with factorization saved; solve only.
         iopti(2) = s_options(s_lin_sol_self_solve_A,zero)
      end do iterative_refinement
```

```
        write (*,*) 'Example 4 for LIN_SOL_SELF is correct.'
        end
```

Output

```
Example 4 for LIN_SOL_SELF is correct.
```

LIN_SOL_LSQ

Solves a rectangular system of linear equations $Ax \cong b$, in a least-squares sense. Using optional arguments, any of several related computations can be performed. These extra tasks include computing and saving the factorization of A using column and row pivoting, representing the determinant of A, computing the generalized inverse matrix $A^\dagger$, or computing the least-squares solution of

$$Ax \cong b$$

or

$$A^T y \cong b,$$

given the factorization of A. An optional argument is provided for computing the following unscaled covariance matrix

$$C = \left(A^T A\right)^{-1}$$

Least-squares solutions, where the unknowns are non-negative or have simple bounds, can be computed with `PARALLEL_NONNEGATIVE_LSQ` and `PARALLEL_BOUNDED_LSQ`. These codes can be restricted to execute without MPI.

Required Arguments

A — Array of size $m \times n$ containing the matrix. (Input [/Output])
If the packaged option `lin_sol_lsq_save_QR` is used then the factorization of `A` is saved in `A`. For efficiency, the diagonal reciprocals of the matrix R are saved in the diagonal entries of `A`.

B — Array of size $m \times nb$ containing the right-hand side matrix. When using the option to solve adjoint systems $A^T x \cong b$, the size of b is $n \times nb$. (Input [/Output])
If the packaged option `lin_sol_lsq_save_QR` is used then input B is used as work storage and is not saved.

X — Array of size $n \times nb$ containing the right-hand side matrix. When using the option to solve adjoint systems $A^T x \cong b$, the size of x is $m \times nb$. (Output)

Optional Arguments

MROWS = `m` (Input)
Uses array `A(1:m, 1:n)` for the input matrix.
Default: `m` = size(`A`, 1)

NCOLS = `n` (Input)

Uses array A(1:m, 1:n) for the input matrix.

Default: n = size(A, 2)

NRHS = `nb` (Input)

Uses the array b(1:, 1:nb) for the input right-hand side matrix.

Default: nb = size(b, 2)

Note that b must be a rank-2 array.

pivots = `pivots(:)` (Output [/Input])

Integer array of size 2 * min(m, n) + 1 that contains the individual row followed by the column interchanges. The last array entry contains the approximate rank of A.

trans = `trans(:)` (Output [/Input])

Array of size 2 * min(m, n) that contains data for the construction of the orthogonal decomposition.

det = `det(1:2)` (Output)

Array of size 2 of the same type and kind as A for representing the products of the determinants of the matrices Q, P, and R. The determinant is represented by two numbers. The first is the base with the sign or complex angle of the result. The second is the exponent. When det(2) is within exponent range, the value of this expression is given by abs (det(1))**det(2) * (det(1))/abs(det(1)). If the matrix is not singular, abs(det(1)) = radix(det); otherwise, det(1) = 0, and det(2) = -huge(abs(det(1))).

ainv = `ainv(:,:)` (Output)

Array with size $n \times m$ of the same type and kind as A(1:m, 1:n). It contains the generalized inverse matrix, $A^{\dagger}$.

cov = `cov(:,:)` (Output)

Array with size $n \times n$ of the same type and kind as A(1:m, 1:n). It contains the unscaled covariance matrix, $C = (A^{T}A)^{-1}$.

iopt = `iopt(:)` (Input)

Derived type array with the same precision as the input matrix; used for passing optional data to the routine. The options are as follows:

Packaged Options for **lin_sol_lsq**		
Option Prefix = ?	Option Name	Option Value
s_, d_, c_, z_	lin_sol_lsq_set_small	1
s_, d_, c_, z_	lin_sol_lsq_save_QR	2
s_, d_, c_, z_	lin_sol_lsq_solve_A	3
s_, d_, c_, z_	lin_sol_lsq_solve_ADJ	4

Packaged Options for lin_sol_lsq		
s_, d_, c_, z_	lin_sol_lsq_no_row_pivoting	5
s_, d_, c_, z_	lin_sol_lsq_no_col_pivoting	6
s_, d_, c_, z_	lin_sol_lsq_scan_for_NaN	7
s_, d_, c_, z_	lin_sol_lsq_no_sing_mess	8

iopt(IO) = ?_options(?_lin_sol_lsq_set_small, *Small*)

Replaces with *Small* if a diagonal term of the matrix *R* is smaller in magnitude than the value *Small*. A solution is approximated based on this replacement in either case.
Default: the smallest number that can be reciprocated safely

iopt(IO) = ?_options(?_lin_sol_lsq_save_QR, ?_dummy)

Saves the factorization of A. Requires the optional arguments "pivots=" and "trans=" if the routine is used for solving further systems with the same matrix. This is the only case where the input arrays A and b are not saved. For efficiency, the diagonal reciprocals of the matrix *R* are saved in the diagonal entries of A.

iopt(IO) = ?_options(?_lin_sol_lsq_solve_A, ?_dummy)

Uses the factorization of A computed and saved to solve $Ax = b$.

iopt(IO) = ?_options(?_lin_sol_lsq_solve_ADJ, ?_dummy)

Uses the factorization of A computed and saved to solve $A^T x = b$.

iopt(IO) = ?_options(?_lin_sol_lsq_no_row_pivoting, ?_dummy)

Does no row pivoting. The array pivots(:), if present, satisfies pivots(i) = i for $i = 1, \ldots, \min(m, n)$.

iopt(IO) = ?_options(?_lin_sol_lsq_no_col_pivoting, ?_dummy)

Does no column pivoting. The array pivots(:), if present, satisfies pivots($i + \min(m, n)$) = i for $i = 1, \ldots, \min(m, n)$.

iopt(IO) = ?_options(?_lin_sol_lsq_scan_for_NaN, ?_dummy)

Examines each input array entry to find the first value such that

```
isNaN(a(i,j)) .or. isNan(b(i,j)) == .true.
```

See the isNaN() function, *Chapter 10*.
Default: Does not scan for NaNs

iopt(IO) = ?_options(?_lin_sol_lsq_no_sing_mess, ?_dummy)

Do not print an error message when *A* is singular or $k < \min(m, n)$.

FORTRAN 90 Interface

Generic:CALL LIN_SOL_LSQ (A, B, X [, …])

Specific:The specific interface names are S_LIN_SOL_LSQ, D_LIN_SOL_LSQ, C_LIN_SOL_LSQ, and Z_LIN_SOL_LSQ.

Description

Routine LIN_SOL_LSQ solves a rectangular system of linear algebraic equations in a least-squares sense. It computes the decomposition of *A* using an orthogonal factorization. This decomposition has the form

$$QAP = \begin{bmatrix} R_{k\times k} & 0 \\ 0 & 0 \end{bmatrix}$$

where the matrices *Q* and *P* are products of elementary orthogonal and permutation matrices. The matrix *R* is $k \times k$, where *k* is the approximate rank of *A*. This value is determined by the value of the parameter *Small*. See Golub and Van Loan (1989, Chapter 5.4) for further details. Note that the use of both row and column pivoting is nonstandard, but the routine defaults to this choice for enhanced reliability.

Fatal and Terminal Error Messages

See the *messages.gls* file for error messages for LIN_SOL_LSQ. These error messages are numbered 241–256; 261–276; 281–296; 301–316.

Examples

Example 1: Solving a Linear Least-squares System

This example solves a linear least-squares system $Cx \cong d$, where

$$C_{m\times n}$$

is a real matrix with $m > n$. The least-squares problem is derived from polynomial data fitting to the function

$$y(x) = e^x + \cos\left(\pi \frac{x}{2}\right)$$

using a discrete set of values in the interval $-1 \le x \le 1$. The polynomial is represented as the series

$$u(x) = \sum_{i=0}^{N} c_i T_i(x)$$

where the $T_i(x)$ are Chebyshev polynomials. It is natural for the problem matrix and solution to have a column or entry corresponding to the subscript zero, which is used in this code. Also, see `operator_ex09`, supplied with the product examples.

```
      use lin_sol_lsq_int
      use rand_gen_int
      use error_option_packet

      implicit none

! This is Example 1 for LIN_SOL_LSQ.

      integer i
      integer, parameter :: m=128, n=8
      real(kind(1d0)), parameter :: one=1d0, zero=0d0
      real(kind(1d0)) A(m,0:n), c(0:n,1), pi_over_2, x(m), y(m,1), &
             u(m), v(m), w(m), delta_x

! Generate a random grid of points.
      call rand_gen(x)

! Transform points to the interval -1,1.
      x = x*2 - one

! Compute the constant 'PI/2'.
      pi_over_2 = atan(one)*2

! Generate known function data on the grid.
      y(1:m,1) = exp(x) + cos(pi_over_2*x)

! Fill in the least-squares matrix for the Chebyshev polynomials.
      A(:,0) = one; A(:,1) = x

      do i=2, n
         A(:,i) = 2*x*A(:,i-1) - A(:,i-2)
      end do

! Solve for the series coefficients.
      call lin_sol_lsq(A, y, c)

! Generate an equally spaced grid on the interval.
      delta_x = 2/real(m-1,kind(one))
      do i=1, m
         x(i) = -one + (i-1)*delta_x
      end do

! Evaluate residuals using backward recurrence formulas.
      u = zero
      v = zero
      do i=n, 0, -1
         w = 2*x*u - v + c(i,1)
         v = u
         u = w
      end do

      y(1:m,1) = exp(x) + cos(pi_over_2*x) - (u-x*v

! Check that n+1 sign changes in the residual curve occur.
```

```
      x = one
      x = sign(x,y(1:m,1))

      if (count(x(1:m-1) /= x(2:m)) >= n+1) then
         write (*,*) 'Example 1 for LIN_SOL_LSQ is correct.'
      end if

      end
```

Output

```
Example 1 for LIN_SOL_LSQ is correct.
```

Example 2: System Solving with the Generalized Inverse

This example solves the same form of the system as Example 1. In this case, the grid of evaluation points is equally spaced. The coefficients are computed using the “smoothing formulas” by rows of the generalized inverse matrix, $A^{\dagger}$, computed using the optional argument “`ainv=`”. Thus, the coefficients are given by the matrix-vector product $c = (A^{\dagger})\,y$, where y is the vector of values of the function $y(x)$ evaluated at the grid of points. Also, see `operator_ex10`, supplied with the product examples.

```
      use lin_sol_lsq_int

      implicit none

! This is Example 2 for LIN_SOL_LSQ.

      integer i
      integer, parameter :: m=128, n=8
      real(kind(1d0)), parameter :: one=1.0d0, zero=0.0d0
      real(kind(1d0)) a(m,0:n), c(0:n,1), pi_over_2, x(m), y(m,1), &
             u(m), v(m), w(m), delta_x, inv(0:n, m)

! Generate an array of equally spaced points on the interval -1,1.

      delta_x = 2/real(m-1,kind(one))
      do i=1, m
         x(i) = -one + (i-1)*delta_x
      end do

! Compute the constant 'PI/2'.

      pi_over_2 = atan(one)*2

! Compute data values on the grid.

      y(1:m,1) = exp(x) + cos(pi_over_2*x)

! Fill in the least-squares matrix for the Chebyshev polynomials.

      a(:,0) = one
      a(:,1) = x

      do i=2, n
         a(:,i) = 2*x*a(:,i-1) - a(:,i-2)
      end do

! Compute the generalized inverse of the least-squares matrix.

      call lin_sol_lsq(a, y, c, nrhs=0, ainv=inv)
```

```
! Compute the series coefficients using the generalized inverse
! as 'smoothing formulas.'

      c(0:n,1) = matmul(inv(0:n,1:m),y(1:m,1))

! Evaluate residuals using backward recurrence formulas.

      u = zero
      v = zero
      do i=n, 0, -1
         w = 2*x*u - v + c(i,1)
         v = u
         u = w
      end do

      y(1:m,1) = exp(x) + cos(pi_over_2*x) - (u-x*v)

! Check that n+2 sign changes in the residual curve occur.
! (This test will fail when n is larger.)

      x = one
      x = sign(x,y(1:m,1))

      if (count(x(1:m-1) /= x(2:m)) == n+2) then
         write (*,*) 'Example 2 for LIN_SOL_LSQ is correct.'
      end if

      end
```

Output

```
Example 2 for LIN_SOL_LSQ is correct.
```

Example 3: Two-Dimensional Data Fitting

This example illustrates the use of radial-basis functions to least-squares fit arbitrarily spaced data points. Let m data values $\{y_i\}$ be given at points in the unit square, $\{p_i\}$. Each p_i is a pair of real values. Then, n points $\{q_j\}$ are chosen on the unit square. A series of *radial-basis functions* is used to represent the data,

$$f(p) = \sum_{j=1}^{n} c_j \left(\|p - q_j\|^2 + \delta^2 \right)^{1/2}$$

where δ^2 is a parameter. This example uses $\delta^2 = 1$, but either larger or smaller values can give a better approximation for user problems. The coefficients $\{c_j\}$ are obtained by solving the following $m \times n$ linear least-squares problem:

$$f(p_j) = y_j$$

This example illustrates an effective use of Fortran 90 array operations to eliminate many details required to build the matrix and right-hand side for the $\{c_j\}$. For this example, the two sets of points $\{p_i\}$ and $\{q_j\}$ are chosen randomly. The values $\{y_j\}$ are computed from the following formula:

$$y_j = e^{-||p_j||^2}$$

The residual function

$$r(p) = e^{-||p||^2} - f(p)$$

is computed at an $N \times N$ square grid of equally spaced points on the unit square. The magnitude of $r(p)$ may be larger at certain points on this grid than the residuals at the given points, $\{p_i\}$. Also, see `operator_ex11`, supplied with the product examples.

```
      use lin_sol_lsq_int
      use rand_gen_int

      implicit none

! This is Example 3 for LIN_SOL_LSQ.

      integer i, j
      integer, parameter :: m=128, n=32, k=2, n_eval=16
      real(kind(1d0)), parameter :: one=1.0d0, delta_sqr=1.0d0
      real(kind(1d0)) a(m,n), b(m,1), c(n,1), p(k,m), q(k,n), &
              x(k*m), y(k*n), t(k,m,n), res(n_eval,n_eval), &
              w(n_eval), delta

! Generate a random set of data points in k=2 space.

      call rand_gen(x)
      p = reshape(x,(/k,m/))

! Generate a random set of center points in k-space.

      call rand_gen(y)
      q = reshape(y,(/k,n/))

! Compute the coefficient matrix for the least-squares system.

      t = spread(p,3,n)
      do j=1, n
        t(1:,:,j) = t(1:,:,j) - spread(q(1:,j),2,m)
      end do

      a = sqrt(sum(t**2,dim=1) + delta_sqr)

! Compute the right hand side of data values.

      b(1:,1) = exp(-sum(p**2,dim=1))

! Compute the solution.

      call lin_sol_lsq(a, b, c)

! Check the results.

      if (sum(abs(matmul(transpose(a),b-matmul(a,c))))/sum(abs(a)) &
          <= sqrt(epsilon(one))) then
        write (*,*) 'Example 3 for LIN_SOL_LSQ is correct.'
      end if

! Evaluate residuals, known function - approximation at a square
```

```
! grid of points.  (This evaluation is only for k=2.)

      delta = one/real(n_eval-1,kind(one))
      do i=1, n_eval
         w(i) = (i-1)*delta
      end do
      res = exp(-(spread(w,1,n_eval)**2 + spread(w,2,n_eval)**2))
      do j=1, n
         res = res - c(j,1)*sqrt((spread(w,1,n_eval) - q(1,j))**2 + &
                    (spread(w,2,n_eval) - q(2,j))**2 + delta_sqr)
      end do

      end
```

Output

```
Example 3 for LIN_SOL_LSQ is correct.
```

Example 4: Least-squares with an Equality Constraint

This example solves a least-squares system $Ax \cong b$ with the constraint that the solution values have a sum equal to the value 1. To solve this system, one heavily weighted row vector and right-hand side component is added to the system corresponding to this constraint. Note that the weight used is

$$\varepsilon^{-1/2}$$

where ε is the machine precision, but any larger value can be used. The fact that `lin_sol_lsq` performs row pivoting in this case is critical for obtaining an accurate solution to the constrained problem solved using weighting. See Golub and Van Loan (1989, Chapter 12) for more information about this method. Also, see `operator_ex12`, supplied with the product examples.

```
      use lin_sol_lsq_int
      use rand_gen_int

      implicit none

! This is Example 4 for LIN_SOL_LSQ.

      integer, parameter :: m=64, n=32
      real(kind(1e0)), parameter :: one=1.0e0
      real(kind(1e0)) :: a(m+1,n), b(m+1,1), x(n,1), y(m*n)

! Generate a random matrix.

      call rand_gen(y)
      a(1:m,1:n) = reshape(y,(/m,n

! Generate a random right hand side.

      call rand_gen(b(1:m,1))

! Heavily weight desired constraint.  All variables sum to one.

      a(m+1,1:n) = one/sqrt(epsilon(one))

      b(m+1,1) = one/sqrt(epsilon(one))

      call lin_sol_lsq(a, b, x)
```

```
      if (abs(sum(x) - one)/sum(abs(x)) <= &
                  sqrt(epsilon(one))) then
         write (*,*) 'Example 4 for LIN_SOL_LSQ is correct.'
      end if

      end
```

Output

```
Example 4 for LIN_SOL_LSQ is correct.
```

LIN_SOL_SVD

Solves a rectangular least-squares system of linear equations $Ax \cong b$ using singular value decomposition

$$A = USV^T$$

With optional arguments, any of several related computations can be performed. These extra tasks include computing the rank of A, the orthogonal $m \times m$ and $n \times n$ matrices U and V, and the $m \times n$ diagonal matrix of singular values, S.

Required Arguments

A — Array of size $m \times n$ containing the matrix. (Input [/Output])
If the packaged option `lin_sol_svd_overwrite_input` is used, this array is not saved on output.

B — Array of size $m \times nb$ containing the right-hand side matrix. (Input [/Output]
If the packaged option `lin_sol_svd_overwrite_input` is used, this array is not saved on output.

X— Array of size $n \times nb$ containing the solution matrix. (Output)

Optional Arguments

MROWS = `m` (Input)
Uses array `A`(1 **:** `m`, 1 **:** `n`) for the input matrix.
Default: `m` = size (`A`, 1)

NCOLS = `n` (Input)
Uses array `A (1:m, 1:n)` for the input matrix.
Default: `n` = size(`A`, 2)

NRHS = `nb` (Input)
Uses the array `b`(1 **:**, 1 **:** `nb`) for the input right-hand side matrix.
Default: `nb` = size(`b`, 2)
Note that `b` must be a rank-2 array.

RANK = `k` (Output)
Number of singular values that are at least as large as the value *Small*. It will satisfy `k` <= min(`m`, `n`).

u = `u(:,:)` (Output)
Array of the same type and kind as `A(1:m, 1:n)`. It contains the $m \times m$ orthogonal matrix U of the singular value decomposition.

s = `s(:)` (Output)
Array of the same precision as `A(1:m, 1:n)`. This array is real even when the matrix data is complex. It contains the $m \times n$ diagonal matrix S in a rank-1 array. The singular values are nonnegative and ordered non-increasing.

v = `v(:,:)` (Output)
Array of the same type and kind as `A(1:m, 1:n)`. It contains the $n \times n$ orthogonal matrix V.

iopt = `iopt(:)` (Input)
Derived type array with the same precision as the input matrix. Used for passing optional data to the routine. The options are as follows:

Packaged Options for `lin_sol_svd`		
Option Prefix = ?	**Option Name**	**Option Value**
`s_, d_, c_, z_`	`lin_sol_svd_set_small`	1
`s_, d_, c_, z_`	`lin_sol_svd_overwrite_input`	2
`s_, d_, c_, z_`	`lin_sol_svd_safe_reciprocal`	3
`s_, d_, c_, z_`	`lin_sol_svd_scan_for_NaN`	4

iopt(IO) = `?_options(?_lin_sol_svd_set_small`, *Small*)
Replaces with zero a diagonal term of the matrix S if it is smaller in magnitude than the value *Small*. This determines the approximate rank of the matrix, which is returned as the "`rank=`" optional argument. A solution is approximated based on this replacement.
Default: the smallest number that can be safely reciprocated

iopt(IO) = `?_options(?_lin_sol_svd_overwrite_input, ?_dummy)`
Does not save the input arrays `A(:,:)` and `b(:,:)`.

iopt(IO) = `?_options(?_lin_sol_svd_safe_reciprocal`, *safe*)
Replaces a denominator term with safe if it is smaller in magnitude than the value *safe*.
Default: the smallest number that can be safely reciprocated

iopt(IO) = `?_options(?_lin_sol_svd_scan_for_NaN, ?_dummy)`
Examines each input array entry to find the first value such that

isNaN(a(i,j)) .or. isNan(b(i,j)) ==.true.

See the `isNaN()` function, *Chapter 10*.
Default: Does not scan for NaNs

FORTRAN 90 Interface

Generic: CALL LIN_SOL_SVD (A, B, X [, …])

Specific: The specific interface names are S_LIN_SOL_SVD, D_LIN_SOL_SVD, C_LIN_SOL_SVD, and Z_LIN_SOL_SVD.

Description

Routine LIN_SOL_SVD solves a rectangular system of linear algebraic equations in a least-squares sense. It computes the factorization of *A* known as the singular value decomposition. This decomposition has the following form:

$A = USV^T$

The matrices *U* and *V* are orthogonal. The matrix *S* is diagonal with the diagonal terms non-increasing. See Golub and Van Loan (1989, Chapters 5.4 and 5.5) for further details.

Fatal, Terminal, and Warning Error Messages

See the *messages.gls* file for error messages for LIN_SOL_SVD. These error messages are numbered 401–412; 421–432; 441–452; 461–472.

Examples

Example 1: Least-squares solution of a Rectangular System

The least-squares solution of a rectangular $m \times n$ system $Ax \cong b$ is obtained. The use of lin_sol_lsq is more efficient in this case since the matrix is of full rank. This example anticipates a problem where the matrix *A* is poorly conditioned or not of full rank; thus, lin_sol_svd is the appropriate routine. Also, see operator_ex13, in *Chapter 10*.

```
      use lin_sol_svd_int
      use rand_gen_int

      implicit none

! This is Example 1 for LIN_SOL_SVD.

      integer, parameter :: m=128, n=32
      real(kind(1d0)), parameter :: one=1d0
      real(kind(1d0)) A(m,n), b(m,1), x(n,1), y(m*n), err

! Generate a random matrix and right-hand side.
      call rand_gen(y)
      A = reshape(y,(/m,n/))
      call rand_gen(b(1:m,1))
```

```
! Compute the least-squares solution matrix of Ax=b.
      call lin_sol_svd(A, b, x)

! Check that the residuals are orthogonal to the
! column vectors of A.
      err = sum(abs(matmul(transpose(A),b-matmul(A,x))))/sum(abs(A))
      if (err <= sqrt(epsilon(one))) then

         write (*,*) 'Example 1 for LIN_SOL_SVD is correct.'
      end if

      end
```

Output

```
Example 1 for LIN_SOL_SVD is correct.
```

Example 2: Polar Decomposition of a Square Matrix

A polar decomposition of an $n \times n$ random matrix is obtained. This decomposition satisfies $A = PQ$, where P is orthogonal and Q is self-adjoint and positive definite.

Given the singular value decomposition

$$A = USV^T$$

the polar decomposition follows from the matrix products

$$P = UV^T \text{and } Q = VSV^T$$

This example uses the optional arguments "u=", "s=", and "v=", then array intrinsic functions to calculate P and Q. Also, see `operator_ex14`, in *Chapter 10*.

```
      use lin_sol_svd_int
      use rand_gen_int

      implicit none

! This is Example 2 for LIN_SOL_SVD.

      integer i
      integer, parameter :: n=32
      real(kind(1d0)), parameter :: one=1.0d0, zero=0.0d0
      real(kind(1d0)) a(n,n), b(n,0), ident(n,n), p(n,n), q(n,n), &
             s_d(n), u_d(n,n), v_d(n,n), x(n,0), y(n*n)

! Generate a random matrix.

      call rand_gen(y)
      a = reshape(y,(/n,n/))

! Compute the singular value decomposition.

      call lin_sol_svd(a, b, x, nrhs=0, s=s_d, &
                u=u_d, v=v_d)

! Compute the (left) orthogonal factor.
```

```
      p = matmul(u_d,transpose(v_d))

! Compute the (right) self-adjoint factor.

      q = matmul(v_d*spread(s_d,1,n),transpose(v_d))

      ident=zero
      do i=1, n
         ident(i,i) = one
      end do

! Check the results.

      if (sum(abs(matmul(p,transpose(p)) - ident))/sum(abs(p)) &
             <= sqrt(epsilon(one))) then
         if (sum(abs(a - matmul(p,q)))/sum(abs(a)) &
             <= sqrt(epsilon(one))) then
            write (*,*) 'Example 2 for LIN_SOL_SVD is correct.'
         end if
      end if

      end
```

Output

```
Example 2 for LIN_SOL_SVD is correct.
```

Example 3: Reduction of an Array of Black and White

An $n \times n$ array A contains entries that are either 0 or 1. The entry is chosen so that as a two-dimensional object with origin at the point (1, 1), the array appears as a black circle of radius $n/4$ centered at the point ($n/2$, $n/2$).

A singular value decomposition

$$A = USV^T$$

is computed, where S is of low rank. Approximations using fewer of these nonzero singular values and vectors suffice to reconstruct A. Also, see `operator_ex15`, supplied with the product examples.

```
      use lin_sol_svd_int
      use rand_gen_int
      use error_option_packet

      implicit none

! This is Example 3 for LIN_SOL_SVD.

      integer i, j, k
      integer, parameter :: n=32
      real(kind(1e0)), parameter :: half=0.5e0, one=1e0, zero=0e0
      real(kind(1e0)) a(n,n), b(n,0), x(n,0), s(n), u(n,n), &
             v(n,n), c(n,n)

! Fill in value one for points inside the circle.
      a = zero
      do i=1, n
         do j=1, n
            if ((i-n/2)**2 + (j-n/2)**2 <= (n/4)**2) a(i,j) = one
         end do
```

```
      end do

! Compute the singular value decomposition.
      call lin_sol_svd(a, b, x, nrhs=0,&
            s=s, u=u, v=v)

! How many terms, to the nearest integer, exactly
! match the circle?
           c = zero; k = count(s > half)
      do i=1, k
        c = c + spread(u(1:n,i),2,n)*spread(v(1:n,i),1,n)*s(i)
        if (count(int(c-a) /= 0) == 0) exit
      end do

      if (i < k) then
         write (*,*) 'Example 3 for LIN_SOL_SVD is correct.'
      end if
      end
```

Output

```
Example 3 for LIN_SOL_SVD is correct.
```

Example 4: Laplace Transform Solution

This example illustrates the solution of a linear least-squares system where the matrix is poorly conditioned. The problem comes from solving the integral equation:

$$\int_0^1 e^{-st} f(t)\,dt = s^{-1}\left(1 - e^{-s}\right) = g(s)$$

The unknown function $f(t) = 1$ is computed. This problem is equivalent to the numerical inversion of the Laplace Transform of the function $g(s)$ using real values of t and s, solving for a function that is nonzero only on the unit interval. The evaluation of the integral uses the following approximate integration rule:

$$\int_0^1 f(t)e^{-st}dt = \sum_{j=1}^{n} f(t_j) \int_{t_j}^{t_{j+1}} e^{-st}dt$$

The points $\{t_j\}$ are chosen equally spaced by using the following:

$$t_j = \frac{j-1}{n}$$

The points $\{s_j\}$ are computed so that the range of $g(s)$ is uniformly sampled. This requires the solution of m equations

$$g(s_i) = g_i = \frac{i}{m+1}$$

for $j = 1, \ldots, n$ and $i = 1, \ldots, m$. Fortran 90 array operations are used to solve for the collocation points $\{s_i\}$ as a single series of steps. Newton's method,

$$s \leftarrow s - \frac{h}{h'}$$

is applied to the array function

$$h(s) = e^{-s} + sg - 1$$

where the following is true:

$$g = [g_1, \ \ldots, \ g_m]^T$$

Note the coefficient matrix for the solution values

$$f = [f(t_1), \ \ldots, \ f(t_n)]^T$$

whose entry at the intersection of row i and column j is equal to the value

$$\int_{t_j}^{t_{j+1}} e^{-s_i t} dt$$

is explicitly integrated and evaluated as an array operation. The solution analysis of the resulting linear least-squares system

$$Af \cong g$$

is obtained by computing the singular value decomposition

$$A = USV^T$$

An approximate solution is computed with the transformed right-hand side

$$b = U^T g$$

followed by using as few of the largest singular values as possible to minimize the following squared error residual:

$$\sum_{j=1}^{n}\left(1-f_j\right)^2$$

This determines an optimal value *k* to use in the approximate solution

$$f=\sum_{j=1}^{k} b_j \frac{v_j}{s_j}$$

Also, see `operator_ex16`, supplied with the product examples.

```
      use lin_sol_svd_int
      use rand_gen_int
      use error_option_packet

      implicit none

! This is Example 4 for LIN_SOL_SVD.

      integer i, j, k
      integer, parameter :: m=64, n=16
      real(kind(1e0)), parameter :: one=1e0, zero=0.0e0
      real(kind(1e0)) :: g(m), s(m), t(n+1), a(m,n), b(m,1), &
               f(n,1), U_S(m,m), V_S(n,n), S_S(n), &
               rms, oldrms
      real(kind(1e0)) :: delta_g, delta_t

      delta_g = one/real(m+1,kind(one))

! Compute which collocation equations to solve.
      do i=1,m
        g(i)=i*delta_g
      end do

! Compute equally spaced quadrature points.
      delta_t =one/real(n,kind(one))
      do j=1,n+1
        t(j)=(j-1)*delta_t
      end do

! Compute collocation points.
      s=m
      solve_equations: do
        s=s-(exp(-s)-(one-s*g))/(g-exp(-s))
        if (sum(abs((one-exp(-s))/s - g)) <= &
              epsilon(one)*sum(g)) &
            exit solve_equations
      end do solve_equations

! Evaluate the integrals over the quadrature points.
      a = (exp(-spread(t(1:n),1,m)*spread(s,2,n)) &
        - exp(-spread(t(2:n+1),1,m)*spread(s,2,n))) / &
          spread(s,2,n)

      b(1:,1)=g

! Compute the singular value decomposition.

      call lin_sol_svd(a, b, f, nrhs=0, &
              rank=k, u=U_S, v=V_S, s=S_S)
```

```
! Singular values that are larger than epsilon determine
! the rank=k.
      k = count(S_S > epsilon(one))
      oldrms = huge(one)
      g = matmul(transpose(U_S), b(1:m,1))

! Find the minimum number of singular values that gives a good
! approximation to f(t) = 1.

      do i=1,k
         f(1:n,1) = matmul(V_S(1:,1:i), g(1:i)/S_S(1:i))
         f = f - one
         rms = sum(f**2)/n
         if (rms > oldrms) exit
         oldrms = rms
      end do

      write (*,"( ' Using this number of singular values, ', &
          &i4 / ' the approximate R.M.S. error is ', 1pe12.4)") &
      i-1, oldrms

      if (sqrt(oldrms) <= delta_t**2) then
         write (*,*) 'Example 4 for LIN_SOL_SVD is correct.'
      end if

      end
```

Output

```
Example 4 for LIN_SOL_SVD is correct.
```

LIN_SOL_TRI

Solves multiple systems of linear equations

$$A_j x_j = y_j, j = 1, \ldots, k$$

Each matrix A_j is tridiagonal with the same dimension, n. The default solution method is based on *LU* factorization computed using cyclic reduction or, optionally, Gaussian elimination with partial pivoting.

Required Arguments

C — Array of size $2n \times k$ containing the upper diagonals of the matrices A_j. Each upper diagonal is entered in array locations `c`$(1 : n - 1, j)$. The data $C(n, 1 : k)$ are not used. (Input [/Output])
The input data is overwritten. See note below.

D — Array of size $2n \times k$ containing the diagonals of the matrices A_j. Each diagonal is entered in array locations `D`$(1 : n, j)$. (Input [/Output])
The input data is overwritten. See note below.

B — Array of size $2n \times k$ containing the lower diagonals of the matrices A_j. Each lower diagonal is entered in array locations `B`$(2 : n, j)$. The data `B`$(1, 1 : k)$ are not used. (Input [/Output])
The input data is overwritten. See note below.

Y — Array of size $2n \times k$ containing the right-hand sides, y_j. Each right-hand side is entered in array locations `Y`$(1 : n, j)$. The computed solution x_j is returned in locations `Y`$(1 : n, j)$. (Input [/Output])

NOTE: The required arguments have the Input data overwritten. If these quantities are used later, they must be saved in user-defined arrays. The routine uses each array's locations (n + 1:2 * n, 1:k) for scratch storage and intermediate data in the LU factorization. The default values for problem dimensions are n = (size (`D`, 1))/2 and k = size (`D`, 2).

Optional Arguments

NCOLS = `n` (Input)
Uses arrays `C`(1 : `n` – 1, 1 : `k`), `D`(1 : `n`, 1 : `k`), and `B`(2 : `n`, 1 : `k`) as the upper, main and lower diagonals for the input tridiagonal matrices. The right-hand sides and solutions are in array `Y`(1 : `n`, 1 : `k`). Note that each of these arrays are rank-2.
Default: `n` = (size(`D`, 1))/2

NPROB = `k` (Input)

The number of systems solved.

Default: *k* = size(`D`, 2)

iopt = `iopt(:)` (Input)

Derived type array with the same precision as the input matrix. Used for passing optional data to the routine. The options are as follows:

Packaged Options for **LIN_SOL_TRI**		
Option Prefix = ?	Option Name	Option Value
`s_, d_, c_, z_`	`lin_sol_tri_set_small`	1
`s_, d_, c_, z_`	`lin_sol_tri_set_jolt`	2
`s_, d_, c_, z_`	`lin_sol_tri_scan_for_NaN`	3
`s_, d_, c_, z_`	`lin_sol_tri_factor_only`	4
`s_, d_, c_, z_`	`lin_sol_tri_solve_only`	5
`s_, d_, c_, z_`	`lin_sol_tri_use_Gauss_elim`	6

iopt(IO) = `?_options(?_lin_sol_tri_set_small`, *Small*)

Whenever a reciprocation is performed on a quantity smaller than *Small*, it is replaced by that value plus 2 × *jolt*.

Default: 0.25 × *epsilon*()

iopt(IO) = `?_options(?_lin_sol_tri_set_jolt`, *jolt*`)`

Default: *epsilon*(), machine precision

iopt(IO) = `?_options(?_lin_sol_tri_scan_for_NaN`, `?_dummy)`

Examines each input array entry to find the first value such that

`isNaN(C(i,j))` .or.

`isNaN(D(i,j))` .or.

`isNaN(B(i,j))` .or.

`isNaN(Y(i,j))` == .true.

See the `isNaN()` function, *Chapter 10*.

Default: Does not scan for NaNs.

iopt(IO) = `?_options(?_lin_sol_tri_factor_only`, `?_dummy)`

Obtain the *LU* factorization of the matrices A_j. Does not solve for a solution.

Default: Factor the matrices and solve the systems.

iopt(IO) = `?_options(?_lin_sol_tri_solve_only, ?_dummy)`

Solve the systems $A_j x_j = y_j$ using the previously computed *LU* factorization.

Default: Factor the matrices and solve the systems.

iopt(IO) = `?_options(?_lin_sol_tri_use_Gauss_elim, ?_dummy)`

The accuracy, numerical stability or efficiency of the cyclic reduction algorithm may be inferior to the use of *LU* factorization with partial pivoting.

Default: Use cyclic reduction to compute the factorization.

FORTRAN 90 Interface

Generic: `CALL LIN_SOL_TRI (C, D, B, Y [, …])`

Specific: The specific interface names are `S_LIN_SOL_TRI`, `D_LIN_SOL_TRI`, `C_LIN_SOL_TRI`, and `Z_LIN_SOL_TRI`.

Description

Routine `lin_sol_tri` solves k systems of tridiagonal linear algebraic equations, each problem of dimension $n \times n$. No relation between k and n is required. See Kershaw, pages 86–88 in Rodrigue (1982) for further details. To deal with poorly conditioned or singular systems, a specific regularizing term is added to each reciprocated value. This technique keeps the factorization process efficient and avoids exceptions from overflow or division by zero. Each occurrence of an array reciprocal a^{-1} is replaced by the expression $(a + t)^{-1}$, where the array temporary t has the value 0 whenever the corresponding entry satisfies $|a| > Small$. Alternately, t has the value $2 \times jolt$. (Every small denominator gives rise to a finite “jolt”.) Since this tridiagonal solver is used in the routines `lin_svd` and `lin_eig_self` for inverse iteration, regularization is required. Users can reset the values of *Small* and *jolt* for their own needs. Using the default values for these parameters, it is generally necessary to scale the tridiagonal matrix so that the maximum magnitude has value approximately one. This is normally not an issue when the systems are nonsingular.

The routine is designed to use cyclic reduction as the default method for computing the *LU* factorization. Using an optional parameter, standard elimination and partial pivoting will be used to compute the factorization. Partial pivoting is numerically stable but is likely to be less efficient than cyclic reduction.

Fatal, Terminal, and Warning Error Messages

See the *messages.gls* file for error messages for `LIN_SOL_TRI`. These error messages are numbered 1081–1086; 1101–1106; 1121–1126; 1141–1146.

Examples

Example 1: Solution of Multiple Tridiagonal Systems

The upper, main and lower diagonals of n systems of size $n \times n$ are generated randomly. A scalar is added to the main diagonal so that the systems are positive definite. A random vector x_j is generated and right-hand sides $y_j = A_j y_j$ are computed. The routine is used to compute the solution, using the A_j and y_j. The results should compare closely with the x_j used to generate the right-hand sides. Also, see `operator_ex17`, supplied with the product examples.

```
      use lin_sol_tri_int
      use rand_gen_int
      use error_option_packet

      implicit none

! This is Example 1 for LIN_SOL_TRI.

      integer i
      integer, parameter :: n=128
      real(kind(1d0)), parameter :: one=1d0, zero=0d0
      real(kind(1d0)) err
      real(kind(1d0)), dimension(2*n,n) :: d, b, c, res(n,n), &
        t(n), x, y

! Generate the upper, main, and lower diagonals of the
! n matrices A_i.  For each system a random vector x is used
! to construct the right-hand side, Ax = y.  The lower part
! of each array remains zero as a result.

      c = zero; d=zero; b=zero; x=zero
      do i = 1, n
         call rand_gen (c(1:n,i))
         call rand_gen (d(1:n,i))
         call rand_gen (b(1:n,i))
         call rand_gen (x(1:n,i))
      end do

! Add scalars to the main diagonal of each system so that
! all systems are positive definite.
      t = sum(c+d+b,DIM=1)
      d(1:n,1:n) = d(1:n,1:n) + spread(t,DIM=1,NCOPIES=n)

! Set Ax = y.  The vector x generates y.  Note the use
! of EOSHIFT and array operations to compute the matrix
! product, n distinct ones as one array operation.

     y(1:n,1:n)=d(1:n,1:n)*x(1:n,1:n) + &
                c(1:n,1:n)*EOSHIFT(x(1:n,1:n),SHIFT=+1,DIM=1) + &
                b(1:n,1:n)*EOSHIFT(x(1:n,1:n),SHIFT=-1,DIM=1)

! Compute the solution returned in y.  (The input values of c,
! d, b, and y are overwritten by lin_sol_tri.)  Check for any
! error messages.

      call lin_sol_tri (c, d, b, y)

! Check the size of the residuals, y-x.  They should be small,
! relative to the size of values in x.
      res = x(1:n,1:n) - y(1:n,1:n)
```

```
       err = sum(abs(res)) / sum(abs(x(1:n,1:n)))
       if (err <= sqrt(epsilon(one))) then
          write (*,*) 'Example 1 for LIN_SOL_TRI is correct.'
       end if

       end
```

Output

```
Example 1 for LIN_SOL_TRI is correct.
```

Example 2: Iterative Refinement and Use of Partial Pivoting

This program unit shows usage that typically gives acceptable accuracy for a large class of problems. Our goal is to use the efficient cyclic reduction algorithm when possible, and keep on using it unless it will fail. In exceptional cases our program switches to the *LU* factorization with partial pivoting. This use of both factorization and solution methods enhances reliability and maintains efficiency on the average. Also, see `operator_ex18`, supplied with the product examples.

```
       use lin_sol_tri_int
       use rand_gen_int

       implicit none

! This is Example 2 for LIN_SOL_TRI.

       integer i, nopt
       integer, parameter :: n=128
       real(kind(1e0)), parameter :: s_one=1e0, s_zero=0e0
       real(kind(1d0)), parameter :: d_one=1d0, d_zero=0d0
       real(kind(1e0)), dimension(2*n,n) :: d, b, c, res(n,n), &
         x, y
       real(kind(1e0)) change_new, change_old, err
       type(s_options) :: iopt(2) = s_options(0,s_zero)
       real(kind(1d0)), dimension(n,n) :: d_save, b_save, c_save, &
              x_save, y_save, x_sol
       logical solve_only


       c = s_zero; d=s_zero; b=s_zero; x=s_zero

! Generate the upper, main, and lower diagonals of the
! matrices A.  A random vector x is used to construct the
! right-hand sides: y=A*x.
       do i = 1, n
          call rand_gen (c(1:n,i))
          call rand_gen (d(1:n,i))
          call rand_gen (b(1:n,i))
          call rand_gen (x(1:n,i))
       end do

! Save double precision copies of the diagonals and the
! right-hand side.
       c_save = c(1:n,1:n); d_save = d(1:n,1:n)
       b_save = b(1:n,1:n); x_save = x(1:n,1:n)
       y_save(1:n,1:n) = d(1:n,1:n)*x_save + &
                 c(1:n,1:n)*EOSHIFT(x_save,SHIFT=+1,DIM=1) + &
                 b(1:n,1:n)*EOSHIFT(x_save,SHIFT=-1,DIM=1)
```

```
! Iterative refinement loop.
      factorization_choice:  do nopt=0, 1

! Set the logical to flag the first time through.

         solve_only = .false.
         x_sol = d_zero
         change_old = huge(s_one)

         iterative_refinement:  do

! This flag causes a copy of data to be moved to work arrays
! and a factorization and solve step to be performed.
            if (.not. solve_only) then
               c(1:n,1:n)=c_save; d(1:n,1:n)=d_save
               b(1:n,1:n)=b_save
            end if

! Compute current residuals, y - A*x, using current x.
            y(1:n,1:n) = -y_save + &
             d_save*x_sol + &
             c_save*EOSHIFT(x_sol,SHIFT=+1,DIM=1) + &
             b_save*EOSHIFT(x_sol,SHIFT=-1,DIM=1)

            call lin_sol_tri (c, d, b, y, iopt=iopt)

            x_sol = x_sol + y(1:n,1:n)

            change_new = sum(abs(y(1:n,1:n)))

! If size of change is not decreasing, stop the iteration.
            if (change_new >= change_old) exit iterative_refinement

            change_old = change_new
            iopt(nopt+1) = s_options(s_lin_sol_tri_solve_only,s_zero)
            solve_only = .true.

         end do iterative_refinement

! Use Gaussian Elimination if Cyclic Reduction did not get an
! accurate solution.
! It is an exceptional event when Gaussian Elimination is required.
         if (sum(abs(x_sol - x_save)) / sum(abs(x_save)) &
           <= sqrt(epsilon(d_one))) exit factorization_choice

         iopt = s_options(0,s_zero)
         iopt(nopt+1) = s_options(s_lin_sol_tri_use_Gauss_elim,s_zero)

      end do factorization_choice

! Check on accuracy of solution.

      res = x(1:n,1:n)- x_save
      err = sum(abs(res)) / sum(abs(x_save))
      if (err <= sqrt(epsilon(d_one))) then
         write (*,*) 'Example 2 for LIN_SOL_TRI is correct.'
      end if

      end
```

Output

```
Example 2 for LIN_SOL_TRI is correct.
```

Example 3: Eigenvectors of Tridiagonal Matrices

The eigenvalues $\lambda_1, \ldots, \lambda_n$ of a tridiagonal real, self-adjoint matrix are computed. Note that the computation is performed using the IMSL MATH/LIBRARY FORTRAN 77 interface to routine EVASB. The user may write this interface based on documentation of the arguments (IMSL 2003, p. 480), or use the module *Numerical_Libraries* as we have done here. The eigenvectors corresponding to $k < n$ of the eigenvalues are required. These vectors are computed using inverse iteration for all the eigenvalues at one step. See Golub and Van Loan (1989, Chapter 7). The eigenvectors are then orthogonalized. Also, see `operator_ex19`, supplied with the product examples.

```
      use lin_sol_tri_int
      use rand_gen_int
      use Numerical_Libraries

      implicit none

! This is Example 3 for LIN_SOL_TRI.

      integer i, j, nopt
      integer, parameter :: n=128, k=n/4, ncoda=1, lda=2
      real(kind(1e0)), parameter :: s_one=1e0, s_zero=0e0
      real(kind(1e0)) A(lda,n), EVAL(k)
      type(s_options) :: iopt(2)=s_options(0,s_zero)
      real(kind(1e0)) d(n), b(n), d_t(2*n,k), c_t(2*n,k), perf_ratio, &
           b_t(2*n,k), y_t(2*n,k), eval_t(k), res(n,k), temp
      logical small

! This flag is used to get the k largest eigenvalues.
      small = .false.

! Generate the main diagonal and the co-diagonal of the
! tridiagonal matrix.

      call rand_gen (b)
      call rand_gen (d)

      A(1,1:)=b; A(2,1:)=d

! Use Numerical Libraries routine for the calculation of k
! largest eigenvalues.

      CALL EVASB (N, K, A, LDA, NCODA, SMALL, EVAL)
      EVAL_T = EVAL


! Use DNFL tridiagonal solver for inverse iteration
! calculation of eigenvectors.
      factorization_choice:  do nopt=0,1

! Create k tridiagonal problems, one for each inverse
! iteration system.
         b_t(1:n,1:k) = spread(b,DIM=2,NCOPIES=k)
         c_t(1:n,1:k) = EOSHIFT(b_t(1:n,1:k),SHIFT=1,DIM=1)
         d_t(1:n,1:k) = spread(d,DIM=2,NCOPIES=k) - &
                        spread(EVAL_T,DIM=1,NCOPIES=n)

! Start the right-hand side at random values, scaled downward
! to account for the expected 'blowup' in the solution.
         do i=1, k
            call rand_gen (y_t(1:n,i))
         end do

! Do two iterations for the eigenvectors.
```

```
          do i=1, 2
             y_t(1:n,1:k) = y_t(1:n,1:k)*epsilon(s_one)
             call lin_sol_tri(c_t, d_t, b_t, y_t, &
                         iopt=iopt)
             iopt(nopt+1) = s_options(s_lin_sol_tri_solve_only,s_zero)
          end do

 ! Orthogonalize the eigenvectors.  (This is the most
 ! intensive part of the computing.)
          do j=1,k-1 ! Forward sweep of HMGS orthogonalization.
             temp=s_one/sqrt(sum(y_t(1:n,j)**2))
             y_t(1:n,j)=y_t(1:n,j)*temp

             y_t(1:n,j+1:k)=y_t(1:n,j+1:k)+ &
             spread(-matmul(y_t(1:n,j),y_t(1:n,j+1:k)), &
          DIM=1,NCOPIES=n)* spread(y_t(1:n,j),DIM=2,NCOPIES=k-j)
          end do
          temp=s_one/sqrt(sum(y_t(1:n,k)**2))
          y_t(1:n,k)=y_t(1:n,k)*temp

          do j=k-1,1,-1 ! Backward sweep of HMGS.
             y_t(1:n,j+1:k)=y_t(1:n,j+1:k)+ &
             spread(-matmul(y_t(1:n,j),y_t(1:n,j+1:k)), &
          DIM=1,NCOPIES=n)* spread(y_t(1:n,j),DIM=2,NCOPIES=k-j)
          end do

 ! See if the performance ratio is smaller than the value one.
 ! If it is not the code will re-solve the systems using Gaussian
 ! Elimination.  This is an exceptional event.  It is a necessary
 ! complication for achieving reliable results.

          res(1:n,1:k) = spread(d,DIM=2,NCOPIES=k)*y_t(1:n,1:k) + &
           spread(b,DIM=2,NCOPIES=k)* &
           EOSHIFT(y_t(1:n,1:k),SHIFT=-1,DIM=1) + &
           EOSHIFT(spread(b,DIM=2,NCOPIES=k)*y_t(1:n,1:k),SHIFT=1) &
           -y_t(1:n,1:k)*spread(EVAL_T(1:k),DIM=1,NCOPIES=n)

 ! If the factorization method is Cyclic Reduction and perf_ratio is
 ! larger than one, re-solve using Gaussian Elimination.  If the
 ! method is already Gaussian Elimination, the loop exits
 ! and perf_ratio is checked at the end.
          perf_ratio = sum(abs(res(1:n,1:k))) / &
                          sum(abs(EVAL_T(1:k))) / &
                          epsilon(s_one) / (5*n)
          if (perf_ratio <= s_one) exit factorization_choice
          iopt(nopt+1) = s_options(s_lin_sol_tri_use_Gauss_elim,s_zero)

       end do factorization_choice

       if (perf_ratio <= s_one) then
          write (*,*) 'Example 3 for LIN_SOL_TRI is correct.'
       end if

       end
```

Output

```
Example 3 for LIN_SOL_TRI is correct.
```

Example 4: Tridiagonal Matrix Solving within Diffusion Equations

The normalized partial differential equation

$$u_t \equiv \frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \equiv u_{xx}$$

is solved for values of $0 \le x \le \pi$ and $t > 0$. A boundary value problem consists of choosing the value

$$u\left(0,t\right) = u_0$$

such that the equation

$$u\left(x_1,t_1\right) = u_1$$

is satisfied. Arbitrary values

$$x_1 = \frac{\pi}{2}, u_1 = \frac{1}{2}$$

and

$$t_1 = 1$$

are used for illustration of the solution process. The one-parameter equation

$$u\left(x_1,t_1\right) - u_1 = 0$$

The variables are changed to

$$v\left(x,t\right) = u\left(x,t\right) - u_0$$

that $v(0, t) = 0$. The function $v(x, t)$ satisfies the differential equation. The one-parameter equation solved is therefore

$$v\left(x_1,t_1\right) - \left(u_1 - u_0\right) = 0$$

To solve this equation for u_0, use the standard technique of the *variational equation*,

$$w \equiv \frac{\partial v}{\partial u_0}$$

Thus

$$\frac{\partial w}{\partial t} = \frac{\partial^2 w}{\partial x^2}$$

Since the initial data for

$$v\left(x,0\right) = -u_0$$

the variational equation initial condition is

$$w(x, 0) = -1$$

This model problem illustrates the method of lines and Galerkin principle implemented with the differential-algebraic solver, D2SPG (IMSL 2003, pp. 889–911). We use the integrator in "reverse communication" mode for evaluating the required functions, derivatives, and solving linear algebraic equations. See Example 4 of routine DASPG for a problem that uses reverse communication. Next see Example 4 of routine IVPAG for the development of the piecewise-linear Galerkin discretization method to solve the differential equation. This present example extends parts of both previous examples and illustrates Fortran 90 constructs. It further illustrates how a user can deal with a defect of an integrator that normally functions using only dense linear algebra factorization methods for solving the corrector equations. See the comments in Brenan et al. (1989, esp. p. 137). Also, see operator_ex20, supplied with the product examples.

```
      use lin_sol_tri_int
      use rand_gen_int
      use Numerical_Libraries

      implicit none

! This is Example 4 for LIN_SOL_TRI.

      integer, parameter :: n=1000, ichap=5, iget=1, iput=2, &
         inum=6, irnum=7
      real(kind(1e0)), parameter :: zero=0e0, one = 1e0
      integer    i, ido, in(50), inr(20), iopt(6), ival(7), &
                iwk(35+n)
      real(kind(1e0))      hx, pi_value, t, u_0, u_1, atol, rtol, sval(2), &
                tend, wk(41+11*n), y(n), ypr(n), a_diag(n), &
                a_off(n), r_diag(n), r_off(n), t_y(n), t_ypr(n), &
                t_g(n), t_diag(2*n,1), t_upper(2*n,1), &
                t_lower(2*n,1), t_sol(2*n,1)
      type(s_options) :: iopti(2)=s_options(0,zero)

      character(2) :: pi(1) = 'pi'
! Define initial data.
      t = 0.0e0
      u_0 = 1
      u_1 = 0.5
      tend = one

! Initial values for the variational equation.
      y = -one; ypr= zero
      pi_value = const(pi)
      hx = pi_value/(n+1)

      a_diag = 2*hx/3
      a_off  = hx/6
      r_diag = -2/hx
      r_off  = 1/hx

! Get integer option numbers.
      iopt(1) = inum
      call iumag ('math', ichap, iget, 1, iopt, in)

! Get floating point option numbers.
      iopt(1) = irnum
      call iumag ('math', ichap, iget, 1, iopt, inr)

! Set for reverse communication evaluation of the DAE.
      iopt(1) = in(26)
      ival(1) = 0
```

```
! Set for use of explicit partial derivatives.
      iopt(2) = in(5)
      ival(2) = 1
! Set for reverse communication evaluation of partials.
      iopt(3) = in(29)
      ival(3) = 0
! Set for reverse communication solution of linear equations.
      iopt(4) = in(31)
      ival(4) = 0
! Storage for the partial derivative array are not allocated or
! required in the integrator.
      iopt(5) = in(34)
      ival(5) = 1
! Set the sizes of iwk, wk for internal checking.
      iopt(6) = in(35)
      ival(6) = 35 + n
      ival(7) = 41 + 11*n
! Set integer options:
      call iumag ('math', ichap, iput, 6, iopt, ival)
! Reset tolerances for integrator:
      atol = 1e-3; rtol= 1e-3
      sval(1) = atol; sval(2) = rtol
      iopt(1) = inr(5)
! Set floating point options:
      call sumag ('math', ichap, iput, 1, iopt, sval)
! Integrate ODE/DAE.  Use dummy external names for g(y,y')
! and partials.
      ido = 1
      Integration_Loop: do

          call d2spg (n, t, tend, ido, y, ypr, dgspg, djspg, iwk, wk)
! Find where g(y,y') goes.  (It only goes in one place here, but can
! vary where divided differences are used for partial derivatives.)
          iopt(1) = in(27)
          call iumag ('math', ichap, iget, 1, iopt, ival)
! Direct user response:
        select case(ido)

        case(1,4)
! This should not occur.
          write (*,*) ' Unexpected return with ido = ', ido
          stop

        case(3)
! Reset options to defaults.  (This is good housekeeping but not
! required for this problem.)
          in = -in
          call iumag ('math', ichap, iput, 50, in, ival)
          inr = -inr
          call sumag ('math', ichap, iput, 20, inr, sval)
          exit Integration_Loop
        case(5)
! Evaluate partials of g(y,y').
          t_y = y; t_ypr = ypr

          t_g = r_diag*t_y + r_off*EOSHIFT(t_y,SHIFT=+1) &
                          + EOSHIFT(r_off*t_y,SHIFT=-1) &
            -  (a_diag*t_ypr + a_off*EOSHIFT(t_ypr,SHIFT=+1) &
                             + EOSHIFT(a_off*t_ypr,SHIFT=-1))
! Move data from the assumed size to assumed shape arrays.
          do i=1, n
             wk(ival(1)+i-1) = t_g(i)
          end do
          cycle Integration_Loop

        case(6)
```

```
! Evaluate partials of g(y,y').
! Get value of c_j for partials.
          iopt(1) = inr(9)
          call sumag ('math', ichap, iget, 1, iopt, sval)

! Subtract c_j from diagonals to compute (partials for y')*c_j.
! The linear system is tridiagonal.
          t_diag(1:n,1) = r_diag - sval(1)*a_diag
          t_upper(1:n,1) = r_off - sval(1)*a_off
          t_lower = EOSHIFT(t_upper,SHIFT=+1,DIM=1)

          cycle Integration_Loop

        case(7)
! Compute the factorization.
          iopti(1) = s_options(s_lin_sol_tri_factor_only,zero)
          call lin_sol_tri (t_upper, t_diag, t_lower, &
                  t_sol, iopt=iopti)
          cycle Integration_Loop

        case(8)
! Solve the system.
          iopti(1) = s_options(s_lin_sol_tri_solve_only,zero)
! Move data from the assumed size to assumed shape arrays.
          t_sol(1:n,1)=wk(ival(1):ival(1)+n-1)

          call lin_sol_tri (t_upper, t_diag, t_lower, &
                    t_sol, iopt=iopti)

! Move data from the assumed shape to assumed size arrays.
          wk(ival(1):ival(1)+n-1)=t_sol(1:n,1)

          cycle Integration_Loop

        case(2)
! Correct initial value to reach u_1 at t=tend.
          u_0 = u_0 - (u_0*y(n/2) - (u_1-u_0)) / (y(n/2) + 1)

! Finish up internally in the integrator.
          ido = 3
          cycle Integration_Loop
      end select
      end do Integration_Loop

      write (*,*) 'The equation u_t = u_xx, with u(0,t) = ', u_0
      write (*,*) 'reaches the value ',u_1, ' at time = ', tend, '.'
      write (*,*) 'Example 4 for LIN_SOL_TRI is correct.'

      end
```

Output

```
Example 4 for LIN_SOL_TRI is correct.
```

LIN_SVD

Computes the singular value decomposition (SVD) of a rectangular matrix, *A*. This gives the decomposition

$$A = USV^T$$

where *V* is an $n \times n$ orthogonal matrix, *U* is an $m \times m$ orthogonal matrix, and *S* is a real, rectangular diagonal matrix.

Required Arguments

A — Array of size $m \times n$ containing the matrix. (Input [/Output])
If the packaged option `lin_svd_overwrite_input` is used, this array is not saved on output.

S — Array of size *min*(*m*, *n*) containing the real singular values. These nonnegative values are in non-increasing order. (Output)

U — Array of size $m \times m$ containing the singular vectors, *U*. (Output)

V — Array of size $n \times n$ containing the singular vectors, *V*. (Output)

Optional Arguments

MROWS = `m` (Input)
Uses array `A`(1**:**`m`, 1**:**`n`) for the input matrix.
Default: `m` = size(`A`, 1)

NCOLS = `n` (Input)
Uses array `A`(1**:**`m`, 1**:**`n`) for the input matrix.
Default: `n` = size(`A`, 2)

RANK = `k` (Output)
Number of singular values that exceed the value *Small*. `RANK` will satisfy `k` <= min(`m`, `n`).

iopt = `iopt(:)` (Input)

Derived type array with the same precision as the input matrix. Used for passing optional data to the routine. The options are as follows:

Packaged Options for **LIN_SVD**		
Option Prefix = ?	Option Name	Option Value
`s_, d_, c_, z_`	`lin_svd_set_small`	1
`s_, d_, c_, z_`	`lin_svd_overwrite_input`	2
`s_, d_, c_, z_`	`lin_svd_scan_for_NaN`	3
`s_, d_, c_, z_`	`lin_svd_use_qr`	4
`s_, d_, c_, z_`	`lin_svd_skip_orth`	5
`s_, d_, c_, z_`	`lin_svd_use_gauss_elim`	6
`s_, d_, c_, z_`	`lin_svd_set_perf_ratio`	7

iopt(IO) = `?_options(?_lin_svd_set_small`, *Small*)

If a singular value is smaller than *Small*, it is defined as zero for the purpose of computing the rank of *A*.

Default: the smallest number that can be reciprocated safely

iopt(IO) = `?_options(?_lin_svd_overwrite_input`, `?_dummy`)

Does not save the input array `A(:, :)`.

iopt(IO) = `?_options(?_lin_svd_scan_for_NaN`, `?_dummy`)

Examines each input array entry to find the first value such that

`isNaN(a(i,j)) == .true.`

See the `isNaN()` function, *Chapter 10*.

Default: The array is not scanned for NaNs.

iopt(IO)= `?_options(?_lin_svd_use_qr`, `?_dummy`)

Uses a rational *QR* algorithm to compute eigenvalues. Accumulate the singular vectors using this algorithm.

Default: singular vectors computed using inverse iteration

iopt(IO) = `?_options(?_lin_svd_skip_Orth`, `?_dummy`)

If the eigenvalues are computed using inverse iteration, skips the final orthogonalization of the vectors. This method results in a more efficient computation. However, the singular vectors, while a complete set, may not be orthogonal.

Default: singular vectors are orthogonalized if obtained using inverse iteration

iopt(IO) = `?_options(?_lin_svd_use_gauss_elim, ?_dummy)`

If the eigenvalues are computed using inverse iteration, uses standard elimination with partial pivoting to solve the inverse iteration problems.

Default: singular vectors computed using cyclic reduction

iopt(IO) = `?_options(?_lin_svd_set_perf_ratio,` *perf_ratio*`)`

Uses residuals for approximate normalized singular vectors if they have a performance index no larger than *perf_ratio*. Otherwise an alternate approach is taken and the singular vectors are computed again: Standard elimination is used instead of cyclic reduction, or the standard *QR* algorithm is used as a backup procedure to inverse iteration. Larger values of *perf_ratio* are less likely to cause these exceptions.

Default: *perf_ratio* = 4

FORTRAN 90 Interface

Generic: `CALL LIN_SVD (A, S, U, V [, …])`

Specific: The specific interface names are `S_LIN_SVD`, `D_LIN_SVD`, `C_LIN_SVD`, and `Z_LIN_SVD`.

Description

Routine `lin_svd` is an implementation of the *QR* algorithm for computing the SVD of rectangular matrices. An orthogonal reduction of the input matrix to upper bidiagonal form is performed. Then, the SVD of a real bidiagonal matrix is calculated. The orthogonal decomposition $AV = US$ results from products of intermediate matrix factors. See Golub and Van Loan (1989, Chapter 8) for details.

Fatal, Terminal, and Warning Error Messages

See the *messages.gls* file for error messages for `LIN_SVD`. These error messages are numbered 1001–1010; 1021–1030; 1041–1050; 1061–1070.

Examples

Example 1: Computing the SVD

The SVD of a square, random matrix A is computed. The residuals $R = AV - US$ are small with respect to working precision. Also, see `operator_ex21`, supplied with the product examples.

```
      use lin_svd_int
```

```
      use rand_gen_int

      implicit none

! This is Example 1 for LIN_SVD.

      integer, parameter :: n=32
      real(kind(1d0)), parameter :: one=1d0
      real(kind(1d0)) err
      real(kind(1d0)), dimension(n,n) :: A, U, V, S(n), y(n*n)

! Generate a random n by n matrix.
      call rand_gen(y)
      A = reshape(y,(/n,n/))

! Compute the singular value decomposition.
      call lin_svd(A, S, U, V)

! Check for small residuals of the expression A*V - U*S.
      err = sum(abs(matmul(A,V) - U*spread(S,dim=1,ncopies=n))) &
                   / sum(abs(S))
      if (err  <= sqrt(epsilon(one))) then
         write (*,*) 'Example 1 for LIN_SVD is correct.'
      end if
      end
```

Output

```
Example 1 for LIN_SVD is correct.
```

Example 2: Linear Least Squares with a Quadratic Constraint

An $m \times n$ matrix equation $Ax \cong b$, $m > n$, is approximated in a least-squares sense. The matrix b is size $m \times k$. Each of the k solution vectors of the matrix x is constrained to have Euclidean length of value $\alpha_j > 0$. The value of α_i is chosen so that the constrained solution is 0.25 the length of the nonregularized or standard least-squares equation. See Golub and Van Loan (1989, Chapter 12) for more details. In the Example 2 code, Newton's method is used to solve for each regularizing parameter of the k systems. The solution is then computed and its length is checked. Also, see operator_ex22, supplied with the product examples.

```
      use lin_svd_int
      use rand_gen_int

      implicit none

! This is Example 2 for LIN_SVD.

      integer, parameter :: m=64, n=32, k=4
      real(kind(1d0)), parameter :: one=1d0, zero=0d0
      real(kind(1d0)) a(m,n), s(n), u(m,m), v(n,n), y(m*max(n,k)), &
             b(m,k), x(n,k), g(m,k), alpha(k), lamda(k), &
             delta_lamda(k), t_g(n,k), s_sq(n), phi(n,k), &
             phi_dot(n,k), rand(k), err

! Generate a random matrix for both A and B.
      call rand_gen(y)
      a = reshape(y,(/m,n/))

      call rand_gen(y)
      b = reshape(y,(/m,k/))
```

```
! Compute the singular value decomposition.
      call lin_svd(a, s, u, v)

! Choose alpha so that the lengths of the regularized solutions
! are 0.25 times lengths of the non-regularized solutions.

      g = matmul(transpose(u),b)
      x = matmul(v,spread(one/s,dim=2,ncopies=k)*g(1:n,1:k))
      alpha = 0.25*sqrt(sum(x**2,dim=1))

      t_g = g(1:n,1:k)*spread(s,dim=2,ncopies=k)
      s_sq = s**2; lamda = zero

      solve_for_lamda:  do
         x=one/(spread(s_sq,dim=2,ncopies=k)+ &
                    spread(lamda,dim=1,ncopies=n))
         phi = (t_g*x)**2; phi_dot = -2*phi*x
         delta_lamda = (sum(phi,dim=1)-alpha**2)/sum(phi_dot,dim=1)

! Make Newton method correction to solve the secular equations for
! lamda.
         lamda = lamda - delta_lamda

         if (sum(abs(delta_lamda)) <= &
             sqrt(epsilon(one))*sum(lamda)) &
                       exit solve_for_lamda

! This is intended to fix up negative solution approximations.
         call rand_gen(rand)
         where (lamda < 0) lamda = s(1) * rand

      end do solve_for_lamda

! Compute solutions and check lengths.
      x = matmul(v,t_g/(spread(s_sq,dim=2,ncopies=k)+ &
                       spread(lamda,dim=1,ncopies=n)))

      err = sum(abs(sum(x**2,dim=1) - alpha**2))/sum(abs(alpha**2))
      if (err <= sqrt(epsilon(one))) then
         write (*,*) 'Example 2 for LIN_SVD is correct.'
      end if

      end
```

Output

```
Example 2 for LIN_SVD is correct.
```

Example 3: Generalized Singular Value Decomposition

The $n \times n$ matrices A and B are expanded in a Generalized Singular Value Decomposition (GSVD). Two $n \times n$ orthogonal matrices, U and V, and a nonsingular matrix X are computed such that

$$AX = U\, diag(c_1, \ldots., c_n)$$

and

$$BX = V\, diag(s_1, \ldots, s_n)$$

The values s_i and c_i are normalized so that

$$s_i^2 + c_i^2 = 1$$

The c_i are nonincreasing, and the s_i are nondecreasing. See Golub and Van Loan (1989, Chapter 8) for more details. Our method is based on computing three SVDs as opposed to the *QR* decomposition and two SVDs outlined in Golub and Van Loan. As a bonus, an SVD of the matrix *X* is obtained, and you can use this information to answer further questions about its conditioning. This form of the decomposition assumes that the matrix

$$D = \begin{bmatrix} A \\ B \end{bmatrix}$$

has all its singular values strictly positive. For alternate problems, where some singular values of *D* are zero, the GSVD becomes

$$U^T A = diag(c_1, \ldots, c_n)W$$

and

$$V^T B = diag(s_1, \ldots, s_n)W$$

The matrix *W* has the same singular values as the matrix *D*. Also, see `operator_ex23`, supplied with the product examples.

```
      use lin_svd_int
      use rand_gen_int

      implicit none

! This is Example 3 for LIN_SVD.

      integer, parameter :: n=32
      integer i
      real(kind(1d0)), parameter :: one=1.0d0
      real(kind(1d0)) a(n,n), b(n,n), d(2*n,n), x(n,n), u_d(2*n,2*n), &
             v_d(n,n), v_c(n,n), u_c(n,n), v_s(n,n), u_s(n,n), &
             y(n*n), s_d(n), c(n), s(n), sc_c(n), sc_s(n), &
             err1, err2

! Generate random square matrices for both A and B.

      call rand_gen(y)
      a = reshape(y,(/n,n/))

      call rand_gen(y)
      b = reshape(y,(/n,n/))

! Construct D; A is on the top; B is on the bottom.

      d(1:n,1:n) = a
      d(n+1:2*n,1:n) = b

! Compute the singular value decompositions used for the GSVD.

      call lin_svd(d, s_d, u_d, v_d)
      call lin_svd(u_d(1:n,1:n), c, u_c, v_c)
      call lin_svd(u_d(n+1:,1:n), s, u_s, v_s)
```

```
! Rearrange c(:) so it is non-increasing.  Move singular
! vectors accordingly.  (The use of temporary objects sc_c and
! x is required.)

      sc_c = c(n:1:-1); c = sc_c
      x = u_c(1:n,n:1:-1); u_c = x
      x = v_c(1:n,n:1:-1); v_c = x

! The columns of v_c and v_s have the same span.  They are
! equivalent by taking the signs of the largest magnitude values
! positive.

      do i=1, n
         sc_c(i) = sign(one,v_c(sum(maxloc(abs(v_c(1:n,i)))),i))
         sc_s(i) = sign(one,v_s(sum(maxloc(abs(v_s(1:n,i)))),i))
      end do

      v_c = v_c*spread(sc_c,dim=1,ncopies=n)
      u_c = u_c*spread(sc_c,dim=1,ncopies=n)

      v_s = v_s*spread(sc_s,dim=1,ncopies=n)
      u_s = u_s*spread(sc_s,dim=1,ncopies=n)

! In this form of the GSVD, the matrix X can be unstable if D
! is ill-conditioned.
      x = matmul(v_d*spread(one/s_d,dim=1,ncopies=n),v_c)

! Check residuals for GSVD, A*X = u_c*diag(c_1, ..., c_n), and
! B*X = u_s*diag(s_1, ..., s_n).
      err1 = sum(abs(matmul(a,x) - u_c*spread(c,dim=1,ncopies=n))) &
              / sum(s_d)
      err2 = sum(abs(matmul(b,x) - u_s*spread(s,dim=1,ncopies=n))) &
              / sum(s_d)
      if (err1 <= sqrt(epsilon(one)) .and. &
          err2 <= sqrt(epsilon(one))) then

         write (*,*) 'Example 3 for LIN_SVD is correct.'
      end if

      end
```

Example 4: Ridge Regression as Cross-Validation with Weighting

This example illustrates a particular choice for the *ridge regression* problem: The least-squares problem $Ax \cong b$ is modified by the addition of a regularizing term to become

$$\min_x\left(\|Ax-b\|_2^2 + \lambda^2\|x\|_2^2 \right)$$

The solution to this problem, with row k deleted, is denoted by $x_k(\lambda)$. Using nonnegative weights ($w_1, \ldots, w_m$), the cross-validation squared error $C(\lambda)$ is given by:

$$mC(\lambda) = \sum_{k=1}^{m} w_k\left(a_k^T x_k(\lambda) - b_k \right)^2$$

With the SVD $A = USV^T$ and product $g = U^T b$, this quantity can be written as

$$mC(\lambda) = \sum_{k=1}^{m} w_k \left(\frac{\left(b_k - \sum_{j=1}^{n} u_{kj} g_j \frac{s_j^2}{\left(s_j^2 + \lambda^2\right)} \right)}{\left(1 - \sum_{j=1}^{n} u_{kj}^2 \frac{s_j^2}{\left(s_j^2 + \lambda^2\right)} \right)} \right)^2$$

This expression is minimized. See Golub and Van Loan (1989, Chapter 12) for more details. In the Example 4 code, *mC*(λ), at *p* = 10 grid points are evaluated using a log-scale with respect to λ, $0.1 s_1 \le \lambda \le 10 s_1$. Array operations and intrinsics are used to evaluate the function and then to choose an approximate minimum. Following the computation of the optimum λ, the regularized solutions are computed. Also, see `operator_ex24`, supplied with the product examples.

```
      use lin_svd_int
      use rand_gen_int

      implicit none

! This is Example 4 for LIN_SVD.

      integer i
      integer, parameter :: m=32, n=16, p=10, k=4
      real(kind(1d0)), parameter :: one=1d0
      real(kind(1d0)) log_lamda, log_lamda_t, delta_log_lamda
      real(kind(1d0)) a(m,n), b(m,k), w(m,k), g(m,k), t(n), s(n), &
              s_sq(n), u(m,m), v(n,n), y(m*max(n,k)),  &
              c_lamda(p,k), lamda(k), x(n,k), res(n,k)

! Generate random rectangular matrices for A and right-hand
! sides, b.
      call rand_gen(y)
      a = reshape(y,(/m,n/))

      call rand_gen(y)
      b = reshape(y,(/m,k/))

! Generate random weights for each of the right-hand sides.
      call rand_gen(y)
      w = reshape(y,(/m,k/))

! Compute the singular value decomposition.
      call lin_svd(a, s, u, v)

      g = matmul(transpose(u),b)
      s_sq = s**2

      log_lamda = log(10.*s(1)); log_lamda_t=log_lamda
      delta_log_lamda = (log_lamda - log(0.1*s(n))) / (p-1)

! Choose lamda to minimize the "cross-validation" weighted
! square error.  First evaluate the error at a grid of points,
! uniform in log_scale.

      cross_validation_error:  do i=1, p
         t = s_sq/(s_sq+exp(log_lamda))
         c_lamda(i,:) = sum(w*((b-matmul(u(1:m,1:n),g(1:n,1:k)* &
                            spread(t,DIM=2,NCOPIES=k)))/ &
                     (one-matmul(u(1:m,1:n)**2, &
```

```
                           spread(t,DIM=2,NCOPIES=k))))**2,DIM=1)
           log_lamda = log_lamda - delta_log_lamda
        end do cross_validation_error

  ! Compute the grid value and lamda corresponding to the minimum.
        do i=1, k
           lamda(i) = exp(log_lamda_t -  delta_log_lamda* &
                                (sum(minloc(c_lamda(1:p,i)))-1))
        end do

  ! Compute the solution using the optimum "cross-validation"
  ! parameter.
        x = matmul(v,g(1:n,1:k)*spread(s,DIM=2,NCOPIES=k)/ &
                       (spread(s_sq,DIM=2,NCOPIES=k)+ &
                        spread(lamda,DIM=1,NCOPIES=n)))
  ! Check the residuals, using normal equations.
        res = matmul(transpose(a),b-matmul(a,x)) - &
                      spread(lamda,DIM=1,NCOPIES=n)*x
        if (sum(abs(res))/sum(s_sq) <= &
                sqrt(epsilon(one))) then
           write (*,*) 'Example 4 for LIN_SVD is correct.'
        end if

        end
```

Output

```
Example 4 for LIN_SVD is correct.
```

Parallel Constrained Least-Squares Solvers

Solving Constrained Least-Squares Systems

The routine PARALLEL_NONNEGATIVE_LSQ is used to solve dense least-squares systems. These are represented by $Ax \cong b$ where *A* is an $m \times n$ coefficient data matrix, *b* is a given right-hand side *m*-vector, and *x* is the solution *n*-vector being computed. Further, there is a constraint requirement, $x \geq 0$. The routine PARALLEL_BOUNDED_LSQ is used when the problem has lower and upper bounds for the solution, $\alpha \leq x \leq \beta$. By making the bounds large, individual constraints can be eliminated. There are no restrictions on the relative sizes of *m* and *n*. When *n* is large, these codes can substantially reduce computer time and storage requirements, compared with using a routine for solving a constrained system and a single processor.

The user provides the matrix partitioned by blocks of columns:

$$A = \left[A_1 | A_2 | \ldots | A_k \right]$$

An individual block of the partitioned matrix, say A_p, is located entirely on the processor with rank $MP\_RANK = p - 1$, where MP_RANK is packaged in the module MPI_SETUP_INT. This module, and the function MP_SETUP() ,define the Fortran Library MPI communicator, MP_LIBRARY_WORLD. See *Chapter 10*, section *Dense Matrix Parallelism Using MPI*.

PARALLEL_NONNEGATIVE_LSQ

MPI REQUIRED

more...

For a detailed description of MPI Requirements see *Dense Matrix Parallelism Using MPI* in *Chapter 10* of this manual.

Solves a linear, non-negative constrained least-squares system.

Usage Notes

```
CALL PARALLEL_NONNEGATIVE_LSQ(A, B, X, RNORM, W, INDEX, IPART,
   IOPT = IOPT)
```

Required Arguments

A(1:M,:)— (Input/Output) Columns of the matrix with limits given by entries in the array `IPART(1:2,1:max(1,MP_NPROCS))`. On output A_k is replaced by the product QA_k, where Q is an orthogonal matrix. The value `SIZE(A,1)` defines the value of `M`. Each processor starts and exits with its piece of the partitioned matrix.

B(1:M) — (Input/Output) Assumed-size array of length `M` containing the right-hand side vector, b. On output b is replaced by the product Qb, where Q is the orthogonal matrix applied to A. All processors in the communicator start and exit with the same vector.

X(1:N) — (Output) Assumed-size array of length `N` containing the solution, $x \geq 0$. The value `SIZE(X)` defines the value of `N`. All processors exit with the same vector.

RNORM — (Output) Scalar that contains the Euclidean or least-squares length of the residual vector, $\|Ax - b\|$. All processors exit with the same value.

W(1:N) — (Output) Assumed-size array of length `N` containing the dual vector, $w = A^T\left(b - Ax\right) \leq 0$. All processors exit with the same vector.

INDEX(1:N) — (Output) Assumed-size array of length N containing the NSETP indices of columns in the positive solution, and the remainder that are at their constraint. The number of positive components in the solution *x* is given by the Fortran intrinsic function value, NSETP=COUNT(X > 0). All processors exit with the same array.

IPART(1:2,1:max(1,MP_NPROCS)) — (Input) Assumed-size array containing the partitioning describing the matrix *A*. The value MP_NPROCS is the number of processors in the communicator, except when MPI has been finalized with a call to the routine MP_SETUP('Final'). This causes MP_NPROCS to be assigned 0. Normally users will give the partitioning to processor of rank = MP_RANK by setting IPART(1,MP_RANK+1) = first column index, and IPART(2,MP_RANK+1) = last column index. The number of columns per node is typically based on their relative computing power. To avoid a node with rank MP_RANK doing any work except communication, set IPART(1,MP_RANK+1) = 0 and IPART(2,MP_RANK+1)= -1. In this exceptional case there is no reference to the array ***A(:,:)*** at that node.

Optional Argument

IOPT(:)— (Input) Assumed-size array of derived type S_OPTIONS or D_OPTIONS. This argument is used to change internal parameters of the algorithm. Normally users will not be concerned about this argument, so they would not include it in the argument list for the routine.

Packaged Options for PARALLEL_NONNEGATIVE_LSQ	
Option Name	Option Value
PNLSQ_SET_TOLERANCE	1
PNLSQ_SET_MAX_ITERATIONS	2
PNLSQ_SET_MIN_RESIDUAL	3

IOPT(IO)=?_OPTIONS(PNLSQ_SET_TOLERANCE, TOLERANCE) Replaces the default rank tolerance for using a column, from EPSILON(TOLERANCE) to TOLERANCE. Increasing the value of TOLERANCE will cause fewer columns to be moved from their constraints, and may cause the minimum residual RNORM to increase.

IOPT(IO)=?_OPTIONS(PNLSQ_SET_MIN_RESIDUAL, RESID) Replaces the default target for the minimum residual vector length from 0 to RESID. Increasing the value of RESID can result in fewer iterations and thus increased efficiency. The descent in the optimization will stop at the first point where the minimum residual RNORM is smaller than RESID. Using this option may result in the dual vector not satisfying its optimality conditions, as noted above.

IOPT(IO)= PNLSQ_SET_MAX_ITERATIONS

IOPT(IO+1)= NEW_MAX_ITERATIONS Replaces the default maximum number of iterations from 3*N to NEW_MAX_ITERATIONS. Note that this option requires two entries in the derived type array.

FORTRAN 90 Interface

Generic: CALL PARALLEL_NONNEGATIVE_LSQ (A, B, X, RNORM, W, INDEX, IPART [, …])

Specific: The specific interface names are S_PARALLEL_NONNEGATIVE_LSQ and D_PARALLEL_NONNEGATIVE_LSQ.

Description

Subroutine PARALLEL_NONNEGATIVE_LSQ solves the linear least-squares system $Ax \cong b, x \geq 0$, using the algorithm *NNLS* found in Lawson and Hanson, (1995), pages 160-161. The code now updates the dual vector w of Step 2, page 161. The remaining new steps involve exchange of required data, using MPI.

Examples

Example 1: Distributed Linear Inequality Constraint Solver

The program PNLSQ_EX1 illustrates the computation of the minimum Euclidean length solution of an $m' \times n'$ system of linear inequality constraints , $Gy \geq h$. The solution algorithm is based on Algorithm *LDP*, page 165-166, *loc. cit*. The rows of $E = \left[\, G{:}h \,\right]$ are partitioned and assigned random values. When the minimum Euclidean length solution to the inequalities has been calculated, the residuals $r = Gy - h \geq 0$ are computed, with the dual variables to the *NNLS* problem indicating the entries of *r* that are precisely zero.

The fact that matrix products involving both *E* and E^T are needed to compute the constrained solution *y* and the residuals *r*, implies that message passing is required. This occurs after the NNLS solution is computed.

```
      PROGRAM PNLSQ_EX1
! Use Parallel_nonnegative_LSQ to solve an inequality
! constraint problem, Gy >= h. This algorithm uses
! Algorithm LDP of Solving Least Squares Problems,
! page 165. The constraints are allocated to the
! processors, by rows, in columns of the array A(:,:).
        USE PNLSQ_INT
        USE MPI_SETUP_INT
        USE RAND_INT
        USE SHOW_INT

        IMPLICIT NONE
        INCLUDE "mpif.h"

        INTEGER, PARAMETER :: MP=500, NP=400, M=NP+1, N=MP
```

```
        REAL(KIND(1D0)), PARAMETER :: ZERO=0D0, ONE=1D0
        REAL(KIND(1D0)), ALLOCATABLE :: &
          A(:,:), B(:), X(:), Y(:), W(:), ASAVE(:,:)
        REAL(KIND(1D0)) RNORM
        INTEGER, ALLOCATABLE :: INDEX(:), IPART(:,:)

        INTEGER K, L, DN, J, JSHIFT, IERROR
        LOGICAL :: PRINT=.false.

! Setup for MPI:
        MP_NPROCS=MP_SETUP()

        DN=N/max(1,max(1,MP_NPROCS))-1
        ALLOCATE(IPART(2,max(1,MP_NPROCS)))

! Spread constraint rows evenly to the processors.
        IPART(1,1)=1
        DO L=2,MP_NPROCS
           IPART(2,L-1)=IPART(1,L-1)+DN
           IPART(1,L)=IPART(2,L-1)+1
        END DO
        IPART(2,MP_NPROCS)=N

! Define the constraint data using random values.
        K=max(0,IPART(2,MP_RANK+1)-IPART(1,MP_RANK+1)+1)
        ALLOCATE(A(M,K), ASAVE(M,K), X(N), W(N), &
          B(M), Y(M), INDEX(N))

! The use of ASAVE can be removed by regenerating
! the data for A(:,:) after the return from
! Parallel_nonnegative_LSQ.
        A=rand(A); ASAVE=A
        IF(MP_RANK == 0 .and. PRINT) &
          CALL SHOW(IPART, &
            "Partition of the constraints to be solved")

! Set the right-hand side to be one in the last component, zero elsewhere.
        B=ZERO;B(M)=ONE

! Solve the dual problem.
        CALL Parallel_nonnegative_LSQ &
          (A, B, X, RNORM, W, INDEX, IPART)

! Each processor multiplies its block times the part of
! the dual corresponding to that part of the partition.
        Y=ZERO
        DO J=IPART(1,MP_RANK+1),IPART(2,MP_RANK+1)
           JSHIFT=J-IPART(1,MP_RANK+1)+1
           Y=Y+ASAVE(:,JSHIFT)*X(J)
        END DO

! Accumulate the pieces from all the processors. Put sum into B(:)
! on rank 0 processor.
        B=Y
        IF(MP_NPROCS > 1) &
          CALL MPI_REDUCE(Y, B, M, MPI_DOUBLE_PRECISION,&
           MPI_SUM, 0, MP_LIBRARY_WORLD, IERROR)
        IF(MP_RANK == 0) THEN

! Compute constrained solution at the root.
! The constraints will have no solution if B(M) = ONE.
! All of these example problems have solutions.
           B(M)=B(M)-ONE;B=-B/B(M)
        END IF

! Send the inequality constraint solution to all nodes.
```

```
        IF(MP_NPROCS > 1) &
          CALL MPI_BCAST(B, M, MPI_DOUBLE_PRECISION, &
           0, MP_LIBRARY_WORLD, IERROR)

! For large problems this printing needs to be removed.
        IF(MP_RANK == 0 .and. PRINT) &
         CALL SHOW(B(1:NP), &
            "Minimal length solution of the constraints")

! Compute residuals of the individual constraints.
! If only the solution is desired, the program ends here.
          X=ZERO
          DO J=IPART(1,MP_RANK+1),IPART(2,MP_RANK+1)
             JSHIFT=J-IPART(1,MP_RANK+1)+1
             X(J)=dot_product(B,ASAVE(:,JSHIFT))
          END DO

! This cleans up residuals that are about rounding
! error unit (times) the size of the constraint
! equation and right-hand side.  They are replaced
! by exact zero.
          WHERE(W == ZERO) X=ZERO; W=X

! Each group of residuals is disjoint, per processor.
! We add all the pieces together for the total set of
! constraints.
          IF(MP_NPROCS > 1) &
            CALL MPI_REDUCE(X, W, N, MPI_DOUBLE_PRECISION,&
              MPI_SUM, 0, MP_LIBRARY_WORLD, IERROR)
          IF(MP_RANK == 0 .and. PRINT) &
            CALL SHOW(W, "Residuals for the constraints")

! See to any errors and shut down MPI.
          MP_NPROCS=MP_SETUP('Final')
          IF(MP_RANK == 0) THEN
            IF(COUNT(W < ZERO) == 0) WRITE(*,*)&
            " Example 1 for PARALLEL_NONNEGATIVE_LSQ is correct."
       END IF
       END
```

Output

```
Example 1 for PARALLEL_NONNEGATIVE_LSQ is correct.
```

Example 2: Distributed Non-negative Least-Squares

The program PNLSQ_EX2 illustrates the computation of the solution to a system of linear least-squares equations with simple constraints: $a_i^T x \cong b_i, i = 1,...m,$ subject to $x \geq 0$. In this example we write the row vectors $\left[a_i^T : b_i \right]$ on a file. This illustrates reading the data by rows and arranging the data by columns, as required by PARALLEL_NONNEGATIVE_LSQ. After reading the data, the right-hand side vector is broadcast to the group before computing a solution, x. The block-size is chosen so that each participating processor receives the same number of columns, except any remaining columns sent to the processor with largest rank. This processor contains the right-hand side before the broadcast.

This example illustrates connecting a *BLACS* 'context' handle and the Fortran Library MPI communicator, MP_LIBRARY_WORLD, described in *Chapter 10*.

```
   PROGRAM PNLSQ_EX2
! Use Parallel_Nonnegative_LSQ to solve a least-squares
! problem, A x = b, with x >= 0. This algorithm uses a
! distributed version of NNLS,  found in the book
! Solving Least Squares Problems, page 165. The data is
! read from a file, by rows, and sent to the processors,
! as array columns.

   USE PNLSQ_INT
   USE SCALAPACK_IO_INT
   USE BLACS_INT

   USE MPI_SETUP_INT
   USE RAND_INT
   USE ERROR_OPTION_PACKET

   IMPLICIT NONE
   INCLUDE "mpif.h"

   INTEGER, PARAMETER :: M=128, N=32, NP=N+1, NIN=10

   real(kind(1d0)), ALLOCATABLE, DIMENSION(:) :: &
     d_A(:,:), A(:,:), B, C, W, X, Y
   real(kind(1d0)) RNORM, ERROR
   INTEGER, ALLOCATABLE :: INDEX(:), IPART(:,:)

   INTEGER I, J, K, L, DN, JSHIFT, IERROR, &
     CONTXT, NPROW, MYROW, MYCOL, DESC_A(9)
   TYPE(d_OPTIONS) IOPT(1)

! Routines with the "BLACS_" prefix are from the
! BLACS library.
   CALL BLACS_PINFO(MP_RANK, MP_NPROCS)

! Make initialization for BLACS.
   CALL BLACS_GET(0,0, CONTXT)

! Define processor grid to be 1 by MP_NPROCS.
   NPROW=1
   CALL BLACS_GRIDINIT(CONTXT, 'N/A', NPROW, MP_NPROCS)

! Get this processor's role in the process grid.
   CALL BLACS_GRIDINFO(CONTXT, NPROW, MP_NPROCS, &
     MYROW, MYCOL)

! Connect BLACS context with communicator MP_LIBRARY_WORLD.
   CALL BLACS_GET(CONTXT, 10, MP_LIBRARY_WORLD)

! Setup for MPI:
   MP_NPROCS=MP_SETUP()

   DN=max(1,NP/MP_NPROCS)
   ALLOCATE(IPART(2,MP_NPROCS))

! Spread columns evenly to the processors.  Any odd
! number of columns are in the processor with highest
! rank.
   IPART(1,:)=1; IPART(2,:)=0
   DO L=2,MP_NPROCS
     IPART(2,L-1)=IPART(1,L-1)+DN
     IPART(1,L)=IPART(2,L-1)+1
   END DO
   IPART(2,MP_NPROCS)=NP
   IPART(2,:)=min(NP,IPART(2,:))
```

```
! Note which processor (L-1) receives the right-hand side.
   DO L=1,MP_NPROCS
     IF(IPART(1,L) <= NP .and. NP <= IPART(2,L)) EXIT
   END DO

   K=max(0,IPART(2,MP_RANK+1)-IPART(1,MP_RANK+1)+1)
   ALLOCATE(d_A(M,K), W(N), X(N), Y(N),&
     B(M), C(M), INDEX(N))

   IF(MP_RANK == 0 ) THEN
     ALLOCATE(A(M,N))
! Define the matrix data using random values.
     A=rand(A); B=rand(B)

! Write the rows of data to an external file.
     OPEN(UNIT=NIN, FILE='Atest.dat', STATUS='UNKNOWN')
     DO I=1,M
       WRITE(NIN,*) (A(I,J),J=1,N), B(I)
     END DO
     CLOSE(NIN)
   ELSE

! No resources are used where this array is not saved.
     ALLOCATE(A(M,0))
   END IF

! Define the matrix descriptor.  This includes the
! right-hand side as an additional column.  The row
! block size, on each processor, is arbitrary, but is
! chosen here to match the column block size.
   DESC_A=(/1, CONTXT, M, NP, DN+1, DN+1, 0, 0, M/)

! Read the data by rows.
   IOPT(1)=ScaLAPACK_READ_BY_ROWS
   CALL ScaLAPACK_READ ("Atest.dat", DESC_A, &
    d_A, IOPT=IOPT)

! Broadcast the right-hand side to all processors.
   JSHIFT=NP-IPART(1,L)+1
   IF(K > 0) B=d_A(:,JSHIFT)
   IF(MP_NPROCS > 1) &
     CALL MPI_BCAST(B, M, MPI_DOUBLE_PRECISION , L-1, &
       MP_LIBRARY_WORLD, IERROR)

! Adjust the partition of columns to ignore the
! last column, which is the right-hand side. It is
! now moved to B(:).
   IPART(2,:)=min(N,IPART(2,:))

! Solve the constrained distributed problem.
       C=B
       CALL Parallel_Nonnegative_LSQ &
       (d_A, B, X, RNORM, W, INDEX, IPART)

! Solve the problem on one processor, with data saved
! for a cross-check.
       IPART(2,:)=0; IPART(2,1)=N; MP_NPROCS=1

! Since all processors execute this code, all arrays
! must be allocated in the main program.
       CALL Parallel_Nonnegative_LSQ &
       (A, C, Y, RNORM, W, INDEX, IPART)

! See to any errors.
       CALL e1pop("Mp_Setup")
```

```
! Check the differences in the two solutions.  Unique solutions
! may differ in the last bits, due to rounding.
   IF(MP_RANK == 0) THEN
     ERROR=SUM(ABS(X-Y))/SUM(Y)
     IF(ERROR <= sqrt(EPSILON(ERROR))) write(*,*) &
       ' Example 2 for PARALLEL_NONNEGATIVE_LSQ is correct.'
     OPEN(UNIT=NIN, FILE='Atest.dat', STATUS='OLD')
     CLOSE(NIN, STATUS='Delete')
   END IF

! Exit from using this process grid.
  CALL BLACS_GRIDEXIT( CONTXT )
  CALL BLACS_EXIT(0)
  END
```

Output

```
Example 2 for PARALLEL_NONNEGATIVE_LSQ is correct.'
```

PARALLEL_BOUNDED_LSQ

more...

NOTE: For a detailed description of MPI Requirements see *Dense Matrix Parallelism Using MPI* in *Chapter 10* of this manual.

Solves a linear least-squares system with bounds on the unknowns.

Usage Notes

```
CALL PARALLEL_BOUNDED_LSQ (A, B, BND, X, RNORM, W, INDEX, IPART, NSETP,
   NSETZ, IOPT=IOPT)
```

Required Arguments

A(1:M,:)— (Input/Output) Columns of the matrix with limits given by entries in the array `IPART(1:2,1:max(1,MP_NPROCS))`. On output A_k is replaced by the product QA_k, where Q is an orthogonal matrix. The value `SIZE(A,1)` defines the value of `M`. Each processor starts and exits with its piece of the partitioned matrix.

B(1:M) — (Input/Output) Assumed-size array of length `M` containing the right-hand side vector, b. On output b is replaced by the product $Q\left(b - Ag\right)$, where Q is the orthogonal matrix applied to A and g is a set of active bounds for the solution. All processors in the communicator start and exit with the same vector.

BND(1:2,1:N) — (Input) Assumed-size array containing the bounds for x. The lower bound α_j is in `BND(1,J)`, and the upper bound β_j is in `BND(2,J)`.

X(1:N) — (Output) Assumed-size array of length `N` containing the solution, $\alpha \le x \le \beta$. The value `SIZE(X)` defines the value of `N`. All processors exit with the same vector.

RNORM — (Output) Scalar that contains the Euclidean or least-squares length of the residual vector, $\|Ax - b\|$. All processors exit with the same value.

W(1:N) — (Output) Assumed-size array of length `N` containing the dual vector, $w = A^T\left(b - Ax\right)$. At a solution exactly one of the following is true for each $j, 1 \le j \le n$,

- $\alpha_j = x_j = \beta_j$, and w_j arbitrary
- $\alpha_j = x_j$, and $w_j \leq 0$
- $x_j = \beta_j$, and $w_j \geq 0$
- $\alpha_j < x_j < \beta_j$, and $w_j = 0$

All processors exit with the same vector.

INDEX(1:N) — (Output) Assumed-size array of length `N` containing the `NSETP` indices of columns in the solution interior to bounds, and the remainder that are at a constraint. All processors exit with the same array.

IPART(1:2,1:max(1,MP_NPROCS)) — (Input) Assumed-size array containing the partitioning describing the matrix *A*. The value `MP_NPROCS` is the number of processors in the communicator, except when MPI has been finalized with a call to the routine `MP_SETUP('Final')`. This causes `MP_NPROCS` to be assigned 0. Normally users will give the partitioning to processor of rank = `MP_RANK` by setting `IPART(1,MP_RANK+1)` = first column index, and `IPART(2,MP_RANK+1)` = last column index. The number of columns per node is typically based on their relative computing power. To avoid a node with rank `MP_RANK` doing any work except communication, set `IPART(1,MP_RANK+1) = 0` and `IPART(2,MP_RANK+1)= -1`. In this exceptional case there is no reference to the array ***A(:,:)*** at that node.

NSETP— (Output) An `INTEGER` indicating the number of solution components not at constraints. The column indices are output in the array `INDEX(:)`.

NSETZ— (Output) An `INTEGER` indicating the solution components held at fixed values. The column indices are output in the array `INDEX(:)`.

Optional Argument

IOPT(:)— (Input) Assumed-size array of derived type `S_OPTIONS` or `D_OPTIONS`. This argument is used to change internal parameters of the algorithm. Normally users will not be concerned about this argument, so they would not include it in the argument list for the routine.

Packaged Options for `PARALLEL_BOUNDED_LSQ`	
Option Name	Option Value
`PBLSQ_SET_TOLERANCE`	1
`PBLSQ_SET_MAX_ITERATIONS`	2
`PBLSQ_SET_MIN_RESIDUAL`	3

IOPT(IO)=?_OPTIONS(PBLSQ_SET_TOLERANCE, TOLERANCE) Replaces the default rank tolerance for using a column, from EPSILON(TOLERANCE) to TOLERANCE. Increasing the value of TOLERANCE will cause fewer columns to be increased from their constraints, and may cause the minimum residual RNORM to increase.

IOPT(IO)=?_OPTIONS(PBLSQ_SET_MIN_RESIDUAL, RESID) Replaces the default target for the minimum residual vector length from 0 to RESID. Increasing the value of RESID can result in fewer iterations and thus increased efficiency. The descent in the optimization will stop at the first point where the minimum residual RNORM is smaller than RESID. Using this option may result in the dual vector not satisfying its optimality conditions, as noted above.

IOPT(IO)= PBLSQ_SET_MAX_ITERATIONS

IOPT(IO+1)= NEW_MAX_ITERATIONS Replaces the default maximum number of iterations from 3*N to NEW_MAX_ITERATIONS. Note that this option requires two entries in the derived type array.

FORTRAN 90 Interface

Generic: CALL PARALLEL_BOUNDED_LSQ (A, B, X [, …])

Specific: The specific interface names are S_PARALLEL_BOUNDED_LSQ and D_PARALLEL_BOUNDED_LSQ.

Description

Subroutine PARALLEL_BOUNDED_LSQ solves the least-squares linear system $Ax \cong b, \alpha \leq x \leq \beta$, using the algorithm *BVLS* found in Lawson and Hanson, (1995), pages 279-283. The new steps involve updating the dual vector and exchange of required data, using MPI. The optional changes to default tolerances, minimum residual, and the number of iterations are new features.

Examples

Example 1: Distributed Equality and Inequality Constraint Solver

The program PBLSQ_EX1 illustrates the computation of the minimum Euclidean length solution of an $m' \times n'$ system of linear inequality constraints , $Gy \geq h$. Additionally the first $f > 0$ of the constraints are equalities. The solution algorithm is based on Algorithm *LDP*, page 165-166, *loc. cit*. By allowing the dual variables to be free, the constraints become equalities. The rows of $E = \left[G:h \right]$ are partitioned and assigned random values. When the minimum Euclidean length solution to the inequalities has been calculated, the residuals $r = Gy - h \geq 0$ are computed, with the dual variables to the *BVLS* problem indicating the entries of r that are exactly zero.

```
      PROGRAM PBLSQ_EX1
! Use Parallel_bounded_LSQ to solve an inequality
! constraint problem, Gy >= h. Force F of the constraints
! to be equalities. This algorithm uses LDP of
! Solving Least Squares Problems, page 165.
! Forcing equality constraints by freeing the dual is
! new here. The constraints are allocated to the
! processors, by rows, in columns of the array A(:,:).
        USE PBLSQ_INT
        USE MPI_SETUP_INT
        USE RAND_INT
        USE SHOW_INT

        IMPLICIT NONE
        INCLUDE "mpif.h"

        INTEGER, PARAMETER :: MP=500, NP=400, M=NP+1, &
          N=MP, F=NP/10

        REAL(KIND(1D0)), PARAMETER :: ZERO=0D0, ONE=1D0
        REAL(KIND(1D0)), ALLOCATABLE :: &
        A(:,:), B(:), BND(:,:), X(:), Y(:), &
          W(:), ASAVE(:,:)
        REAL(KIND(1D0)) RNORM
        INTEGER, ALLOCATABLE :: INDEX(:), IPART(:,:)

        INTEGER K, L, DN, J, JSHIFT, IERROR, NSETP, NSETZ
        LOGICAL :: PRINT=.false.

! Setup for MPI:
        MP_NPROCS=MP_SETUP()

        DN=N/max(1,max(1,MP_NPROCS))-1
        ALLOCATE(IPART(2,max(1,MP_NPROCS)))

! Spread constraint rows evenly to the processors.
        IPART(1,1)=1
        DO L=2,MP_NPROCS
           IPART(2,L-1)=IPART(1,L-1)+DN
           IPART(1,L)=IPART(2,L-1)+1
        END DO
        IPART(2,MP_NPROCS)=N

! Define the constraints using random data.
        K=max(0,IPART(2,MP_RANK+1)-IPART(1,MP_RANK+1)+1)
        ALLOCATE(A(M,K), ASAVE(M,K), BND(2,N), &
          X(N), W(N), B(M), Y(M), INDEX(N))

! The use of ASAVE can be replaced by regenerating the
! data for A(:,:) after the return from
! Parallel_bounded_LSQ
        A=rand(A); ASAVE=A
        IF(MP_RANK == 0 .and. PRINT) &
          call show(IPART,&
            "Partition of the constraints to be solved")

! Set the right-hand side to be one in the last
! component, zero elsewhere.
        B=ZERO;B(M)=ONE

! Solve the dual problem. Letting the dual variable
! have no constraint forces an equality constraint
! for the primal problem.
        BND(1,1:F)=-HUGE(ONE); BND(1,F+1:)=ZERO
        BND(2,:)=HUGE(ONE)
```

```
         CALL Parallel_bounded_LSQ &
           (A, B, BND, X, RNORM, W, INDEX, IPART, &
             NSETP, NSETZ)

 ! Each processor multiplies its block times the part
 ! of the dual corresponding to that partition.
         Y=ZERO
         DO J=IPART(1,MP_RANK+1),IPART(2,MP_RANK+1)
            JSHIFT=J-IPART(1,MP_RANK+1)+1
            Y=Y+ASAVE(:,JSHIFT)*X(J)
         END DO

 ! Accumulate the pieces from all the processors.
 ! Put sum into B(:) on rank 0 processor.
         B=Y
         IF(MP_NPROCS > 1) &
           CALL MPI_REDUCE(Y, B, M, MPI_DOUBLE_PRECISION,&
            MPI_SUM, 0, MP_LIBRARY_WORLD, IERROR)
         IF(MP_RANK == 0) THEN

 ! Compute constraint solution at the root.
 ! The constraints will have no solution if B(M) = ONE.
 ! All of these example problems have solutions.
            B(M)=B(M)-ONE;B=-B/B(M)
         END IF

 ! Send the inequality constraint or primal solution to all nodes.
   IF(MP_NPROCS > 1) &
     CALL MPI_BCAST(B, M, MPI_DOUBLE_PRECISION, 0, &
       MP_LIBRARY_WORLD, IERROR)

 ! For large problems this printing may need to be removed.
         IF(MP_RANK == 0 .and. PRINT) &
           call show(B(1:NP), &
             "Minimal length solution of the constraints")

 ! Compute residuals of the individual constraints.
         X=ZERO
         DO J=IPART(1,MP_RANK+1),IPART(2,MP_RANK+1)
            JSHIFT=J-IPART(1,MP_RANK+1)+1
            X(J)=dot_product(B,ASAVE(:,JSHIFT))
         END DO

 ! This cleans up residuals that are about rounding error
 ! unit (times) the size of the constraint equation and
 ! right-hand side.  They are replaced by exact zero.
         WHERE(W == ZERO) X=ZERO
         W=X

 ! Each group of residuals is disjoint, per processor.
 ! We add all the pieces together for the total set of
 ! constraints.
       IF(MP_NPROCS > 1) &
         CALL MPI_REDUCE(X, W, N, MPI_DOUBLE_PRECISION, &
           MPI_SUM, 0, MP_LIBRARY_WORLD, IERROR)
         IF(MP_RANK == 0 .and. PRINT) &
           call show(W, "Residuals for the constraints")

 ! See to any errors and shut down MPI.
         MP_NPROCS=MP_SETUP('Final')
         IF(MP_RANK == 0) THEN
           IF(COUNT(W < ZERO) == 0 .and.&
            COUNT(W == ZERO) >= F) WRITE(*,*)&
             " Example 1 for PARALLEL_BOUNDED_LSQ is correct."
         END IF
      END
```

Output

```
Example 1 for PARALLEL_BOUNDED_LSQ is correct.
```

Example 2: Distributed Newton-Raphson Method with Step Control

The program PBLSQ_EX2 illustrates the computation of the solution of a non-linear system of equations. We use a constrained Newton-Raphson method.
This algorithm works with the problem chosen for illustration. The step-size control used here, employing only simple bounds, *may not work* on other non-linear systems of equations. Therefore we do not recommend the simple non-linear solving technique illustrated here for an *arbitrary* problem. The test case is *Brown's Almost Linear Problem*, Moré, et al. (1982). The components are given by:

- $f_i(x) = x_i + \sum_{j=1}^{n} x_j - (n+1), \quad i = 1, \ \ldots, \ n-1$
- $f_n(x) = x_1 \ \ldots \ x_n - 1$

The functions are zero at the point $x = \left(\delta, \ldots \delta, \delta^{1-n}\right)^T$, where $\delta > 1$ is a particular root of the polynomial equation $n\delta^n - \left(n+1\right)\delta^{n-1} + 1 = 0$. To avoid convergence to the local minimum $x = \left(0, \ldots, 0n+1\right)^T$, we start at the standard point $x = \left(1/2, \ldots 1/2, 1/2\right)^T$ and develop the Newton method using the linear terms $f\left(x-y\right) \approx f\left(x\right) - J\left(x\right)y \cong 0$, where $J\left(x\right)$ is the Jacobian matrix. The update is constrained so that the first $n-1$ components satisfy $x_j - y_j \geq 1/2$, or $y_j \leq x_j - 1/2$. The last component is bounded from both sides, $0 < x_n - y_n \leq 1/2$, or $x_n > y_n \geq \left(x_n - 1/2\right)$. These bounds avoid the local minimum and allow us to replace the last equation by $\sum_{j=1}^{n} \ln\left(x_j\right) = 0$, which is better scaled than the original. The positive lower bound for $x_n - y_n$ is replaced by the strict bound, EPSILON(1D0), the arithmetic precision, which restricts the relative accuracy of x_n. The input for routine PARALLEL_BOUNDED_LSQ expects each processor to obtain that part of $J\left(x\right)$ it owns. Those columns of the Jacobian matrix correspond to the partition given in the array IPART(:,:). Here the columns of the matrix are evaluated, in parallel, on the nodes where they are required.

```
      PROGRAM PBLSQ_EX2
! Use Parallel_bounded_LSQ to solve a non-linear system
! of equations. The example is an ACM-TOMS test problem,
! except for the larger size.  It is "Brown's Almost Linear
! Function."
        USE ERROR_OPTION_PACKET
        USE PBLSQ_INT
        USE MPI_SETUP_INT
        USE SHOW_INT
        USE Numerical_Libraries, ONLY : N1RTY

        IMPLICIT NONE

        INTEGER, PARAMETER :: N=200, MAXIT=5
```

```
         REAL(KIND(1D0)), PARAMETER :: ZERO=0D0, ONE=1D0,&
           HALF=5D-1, TWO=2D0
         REAL(KIND(1D0)), ALLOCATABLE :: &
          A(:,:), B(:), BND(:,:), X(:), Y(:), W(:)
         REAL(KIND(1D0)) RNORM
         INTEGER, ALLOCATABLE :: INDEX(:), IPART(:,:)

         INTEGER K, L, DN, J, JSHIFT, IERROR, NSETP, &
           NSETZ, ITER
         LOGICAL :: PRINT=.false.
         TYPE(D_OPTIONS) IOPT(3)

! Setup for MPI:
         MP_NPROCS=MP_SETUP()

         DN=N/max(1,max(1,MP_NPROCS))-1
         ALLOCATE(IPART(2,max(1,MP_NPROCS)))

! Spread Jacobian matrix columns evenly to the processors.
         IPART(1,1)=1
         DO L=2,MP_NPROCS
            IPART(2,L-1)=IPART(1,L-1)+DN
            IPART(1,L)=IPART(2,L-1)+1
         END DO
         IPART(2,MP_NPROCS)=N

         K=max(0,IPART(2,MP_RANK+1)-IPART(1,MP_RANK+1)+1)
         ALLOCATE(A(N,K), BND(2,N), &
           X(N), W(N), B(N), Y(N), INDEX(N))

! This is Newton's method on "Brown's almost
! linear function."
         X=HALF
         ITER=0

! Turn off messages and stopping for FATAL class errors.
         CALL ERSET (4, 0, 0)

NEWTON_METHOD: DO

! Set bounds for the values after the step is taken.
! All variables are positive and bounded below by HALF,
! except for variable N, which has an upper bound of HALF.
         BND(1,1:N-1)=-HUGE(ONE)
         BND(2,1:N-1)=X(1:N-1)-HALF
         BND(1,N)=X(N)-HALF
         BND(2,N)=X(N)-EPSILON(ONE)

! Compute the residual function.
         B(1:N-1)=SUM(X)+X(1:N-1)-(N+1)
         B(N)=LOG(PRODUCT(X))
         if(mp_rank == 0 .and. PRINT) THEN
           CALL SHOW(B, &
             "Developing non-linear function residual")
         END IF
         IF (MAXVAL(ABS(B(1:N-1))) <= SQRT(EPSILON(ONE)))&
           EXIT NEWTON_METHOD

! Compute the derivatives local to each processor.
         A(1:N-1,:)=ONE
         DO J=1,N-1
           IF(J < IPART(1,MP_RANK+1)) CYCLE
           IF(J > IPART(2,MP_RANK+1)) CYCLE
           JSHIFT=J-IPART(1,MP_RANK+1)+1
           A(J,JSHIFT)=TWO
         END DO
```

```
        A(N,:)=ONE/X(IPART(1,MP_RANK+1):IPART(2,MP_RANK+1))

! Reset the linear independence tolerance.
        IOPT(1)=D_OPTIONS(PBLSQ_SET_TOLERANCE,&
          sqrt(EPSILON(ONE)))
        IOPT(2)=PBLSQ_SET_MAX_ITERATIONS

! If N iterations was not enough on a previous iteration, reset to 2*N.
        IF(N1RTY(1) == 0) THEN
          IOPT(3)=N
        ELSE
          IOPT(3)=2*N
          CALL E1POP('MP_SETUP')
          CALL E1PSH('MP_SETUP')
        END IF

        CALL parallel_bounded_LSQ &
          (A, B, BND, Y, RNORM, W, INDEX, IPART, NSETP, &
            NSETZ,IOPT=IOPT)

! The array Y(:) contains the constrained Newton step.
! Update the variables.
        X=X-Y

        IF(mp_rank == 0 .and. PRINT) THEN
          CALL show(BND, "Bounds for the moves")
          CALL SHOW(X, "Developing Solution")
          CALL SHOW((/RNORM/), &
            "Linear problem residual norm")
        END IF

! This is a safety measure for not taking too many steps.
       ITER=ITER+1
       IF(ITER > MAXIT) EXIT NEWTON_METHOD
         END DO NEWTON_METHOD

      IF(MP_RANK == 0) THEN
        IF(ITER <= MAXIT) WRITE(*,*)&
        " Example 2 for PARALLEL_BOUNDED_LSQ is correct."
      END IF

! See to any errors and shut down MPI.
        MP_NPROCS=MP_SETUP('Final')

     END
```

LSARG

more... more...

Solves a real general system of linear equations with iterative refinement.

Required Arguments

A — `N` by `N` matrix containing the coefficients of the linear system. (Input)

B — Vector of length `N` containing the right-hand side of the linear system. (Input)

X — Vector of length `N` containing the solution to the linear system. (Output)

Optional Arguments

N — Number of equations. (Input)
Default: `N` = size (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = size (`A`,1).

IPATH — Path indicator. (Input)

`IPATH` **=** 1 means the system $AX = B$ is solved.

`IPATH` **=** 2 means the system $A^T X = B$ is solved.

Default: `IPATH` = 1.

FORTRAN 90 Interface

Generic: `CALL LSARG (A, B, X [, …])`

Specific: The specific interface names are `S_LSARG` and `D_LSARG`.

FORTRAN 77 Interface

Single: `CALL LSARG (N, A, LDA, B, IPATH, X)`

Double: The double precision name is `DLSARG`

ScaLAPACK Interface

Generic: `CALL LSARG (A0, B0, X0 [, …])`

Specific: The specific interface names are `S_LSARG` and `D_LSARG`.

See the *ScaLAPACK Usage Notes* below for a description of the arguments for distributed computing.

Description

Routine `LSARG` solves a system of linear algebraic equations having a real general coefficient matrix. It first uses routine `LFCRG` to compute an *LU* factorization of the coefficient matrix and to estimate the condition number of the matrix. The solution of the linear system is then found using the iterative refinement routine `LFIRG`. The underlying code is based on either LINPACK , LAPACK, or ScaLAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see *Using ScaLAPACK, LAPACK, LINPACK, and EISPACK* in the Introduction section of this manual.

`LSARG` fails if *U*, the upper triangular part of the factorization, has a zero diagonal element or if the iterative refinement algorithm fails to converge. These errors occur only if *A* is singular or very close to a singular matrix.

If the estimated condition number is greater than $1/\varepsilon$ (where ε is machine precision), a warning error is issued. This indicates that very small changes in *A* can cause very large changes in the solution *x*. Iterative refinement can sometimes find the solution to such a system. `LSARG` solves the problem that is represented in the computer; however, this problem may differ from the problem whose solution is desired.

Comments

1. Workspace may be explicitly provided, if desired, by use of `L2ARG/DL2ARG`. The reference is:

   `CALL L2ARG (N, A, LDA, B, IPATH, X, FACT, IPVT, WK)`

   The additional arguments are as follows:

   FACT — Work vector of length N^2 containing the *LU* factorization of `A` on output.

   IPVT — Integer work vector of length `N` containing the pivoting information for the *LU* factorization of `A` on output.

   WK — Work vector of length `N`.

2 ***Informational errors***

Type	Code	Description
3	1	The input matrix is too ill-conditioned. The solution might not be accurate.
4	2	The input matrix is singular.

ScaLAPACK Usage Notes

The arguments which differ from the standard version of this routine are:

A0 — `MXLDA` by `MXCOL` local matrix containing the local portions of the distributed matrix `A`. `A` contains the coefficients of the linear system. (Input)

B0 — Local vector of length `MXLDA` containing the local portions of the distributed vector `B`. `B` contains the right-hand side of the linear system. (Input)

X0 — Local vector of length `MXLDA` containing the local portions of the distributed vector `X`. `X` contains the solution to the linear system. (Output)

All other arguments are global and are the same as described for the standard version of the routine. In the argument descriptions above, `MXLDA` and `MXCOL` can be obtained through a call to `SCALAPACK_GETDIM` (see *Utilities*) after a call to `SCALAPACK_SETUP` (see *Utilities*) has been made. See the ScaLAPACK Example below.

Examples

Example

A system of three linear equations is solved. The coefficient matrix has real general form and the right-hand-side vector *b* has three elements.

```
      USE LSARG_INT
      USE WRRRN_INT
      IMPLICIT NONE
!                                 Declare variables
      INTEGER    LDA, N
      PARAMETER  (LDA=3, N=3)

      REAL    A(LDA,N), B(N), X(N)
!                                 Set values for A and B
      A(1,:) = (/ 33.0,  16.0,  72.0/)
      A(2,:) = (/-24.0, -10.0, -57.0/)
      A(3,:) = (/ 18.0, -11.0,   7.0/)
!
      B =      (/129.0, -96.0,   8.5/)

!                                 Solve the system of equations
      CALL LSARG (A, B, X)
!                                Print results
```

```
      CALL WRRRN ('X', X, 1, N, 1)
      END
```

Output

```
             X
    1        2        3
1.000    1.500    1.000
```

ScaLAPACK Example

The same system of three linear equations is solved as a distributed computing example. The coefficient matrix has real general form and the right-hand-side vector *b* has three elements. `SCALAPACK_MAP` and `SCALAPACK_UNMAP` are IMSL utility routines (see *Utilities*) used to map and unmap arrays to and from the processor grid. They are used here for brevity. `DESCINIT` is a ScaLAPACK tools routine which initializes the descriptors for the local arrays.

```
      USE MPI_SETUP_INT
      USE LSARG_INT
      USE WRRRN_INT
      USE SCALAPACK_SUPPORT
      IMPLICIT NONE
      INCLUDE 'mpif.h'
!                                 Declare variables
      INTEGER    N, DESCA(9), DESCX(9)
      INTEGER       INFO, MXLDA, MXCOL
      REAL, ALLOCATABLE ::        A(:,:), B(:), X(:)
      REAL, ALLOCATABLE ::        A0(:,:), B0(:), X0(:)
      PARAMETER  (N=3)
!                                 Set up for MPI
      MP_NPROCS = MP_SETUP()
      IF (MP_RANK .EQ. 0) THEN
          ALLOCATE (A(N,N), B(N), X(N))
!                                 Set values for A and B
          A(1,:) = (/ 33.0,  16.0,  72.0/)
          A(2,:) = (/-24.0, -10.0, -57.0/)
          A(3,:) = (/ 18.0, -11.0,   7.0/)
!
          B = (/129.0, -96.0,  8.5/)
      ENDIF
!                                  Set up a 1D processor grid and define
!                                  its context id, MP_ICTXT
      CALL SCALAPACK_SETUP(N, N, .TRUE., .TRUE.)
!                                  Get the array descriptor entities MXLDA,
!                                  AND MXCOL
      CALL SCALAPACK_GETDIM(N, N, MP_MB, MP_NB, MXLDA, MXCOL)
!                                  Set up the array descriptors
      CALL DESCINIT(DESCA, N, N, MP_MB, MP_NB, 0, 0, MP_ICTXT, MXLDA, INFO)
      CALL DESCINIT(DESCX, N, 1, MP_MB, 1, 0, 0, MP_ICTXT, MXLDA, INFO)
!                Allocate space for the local arrays
      ALLOCATE (A0(MXLDA,MXCOL), B0(MXLDA), X0(MXLDA))
!                                 Map input arrays to the processor grid
      CALL SCALAPACK_MAP(A, DESCA, A0)
      CALL SCALAPACK_MAP(B, DESCX, B0)
!                                  Solve the system of equations
      CALL LSARG (A0, B0, X0)
!                                  Unmap the results from the distributed
!                                  arrays back to a non-distributed array.
!                                  After the unmap, only Rank=0 has the full
!                                  array.
```

```
      CALL SCALAPACK_UNMAP(X0, DESCX, X)
!                                   Print results.
!                                   Only Rank=0 has the solution, X.
      IF (MP_RANK .EQ. 0) CALL WRRRN ('X', X, 1, N, 1)
      IF (MP_RANK .EQ. 0) DEALLOCATE(A, B, X)
      DEALLOCATE(A0, B0, X0)
!                                   Exit ScaLAPACK usage
      CALL SCALAPACK_EXIT(MP_ICTXT)
!                                   Shut down MPI
      MP_NPROCS = MP_SETUP('FINAL')
      END
```

Output

```
            X
     1       2       3
 1.000   1.500   1.000
```

LSLRG

more...

more...

Solves a real general system of linear equations without iterative refinement.

Required Arguments

A — N by N matrix containing the coefficients of the linear system. (Input)

B — Vector of length N containing the right-hand side of the linear system. (Input)

X — Vector of length N containing the solution to the linear system. (Output)
If B is not needed, B and X can share the same storage locations

Optional Arguments

N — Number of equations. (Input)
Default: N = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

IPATH — Path indicator. (Input)
IPATH = 1 means the system $AX = B$ is solved. IPATH = 2 means the system $A^T X = B$ is solved.
Default: IPATH = 1.

FORTRAN 90 Interface

Generic: CALL LSLRG (A, B, X [, …])

Specific: The specific interface names are S_LSLRG and D_LSLRG.

FORTRAN 77 Interface

Single: CALL LSLRG (N, A, LDA, B, IPATH, X)

Double: The double precision name is DLSLRG.

ScaLAPACK Interface

Generic: CALL LSLRG (A0, B0, X0 [, …])

Specific: The specific interface names are S_LSLRG and D_LSLRG.

See the *ScaLAPACK Usage Notes* below for a description of the arguments for distributed computing.

Description

Routine LSLRG solves a system of linear algebraic equations having a real general coefficient matrix. The underlying code is based on either LINPACK , LAPACK, or ScaLAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see *Using ScaLAPACK, LAPACK, LINPACK, and EISPACK* in the Introduction section of this manual. LSLRG first uses the routine LFCRG to compute an *LU* factorization of the coefficient matrix based on Gauss elimination with partial pivoting. Experiments were analyzed to determine efficient implementations on several different computers. For some supercomputers, particularly those with efficient vendor-supplied BLAS, versions that call Level 1, 2 and 3 BLAS are used. The remaining computers use a factorization method provided to us by Dr. Leonard J. Harding of the University of Michigan. Harding's work involves "loop unrolling and jamming" techniques that achieve excellent performance on many computers. Using an option, LSLRG will estimate the condition number of the matrix. The solution of the linear system is then found using LFSRG.

The routine LSLRG fails if U, the upper triangular part of the factorization, has a zero diagonal element. This occurs only if A is close to a singular matrix.

If the estimated condition number is greater than $1/\varepsilon$ (where ε is machine precision), a warning error is issued. This indicates that small changes in A can cause large changes in the solution x. If the coefficient matrix is ill-conditioned or poorly scaled, it is recommended that either LIN_SOL_SVD or LSARG be used.

Comments

1. Workspace may be explicitly provided, if desired, by use of L2LRG/DL2LRG. The reference is:

   CALL L2LRG (N, A, LDA, B, IPATH, X, FACT, IPVT, WK)

   The additional arguments are as follows:

FACT — N × N work array containing the *LU* factorization of A on output. If A is not needed, A and FACT can share the same storage locations. See Item 3 below to avoid memory bank conflicts.

IPVT — Integer work vector of length N containing the pivoting information for the *LU* factorization of A on output.

WK — Work vector of length N.

2. Informational errors

Type	Code	Description
3	1	The input matrix is too ill-conditioned. The solution might not be accurate.
4	2	The input matrix is singular.

3. *Integer Options* with *Chapter 11, Options Manager*

16This option uses four values to solve memory bank conflict (access inefficiency) problems. In routine L2LRG the leading dimension of FACT is increased by IVAL(3) when N is a multiple of IVAL(4). The values IVAL(3) and IVAL(4) are temporarily replaced by IVAL(1) and IVAL(2); respectively, in LSLRG. Additional memory allocation for FACT and option value restoration are done automatically in LSLRG. Users directly calling L2LRG can allocate additional space for FACT and set IVAL(3) and IVAL(4) so that memory bank conflicts no longer cause inefficiencies. There is no requirement that users change existing applications that use LSLRG or L2LRG. Default values for the option are
IVAL(*) = 1, 16, 0, 1.

17This option has two values that determine if the L_1 condition number is to be computed. Routine LSLRG temporarily replaces IVAL(2) by IVAL(1). The routine L2CRG computes the condition number if IVAL(2) = 2. Otherwise L2CRG skips this computation. LSLRG restores the option. Default values for the option are
IVAL(*) = 1, 2.

ScaLAPACK Usage Notes

The arguments which differ from the standard version of this routine are:

A0 — MXLDA by MXCOL local matrix containing the local portions of the distributed matrix A. A contains the coefficients of the linear system. (Input)

B0 — Local vector of length MXLDA containing the local portions of the distributed vector B. B contains the right-hand side of the linear system. (Input)

X0 — Local vector of length MXLDA containing the local portions of the distributed vector X. X contains the solution to the linear system. (Output)

All other arguments are global and are the same as described for the standard version of the routine. In the argument descriptions above, MXLDA and MXCOL can be obtained through a call to SCALAPACK_GETDIM (see *Utilities*) after a call to SCALAPACK_SETUP (see *Utilities*) has been made. See the ScaLAPACK Example below.

Examples

Example 1

A system of three linear equations is solved. The coefficient matrix has real general form and the right-hand-side vector *b* has three elements.

```
      USE LSLRG_INT
      USE WRRRN_INT
      IMPLICIT NONE
!                                 Declare variables
      INTEGER    LDA, N
      PARAMETER  (LDA=3, N=3)

      REAL    A(LDA,N), B(N), X(N)
!                                 Set values for A and B
      A(1,:) = (/ 33.0,  16.0,  72.0/)
      A(2,:) = (/-24.0, -10.0, -57.0/)
      A(3,:) = (/ 18.0, -11.0,   7.0/)
!
      B = (/129.0 -96.0   8.5/)

!                                 Solve the system of equations
      CALL LSLRG (A, B, X)
!                                Print results
      CALL WRRRN ('X', X, 1, N, 1)
      END
```

Output

```
           X
    1        2        3
1.000    1.500    1.000
```

Example 2

A system of N = 16 linear equations is solved using the routine L2LRG. The option manager is used to eliminate memory bank conflict inefficiencies that may occur when the matrix dimension is a multiple of 16. The leading dimension of FACT=A is increased from N to N+IVAL(3)=17, since N=16=IVAL(4). The data used for the test is a nonsymmetric Hadamard matrix and a right-hand side generated by a known solution, $x_j = j$, $j = 1, \ldots, N$.

```
      USE L2LRG_INT
      USE IUMAG_INT
      USE WRRRN_INT
      USE SGEMV_INT
      IMPLICIT NONE
!                                 Declare variables
      INTEGER    LDA, N
      PARAMETER  (LDA=17, N=16)
```

```
!                                  SPECIFICATIONS FOR PARAMETERS
      INTEGER    ICHP, IPATH, IPUT, KBANK
      REAL       ONE, ZERO
      PARAMETER  (ICHP=1, IPATH=1, IPUT=2, KBANK=16, ONE=1.0E0, &
                 ZERO=0.0E0)
!                                  SPECIFICATIONS FOR LOCAL VARIABLES
      INTEGER    I, IPVT(N), J, K, NN
      REAL       A(LDA,N), B(N), WK(N), X(N)
!                                  SPECIFICATIONS FOR SAVE VARIABLES
      INTEGER    IOPT(1), IVAL(4)
      SAVE       IVAL
!                                Data for option values.
      DATA IVAL/1, 16, 1, 16/
!                                  Set values for A and B:
      A(1,1) = ONE
      NN     = 1
!                                  Generate Hadamard matrix.
      DO 20  K=1, 4
         DO 10  J=1, NN
            DO 10  I=1, NN
               A(NN+I,J)  = -A(I,J)
               A(I,NN+J)  = A(I,J)
               A(NN+I,NN+J) = A(I,J)
   10    CONTINUE
         NN = NN + NN
   20 CONTINUE
!                                  Generate right-hand-side.
      DO 30  J=1, N
         X(J) = J
   30 CONTINUE
!                                  Set B = A*X.
      CALL SGEMV ('N', N, N, ONE, A, LDA, X, 1, ZERO, B, 1)
!                                  Clear solution array.
         X = ZERO

!                                  Set option to avoid memory
!                                  bank conflicts.
      IOPT(1) = KBANK
      CALL IUMAG ('MATH', ICHP, IPUT, 1, IOPT, IVAL)
!                                  Solve A*X = B.
      CALL L2LRG (N, A, LDA, B, IPATH, X, A, IPVT, WK)
!                                  Print results
      CALL WRRRN ('X', X, 1, N, 1)
      END
```

Output

```
                                         X
   1       2       3       4       5       6       7       8       9      10
1.00    2.00    3.00    4.00    5.00    6.00    7.00    8.00    9.00   10.00

    11      12      13      14      15      16
 11.00   12.00   13.00   14.00   15.00   16.00
```

ScaLAPACK Example

The same system of three linear equations is solved as a distributed computing example. The coefficient matrix has real general form and the right-hand-side vector *b* has three elements. `SCALAPACK_MAP` and `SCALAPACK_UNMAP` are IMSL utility routines (see *Chapter 11, "Utilities"*) used to map and unmap arrays to and from the processor grid. They are used here for brevity. `DESCINIT` is a ScaLAPACK tools routine which initializes the descriptors for the local arrays.

```
      USE MPI_SETUP_INT
      USE LSLRG_INT
      USE WRRRN_INT
      USE SCALAPACK_SUPPORT
      IMPLICIT NONE
      INCLUDE 'mpif.h'
!                                  Declare variables
      INTEGER    N, DESCA(9), DESCX(9)
      INTEGER       INFO, MXCOL, MXLDA
      REAL, ALLOCATABLE ::        A(:,:), B(:), X(:)
      REAL, ALLOCATABLE ::        A0(:,:), B0(:), X0(:)
      PARAMETER  (N=3)
!                                  Set up for MPI
      MP_NPROCS = MP_SETUP()
      IF(MP_RANK .EQ. 0) THEN
          ALLOCATE (A(N,N), B(N), X(N))
!                                  Set values for A and B
          A(1,:) = (/ 33.0,  16.0,  72.0/)
          A(2,:) = (/-24.0, -10.0, -57.0/)
          A(3,:) = (/ 18.0, -11.0,   7.0/)
!
          B = (/129.0, -96.0,  8.5/)
      ENDIF
!                                   Set up a 1D processor grid and define
!                                   its context id, MP_ICTXT
      CALL SCALAPACK_SETUP(N, N, .TRUE., .TRUE.)
!                                   Get the array descriptor entities MXLDA,
!                                   and MXCOL
      CALL SCALAPACK_GETDIM(N, N, MP_MB, MP_NB, MXLDA, MXCOL)
!                                   Set up the array descriptors
      CALL DESCINIT(DESCA, N, N, MP_MB, MP_NB, 0, 0, MP_ICTXT, MXLDA, INFO)
      CALL DESCINIT(DESCX, N, 1, MP_MB, 1, 0, 0, MP_ICTXT, MXLDA, INFO)
!                Allocate space for the local arrays
      ALLOCATE (A0(MXLDA,MXCOL), B0(MXLDA), X0(MXLDA))
!                                  Map input arrays to the processor grid
      CALL SCALAPACK_MAP(A, DESCA, A0)
      CALL SCALAPACK_MAP(B, DESCX, B0)
!                                  Solve the system of equations
      CALL LSLRG (A0, B0, X0)
!                                  Unmap the results from the distributed
!                                  arrays back to a non-distributed array.
!                                  After the unmap, only Rank=0 has the full
!                                  array.
      CALL SCALAPACK_UNMAP(X0, DESCX, X)
!                                  Print results
!                                  Only Rank=0 has the solution, X.
      IF(MP_RANK .EQ. 0)CALL WRRRN ('X', X, 1, N, 1)
      IF (MP_RANK .EQ. 0) DEALLOCATE(A, B, X)
      DEALLOCATE(A0, B0, X0)
!                                  Exit ScaLAPACK usage
      CALL SCALAPACK_EXIT(MP_ICTXT)
!                                  Shut down MPI
      MP_NPROCS = MP_SETUP('FINAL')
      END
```

Output

```
          X
    1        2        3
1.000    1.500    1.000
```

LFCRG

more...

more...

Computes the *LU* factorization of a real general matrix and estimates its L_1 condition number.

Required Arguments

A — `N` by `N` matrix to be factored. (Input)

FACT — `N` by `N` matrix containing the *LU* factorization of the matrix `A`. (Output)
If *A* is not needed, `A` and `FACT` can share the same storage locations.

IPVT — Vector of length `N` containing the pivoting information for the *LU* factorization. (Output)

RCOND — Scalar containing an estimate of the reciprocal of the L_1 condition number of `A`. (Output)

Optional Arguments

N — Order of the matrix. (Input)
Default: `N` = size (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = size (`A`,1).

LDFACT — Leading dimension of `FACT` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDFACT` = size (`FACT`,1).

FORTRAN 90 Interface

Generic: `CALL LFCRG (A, FACT, IPVT, RCOND, [, …])`

Specific: The specific interface names are `S_LFCRG` and `D_LFCRG`.

FORTRAN 77 Interface

Single: CALL LFCRG (N, A, LDA, FACT, LDFACT, IPVT, RCOND)

Double: The double precision name is DLFCRG.

ScaLAPACK Interface

Generic: CALL LFCRG (A0, FACT0, IPVT0, RCOND [, …])

Specific: The specific interface names are S_LFCRG and D_LFCRG.

See the ScaLAPACK Usage Notes below for a description of the arguments for distributed computing.

Description

Routine LFCRG performs an *LU* factorization of a real general coefficient matrix. It also estimates the condition number of the matrix. The underlying code is based on either LINPACK , LAPACK, or ScaLAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see *Using ScaLAPACK, LAPACK, LINPACK, and EISPACK* in the Introduction section of this manual. The *LU* factorization is done using scaled partial pivoting. Scaled partial pivoting differs from partial pivoting in that the pivoting strategy is the same as if each row were scaled to have the same ∞-norm. Otherwise, partial pivoting is used.

The L_1 condition number of the matrix A is defined to be $\kappa(A) = \|A\|_1\|A^{-1}\|_1$. Since it is expensive to compute $\|A^{-1}\|_1$, the condition number is only estimated. The estimation algorithm is the same as used by LINPACK and is described in a paper by Cline et al. (1979).

If the estimated condition number is greater than $1/\varepsilon$ (where ε is machine precision), a warning error is issued. This indicates that very small changes in A can cause very large changes in the solution x. Iterative refinement can sometimes find the solution to such a system.

LFCRG fails if U, the upper triangular part of the factorization, has a zero diagonal element. This can occur only if A either is singular or is very close to a singular matrix.

The *LU* factors are returned in a form that is compatible with routines LFIRG, LFSRG and LFDRG. To solve systems of equations with multiple right-hand-side vectors, use LFCRG followed by either LFIRG or LFSRG called once for each right-hand side. The routine LFDRG can be called to compute the determinant of the coefficient matrix after LFCRG has performed the factorization.

Let F be the matrix FACT and let p be the vector IPVT. The triangular matrix U is stored in the upper triangle of F. The strict lower triangle of F contains the information needed to reconstruct L using

$$L^{-1} = L_{N-1}P_{N-1} \ldots L_1P_1$$

where P_k is the identity matrix with rows k and p_k interchanged and L_k is the identity with F_{ik} for $i = k + 1, \ldots, N$ inserted below the diagonal. The strict lower half of F can also be thought of as containing the negative of the multipliers. LFCRG is based on the LINPACK routine SGECO; see Dongarra et al. (1979). SGECO uses unscaled partial pivoting.

Comments

1. Workspace may be explicitly provided, if desired, by use of L2CRG/DL2CRG. The reference is:

   CALL L2CRG (N, A, LDA, FACT, LDFACT, IPVT, RCOND, WK)

   The additional argument is

   WK — Work vector of length N.

2. Informational errors

Type	Code	Description
3	1	The input matrix is algorithmically singular.
4	2	The input matrix is singular.

ScaLAPACK Usage Notes

The arguments which differ from the standard version of this routine are:

A0 — MXLDA by MXCOL local matrix containing the local portions of the distributed matrix A. A contains the matrix to be factored. (Input)

FACT0 — MXLDA by MXCOL local matrix containing the local portions of the distributed matrix FACT. FACT contains the *LU* factorization of the matrix A. (Output)

IPVT0 — Local vector of length MXLDA containing the local portions of the distributed vector IPVT. IPVT contains the pivoting information for the *LU* factorization. (Output)

All other arguments are global and are the same as described for the standard version of the routine. In the argument descriptions above, MXLDA and MXCOL can be obtained through a call to SCALAPACK_GETDIM (see *Utilities*) after a call to SCALAPACK_SETUP (see *Utilities*) has been made. See the *ScaLAPACK Example* below.

Examples

Example 1

The inverse of a 3 × 3 matrix is computed. `LFCRG` is called to factor the matrix and to check for singularity or ill-conditioning. `LFIRG` is called to determine the columns of the inverse.

```
      USE LFCRG_INT
      USE UMACH_INT
      USE LFIRG_INT
      USE WRRRN_INT
!                                 Declare variables
      PARAMETER  (LDA=3, LDFACT=3, N=3)
      INTEGER    IPVT(N), J, NOUT
      REAL       A(LDA,N), AINV(LDA,N), FACT(LDFACT,N), RCOND, &
                 RES(N), RJ(N)
!                                 Set values for A
          A(1,:) = (/ 1.0,  3.0,  3.0/)
          A(2,:) = (/ 1.0,  3.0,  4.0/)
          A(3,:) = (/ 1.0,  4.0,  3.0/)!
      CALL LFCRG (A, FACT, IPVT, RCOND)
!                                 Print the reciprocal condition number
!                                 and the L1 condition number
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99998) RCOND, 1.0E0/RCOND
!                                 Set up the columns of the identity
!                                 matrix one at a time in RJ
      RJ = 0.0E0
      DO 10  J=1, N
         RJ(J) = 1.0
!                                 RJ is the J-th column of the identity
!                                 matrix so the following LFIRG
!                                 reference places the J-th column of
!                                 the inverse of A in the J-th column
!                                 of AINV
         CALL LFIRG (A, FACT, IPVT, RJ, AINV(:,J), RES)
         RJ(J) = 0.0
   10 CONTINUE
!                                 Print results
      CALL WRRRN ('AINV', AINV)
!
99998 FORMAT ('  RCOND = ',F5.3,/,'  L1 Condition number = ',F6.3)
      END
```

Output

```
RCOND < .02
L1 Condition number < 100.0

          AINV
        1       2       3
1   7.000  -3.000  -3.000
2  -1.000   0.000   1.000
3  -1.000   1.000   0.000
```

ScaLAPACK Example

The inverse of the same 3 × 3 matrix is computed as a distributed example. LFCRG is called to factor the matrix and to check for singularity or ill-conditioning. LFIRG is called to determine the columns of the inverse. SCALAPACK_MAP and SCALAPACK_UNMAP are IMSL utility routines (see Chapter 11, "Utilities") used to map and unmap arrays to and from the processor grid. They are used here for brevity. DESCINIT is a ScaLAPACK tools routine which initializes the descriptors for the local arrays.

```
      USE MPI_SETUP_INT
      USE LFCRG_INT
      USE UMACH_INT
      USE LFIRG_INT
      USE WRRRN_INT
      USE SCALAPACK_SUPPORT
      IMPLICIT NONE
      INCLUDE 'mpif.h'
!                                 Declare variables
      INTEGER     J, LDA, N, DESCA(9), DESCL(9)
      INTEGER     INFO, MXCOL, MXLDA, NOUT
      INTEGER, ALLOCATABLE ::     IPVT0(:)
      REAL, ALLOCATABLE ::        A(:,:), AINV(:,:), X0(:), RJ(:)
      REAL, ALLOCATABLE ::        A0(:,:), FACT0(:,:), RES0(:), RJ0(:)
      REAL        RCOND
      PARAMETER  (LDA=3, N=3)
!                                 Set up for MPI
      MP_NPROCS = MP_SETUP()
      IF(MP_RANK .EQ. 0) THEN
          ALLOCATE (A(LDA,N), AINV(LDA,N))
!                                 Set values for A
          A(1,:) = (/ 1.0,  3.0,  3.0/)
          A(2,:) = (/ 1.0,  3.0,  4.0/)
          A(3,:) = (/ 1.0,  4.0,  3.0/)
      ENDIF
!                                  Set up a 1D processor grid and define
!                                  its context id, MP_ICTXT
      CALL SCALAPACK_SETUP(N, N, .TRUE., .TRUE.)
!                                  Get the array descriptor entities MXLDA,
!                                  and MXCOL
      CALL SCALAPACK_GETDIM(N, N, MP_MB, MP_NB, MXLDA, MXCOL)
!                                  Set up the array descriptors
      CALL DESCINIT(DESCA, N, N, MP_MB, MP_NB, 0, 0, MP_ICTXT, MXLDA, INFO)
      CALL DESCINIT(DESCL, N, 1, MP_MB, 1, 0, 0, MP_ICTXT, MXLDA, INFO)
!                                  Allocate space for the local arrays
      ALLOCATE(A0(MXLDA,MXCOL), X0(MXLDA),FACT0(MXLDA,MXCOL), RJ(N), &
               RJ0(MXLDA), RES0(MXLDA), IPVT0(MXLDA))
!                                 Map input arrays to the processor grid
      CALL SCALAPACK_MAP(A, DESCA, A0)
!                                 Call the factorization routine
      CALL LFCRG (A0, FACT0, IPVT0, RCOND)
!                                 Print the reciprocal condition number
!                                 and the L1 condition number
      IF(MP_RANK .EQ. 0) THEN
         CALL UMACH (2, NOUT)
         WRITE (NOUT,99998) RCOND, 1.0E0/RCOND
      ENDIF
!                                 Set up the columns of the identity
!                                 matrix one at a time in RJ
      RJ = 0.0E0
      DO 10  J=1, N
         RJ(J) = 1.0
         CALL SCALAPACK_MAP(RJ, DESCL, RJ0)
!                                 RJ is the J-th column of the identity
```

```
!                                  matrix so the following LFIRG
!                                  reference computes the J-th column of
!                                  the inverse of A
         CALL LFIRG (A0, FACT0, IPVT0, RJ0, X0, RES0)
         RJ(J) = 0.0
         CALL SCALAPACK_UNMAP(X0, DESCL, AINV(:,J))
   10 CONTINUE
!                                  Print results
!                                  Only Rank=0 has the solution, X.
      IF(MP_RANK.EQ.0) CALL WRRRN ('AINV', AINV)
      IF (MP_RANK .EQ. 0) DEALLOCATE(A, AINV)
      DEALLOCATE(A0, IPVT0, FACT0, RES0, RJ, RJ0, X0)
!                                 Exit ScaLAPACK usage
      CALL SCALAPACK_EXIT(MP_ICTXT)
!                                 Shut down MPI
      MP_NPROCS = MP_SETUP('FINAL')
99998 FORMAT ('  RCOND = ',F5.3,/,'  L1 Condition number = ',F6.3)
      END
```

Output

```
RCOND < .02
L1 Condition number < 100.0

          AINV
        1       2       3
1   7.000  -3.000  -3.000
2  -1.000   0.000   1.000
3  -1.000   1.000   0.000
```

LFTRG

more...

more...

Computes the *LU* factorization of a real general matrix.

Required Arguments

A — `N` by `N` matrix to be factored. (Input)

FACT — `N` by `N` matrix containing the *LU* factorization of the matrix `A`. (Output)
If *A* is not needed, `A` and `FACT` can share the same storage locations.

IPVT — Vector of length `N` containing the pivoting information for the *LU* factorization. (Output)

Optional Arguments

N — Order of the matrix. (Input)
Default: `N` = size (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = size (`A`,1).

LDFACT — Leading dimension of `FACT` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDFACT` = size (`FACT`,1).

FORTRAN 90 Interface

Generic:`CALL LFTRG (A, FACT, IPVT [, …])`

Specific: The specific interface names are `S_LFTRG` and `D_LFTRG`.

FORTRAN 77 Interface

Single: `CALL LFTRG (N, A, LDA, FACT, LDFACT, IPVT)`

Double: The double precision name is `DLFTRG`.

ScaLAPACK Interface

Generic: `CALL LFTRG (A0, FACT0, IPVT0 [, …])`

Specific: The specific interface names are `S_LFTRG` and `D_LFTRG`.

See the *ScaLAPACK Usage Notes* below for a description of the arguments for distributed computing.

Description

Routine `LFTRG` performs an *LU* factorization of a real general coefficient matrix. The underlying code is based on either LINPACK , LAPACK, or ScaLAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see *Using ScaLAPACK, LAPACK, LINPACK, and EISPACK* in the Introduction section of this manual. The *LU* factorization is done using scaled partial pivoting. Scaled partial pivoting differs from partial pivoting in that the pivoting strategy is the same as if each row were scaled to have the same norm. Otherwise, partial pivoting is used.

The routine `LFTRG` fails if *U*, the upper triangular part of the factorization, has a zero diagonal element. This can occur only if *A* is singular or very close to a singular matrix.

The *LU* factors are returned in a form that is compatible with routines `LFIRG`, `LFSRG` and `LFDRG`. To solve systems of equations with multiple right-hand-side vectors, use `LFTRG` followed by either `LFIRG` or `LFSRG` called once for each right-hand side. The routine `LFDRG` can be called to compute the determinant of the coefficient matrix after `LFTRG` has performed the factorization. Let *F* be the matrix `FACT` and let *p* be the vector `IPVT`. The triangular matrix *U* is stored in the upper triangle of *F*. The strict lower triangle of *F* contains the information needed to reconstruct L^{-1} using

$$L^{-1} = L_{N-1} P_{N-1} \dots L_1 P_1$$

where P_k is the identity matrix with rows k and p_k interchanged and L_k is the identity with F_{ik} for $i = k + 1, \dots N$ inserted below the diagonal. The strict lower half of *F* can also be thought of as containing the negative of the multipliers.

Routine `LFTRG` is based on the LINPACK routine `SGEFA`. See Dongarra et al. (1979). The routine `SGEFA` uses partial pivoting.

Comments

1. Workspace may be explicitly provided, if desired, by use of L2TRG/ DL2TRG. The reference is:

   CALL L2TRG (N, A, LDA, FACT, LDFACT, IPVT, WK)

   The additional argument is:

   WK — Work vector of length N used for scaling.

2. Informational error

Type	Code	Description
4	2	The input matrix is singular.

ScaLAPACK Usage Notes

The arguments which differ from the standard version of this routine are:

A0 — MXLDA by MXCOL local matrix containing the local portions of the distributed matrix A. A contains the matrix to be factored. (Input)

FACT0 — MXLDA by MXCOL local matrix containing the local portions of the distributed matrix FACT. FACT contains the *LU* factorization of the matrix A. (Output)

IPVT0 — Local vector of length MXLDA containing the local portions of the distributed vector IPVT. IPVT contains the pivoting information for the *LU* factorization. (Output)

All other arguments are global and are the same as described for the standard version of the routine. In the argument descriptions above, MXLDA and MXCOL can be obtained through a call to SCALAPACK_GETDIM (see *Utilities*) after a call to SCALAPACK_SETUP (see *Utilities*) has been made. See the ScaLAPACK Example below.

Examples

Example 1

A linear system with multiple right-hand sides is solved. Routine LFTRG is called to factor the coefficient matrix. The routine LFSRG is called to compute the two solutions for the two right-hand sides. In this case, the coefficient matrix is assumed to be well-conditioned and correctly scaled. Otherwise, it would be better to call LFCRG to perform the factorization, and LFIRG to compute the solutions.

```
      USE LFTRG_INT
      USE LFSRG_INT
      USE WRRRN_INT
!                                 Declare variables
      PARAMETER  (LDA=3, LDFACT=3, N=3)
```

```
      INTEGER    IPVT(N), J
      REAL       A(LDA,LDA), B(N,2), FACT(LDFACT,LDFACT), X(N,2)
!
!                                Set values for A and B
!
!                                A = (  1.0   3.0   3.0)
!                                    (  1.0   3.0   4.0)
!                                    (  1.0   4.0   3.0)
!
!                                B = (  1.0  10.0)
!                                    (  4.0  14.0)
!                                    ( -1.0   9.0)
!
      DATA A/1.0, 1.0, 1.0, 3.0, 3.0, 4.0, 3.0, 4.0, 3.0/
      DATA B/1.0, 4.0, -1.0, 10.0, 14.0, 9.0/
!
      CALL LFTRG (A,  FACT,  IPVT)
!                                Solve for the two right-hand sides
      DO 10  J=1, 2
         CALL LFSRG (FACT, IPVT, B(:,J), X(:,J))
   10 CONTINUE
!                                Print results
      CALL WRRRN ('X', X)
      END
```

Output

```
         X
        1        2
1  -2.000    1.000
2  -2.000   -1.000
3   3.000    4.000
```

ScaLAPACK Example

A linear system with multiple right-hand sides is solved. Routine LFTRG is called to factor the coefficient matrix. The routine LFSRG is called to compute the two solutions for the two right-hand sides. In this case, the coefficient matrix is assumed to be well-conditioned and correctly scaled. Otherwise, it would be better to call LFCRG to perform the factorization, and LFIRG to compute the solutions. SCALAPACK_MAP and SCALAPACK_UNMAP are IMSL utility routines (see *Chapter 11, "Utilities"*) used to map and unmap arrays to and from the processor grid. They are used here for brevity. DESCINIT is a ScaLAPACK tools routine which initializes the descriptors for the local arrays.

```
      USE MPI_SETUP_INT
      USE LFTRG_INT
      USE LFSRG_INT
      USE WRRRN_INT
      USE SCALAPACK_SUPPORT
      IMPLICIT NONE
      INCLUDE 'mpif.h'
!                                Declare variables
      INTEGER     J, LDA, N, DESCA(9), DESCL(9)
      INTEGER     INFO, MXCOL, MXLDA
      INTEGER, ALLOCATABLE ::     IPVT0(:)
      REAL, ALLOCATABLE ::        A(:,:), B(:,:), X(:,:), X0(:)
      REAL, ALLOCATABLE ::        A0(:,:), FACT0(:,:), B0(:)
      PARAMETER  (LDA=3, N=3)
!                                Set up for MPI
      MP_NPROCS = MP_SETUP()
```

```
      IF(MP_RANK .EQ. 0) THEN
          ALLOCATE (A(LDA,N), B(N,2), X(N,2))
!                                 Set values for A and B
          A(1,:) = (/ 1.0,  3.0,  3.0/)
          A(2,:) = (/ 1.0,  3.0,  4.0/)
          A(3,:) = (/ 1.0,  4.0,  3.0/)
!
          B(1,:) = (/ 1.0, 10.0/)
          B(2,:) = (/ 4.0, 14.0/)
          B(3,:) = (/-1.0, 9.0/)
      ENDIF
!                                  Set up a 1D processor grid and define
!                                  its context id, MP_ICTXT
      CALL SCALAPACK_SETUP(N, N, .TRUE., .TRUE.)
!                                  Get the array descriptor entities MXLDA,
!                                  and MXCOL
      CALL SCALAPACK_GETDIM(N, N, MP_MB, MP_NB, MXLDA, MXCOL)
!                                  Set up the array descriptors
      CALL DESCINIT(DESCA, N, N, MP_MB, MP_NB, 0, 0, MP_ICTXT, MXLDA, INFO)
      CALL DESCINIT(DESCL, N, 1, MP_MB, 1, 0, 0, MP_ICTXT, MXLDA, INFO)
!                                  Allocate space for the local arrays
      ALLOCATE(A0(MXLDA,MXCOL), X0(MXLDA),FACT0(MXLDA,MXCOL), B0(MXLDA), &
               IPVT0(MXLDA))
!                                  Map input arrays to the processor grid
      CALL SCALAPACK_MAP(A, DESCA, A0)
!                                 Call the factorization routine
      CALL LFTRG (A0, FACT0, IPVT0)
!                                 Set up the columns of the B
!                                 matrix one at a time in X0
      DO 10  J=1, 2
         CALL SCALAPACK_MAP(B(:,j), DESCL, B0)
!                                 Solve for the J-th column of X
         CALL LFSRG (FACT0, IPVT0, B0, X0)
         CALL SCALAPACK_UNMAP(X0, DESCL, X(:,J))
   10 CONTINUE
!                                 Print results.
!                                 Only Rank=0 has the solution, X.
      IF(MP_RANK.EQ.0) CALL WRRRN ('X', X)
      IF (MP_RANK .EQ. 0) DEALLOCATE(A, B, X)
      DEALLOCATE(A0, B0, IPVT0, FACT0, X0)
!                                 Exit ScaLAPACK usage
      CALL SCALAPACK_EXIT(MP_ICTXT)
!                                 Shut down MPI
      MP_NPROCS = MP_SETUP('FINAL')
      END
```

Output

```
         X
        1        2
1  -2.000   1.000
2  -2.000  -1.000
3   3.000   4.000
```

LFSRG

more...

more...

Solves a real general system of linear equations given the *LU* factorization of the coefficient matrix.

Required Arguments

FACT — `N` by `N` matrix containing the *LU* factorization of the coefficient matrix `A` as output from routine `LFCRG` or `LFTRG`. (Input)

IPVT — Vector of length `N` containing the pivoting information for the *LU* factorization of `A` as output from subroutine `LFCRG` or `LFTRG`. (Input).

B — Vector of length `N` containing the right-hand side of the linear system. (Input)

X — Vector of length `N` containing the solution to the linear system. (Output)
If `B` is not needed, `B` and `X` can share the same storage locations.

Optional Arguments

N — Number of equations. (Input)
Default: `N` = size (`FACT`, `2`).

LDFACT — Leading dimension of `FACT` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDFACT` = size (`FACT`, `1`).

IPATH — Path indicator. (Input)

`IPATH` = 1 means the system $AX = B$ is solved.

`IPATH` = 2 means the system $A^T X = B$ is solved.

Default: `IPATH` = 1.

FORTRAN 90 Interface

Generic: CALL LFSRG (FACT, IPVT, B, X [, …])

Specific: The specific interface names are S_LFSRG and D_LFSRG.

FORTRAN 77 Interface

Single: CALL LFSRG (N, FACT, LDFACT, IPVT, B, IPATH, X)

Double: The double precision name is DLFSRG.

ScaLAPACK Interface

Generic: CALL LFSRG (FACT0, IPVT0, B0, X0 [, …])

Specific: The specific interface names are S_LFSRG and D_LFSRG.

See the *ScaLAPACK Usage Notes* below for a description of the arguments for distributed computing.

Description

Routine LFSRG computes the solution of a system of linear algebraic equations having a real general coefficient matrix. To compute the solution, the coefficient matrix must first undergo an *LU* factorization. This may be done by calling either LFCRG or LFTRG. The solution to $Ax = b$ is found by solving the triangular systems $Ly = b$ and $Ux = y$. The forward elimination step consists of solving the system $Ly = b$ by applying the same permutations and elimination operations to b that were applied to the columns of A in the factorization routine. The backward substitution step consists of solving the triangular system $Ux = y$ for x.

LFSRG and LFIRG both solve a linear system given its *LU* factorization. LFIRG generally takes more time and produces a more accurate answer than LFSRG. Each iteration of the iterative refinement algorithm used by LFIRG calls LFSRG. The underlying code is based on either LINPACK , LAPACK, or ScaLAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see *Using ScaLAPACK, LAPACK, LINPACK, and EISPACK* in the Introduction section of this manual.

ScaLAPACK Usage Notes

The arguments which differ from the standard version of this routine are:

FACT0 — MXLDA by MXCOL local matrix containing the local portions of the distributed matrix FACT as output from routine LFCRG. FACT contains the *LU* factorization of the matrix A. (Input)

IPVT0 — Local vector of length MXLDA containing the local portions of the distributed vector IPVT. IPVT contains the pivoting information for the *LU* factorization as output from subroutine LFCRG or LFTRG/DLFTRG. (Input)

B0 — Local vector of length MXLDA containing the local portions of the distributed vector B. B contains the right-hand side of the linear system. (Input)

X0 — Local vector of length MXLDA containing the local portions of the distributed vector X. X contains the solution to the linear system. (Output)
If B is not needed, B and X can share the same storage locations.

All other arguments are global and are the same as described for the standard version of the routine. In the argument descriptions above, MXLDA and MXCOL can be obtained through a call to SCALAPACK_GETDIM (see *Utilities*) after a call to SCALAPACK_SETUP (see *Utilities*) has been made. See the ScaLAPACK Example below.

Examples

Example

The inverse is computed for a real general 3 × 3 matrix. The input matrix is assumed to be well-conditioned, hence, LFTRG is used rather than LFCRG.

```
      USE LFSRG_INT
      USE LFTRG_INT
      USE WRRRN_INT
!                                 Declare variables
      PARAMETER  (LDA=3, LDFACT=3, N=3)
      INTEGER    I, IPVT(N), J
      REAL       A(LDA,LDA), AINV(LDA,LDA), FACT(LDFACT,LDFACT), RJ(N)
!
!                                 Set values for A
          A(1,:) = (/ 1.0,  3.0,  3.0/)
          A(2,:) = (/ 1.0,  3.0,  4.0/)
          A(3,:) = (/ 1.0,  4.0,  3.0/)
!
      CALL LFTRG (A, FACT, IPVT)
!                                 Set up the columns of the identity
!                                 matrix one at a time in RJ
      RJ = 0.0E0
      DO 10  J=1, N
         RJ(J) = 1.0
!                                 RJ is the J-th column of the identity
!                                 matrix so the following LFSRG
!                                 reference places the J-th column of
!                                 the inverse of A in the J-th column
!                                 of AINV
         CALL LFSRG (FACT, IPVT, RJ, AINV(:,J))
         RJ(J) = 0.0
   10 CONTINUE
!                                 Print results
      CALL WRRRN ('AINV', AINV)
      END
```

Output

```
           AINV
        1        2        3
1   7.000   -3.000   -3.000
2  -1.000    0.000    1.000
3  -1.000    1.000    0.000
```

ScaLAPACK Example

The inverse of the same 3 × 3 matrix is computed as a distributed example. The input matrix is assumed to be well-conditioned, hence, LFTRG is used rather than LFCRG. LFSRG is called to determine the columns of the inverse. SCALAPACK_MAP and SCALAPACK_UNMAP are IMSL utility routines (see *Chapter 11, “Utilities”*) used to map and unmap arrays to and from the processor grid. They are used here for brevity. DESCINIT is a ScaLAPACK tools routine which initializes the descriptors for the local arrays.

```
      USE MPI_SETUP_INT
      USE LFTRG_INT
      USE UMACH_INT
      USE LFSRG_INT
      USE WRRRN_INT
      USE SCALAPACK_SUPPORT
      IMPLICIT NONE
      INCLUDE 'mpif.h'
!                                 Declare variables
      INTEGER     J, LDA, N, DESCA(9), DESCL(9)
      INTEGER     INFO, MXCOL, MXLDA
      INTEGER, ALLOCATABLE ::     IPVT0(:)
      REAL, ALLOCATABLE ::        A(:,:), AINV(:,:), X0(:), RJ(:)
      REAL, ALLOCATABLE ::        A0(:,:), FACT0(:,:), RJ0(:)
      PARAMETER  (LDA=3, N=3)
!                                 Set up for MPI
      MP_NPROCS = MP_SETUP()
      IF(MP_RANK .EQ. 0) THEN
          ALLOCATE (A(LDA,N), AINV(LDA,N))
!                                 Set values for A
          A(1,:) = (/ 1.0,  3.0,  3.0/)
          A(2,:) = (/ 1.0,  3.0,  4.0/)
          A(3,:) = (/ 1.0,  4.0,  3.0/)
      ENDIF
!                                  Set up a 1D processor grid and define
!                                  its context id, MP_ICTXT
      CALL SCALAPACK_SETUP(N, N, .TRUE., .TRUE.)
!                                  Get the array descriptor entities MXLDA,
!                                  and MXCOL
      CALL SCALAPACK_GETDIM(N, N, MP_MB, MP_NB, MXLDA, MXCOL)
!                                  Set up the array descriptors
      CALL DESCINIT(DESCA, N, N, MP_MB, MP_NB, 0, 0, MP_ICTXT, MXLDA, INFO)
      CALL DESCINIT(DESCL, N, 1, MP_MB, 1, 0, 0, MP_ICTXT, MXLDA, INFO)
!                                  Allocate space for the local arrays
      ALLOCATE(A0(MXLDA,MXCOL), X0(MXLDA),FACT0(MXLDA,MXCOL), RJ(N), &
               RJ0(MXLDA), IPVT0(MXLDA))
!                                  Map input arrays to the processor grid
      CALL SCALAPACK_MAP(A, DESCA, A0)
!                                  Call the factorization routine
      CALL LFTRG (A0, FACT0, IPVT0)
!                                 Set up the columns of the identity
!                                 matrix one at a time in RJ
      RJ = 0.0E0
      DO 10  J=1, N
         RJ(J) = 1.0
```

```
          CALL SCALAPACK_MAP(RJ, DESCL, RJ0)
!                                 RJ is the J-th column of the identity
!                                 matrix so the following LFIRG
!                                 reference computes the J-th column of
!                                 the inverse of A
          CALL LFSRG (FACT0, IPVT0, RJ0, X0)
          RJ(J) = 0.0
          CALL SCALAPACK_UNMAP(X0, DESCL, AINV(:,J))
   10 CONTINUE
!                                 Print results
!                                 Only Rank=0 has the solution, AINV.
      IF(MP_RANK.EQ.0) CALL WRRRN ('AINV', AINV)
      IF (MP_RANK .EQ. 0) DEALLOCATE(A, AINV)
      DEALLOCATE(A0, IPVT0, FACT0, RJ, RJ0, X0)
!                                Exit ScaLAPACK usage
      CALL SCALAPACK_EXIT(MP_ICTXT)

!                                Shut down MPI
      MP_NPROCS = MP_SETUP('FINAL')
      END
```

Output

```
            AINV
          1        2        3
1    7.000   -3.000   -3.000
2   -1.000    0.000    1.000
3   -1.000    1.000    0.000
```

LFIRG

more...

more...

Uses iterative refinement to improve the solution of a real general system of linear equations.

Required Arguments

A — `N` by `N` matrix containing the coefficient matrix of the linear system. (Input)

FACT — `N` by `N` matrix containing the *LU* factorization of the coefficient matrix `A` as output from routine `LFCRG`/`DLFCRG` or `LFTRG`/`DLFTRG`. (Input).

IPVT — Vector of length `N` containing the pivoting information for the *LU* factorization of `A` as output from routine `LFCRG`/`DLFCRG` or `LFTRG`/`DLFTRG`. (Input)

B — Vector of length `N` containing the right-hand side of the linear system. (Input).

X — Vector of length `N` containing the solution to the linear system. (Output)

RES — Vector of length `N` containing the final correction at the improved solution. (Output)

Optional Arguments

N — Number of equations. (Input)
Default: `N` = size (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = size (`A`,1).

LDFACT — Leading dimension of `FACT` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDFACT` = size (`FACT`,1).

IPATH — Path indicator. (Input)

`IPATH` = 1 means the system $A * X = B$ is solved.

IPATH = 2 means the system $A^T X = B$ is solved.

Default: IPATH = 1.

FORTRAN 90 Interface

Generic: CALL LFIRG (A, FACT, IPVT, B, X, RES [, …])

Specific: The specific interface names are S_LFIRG and D_LFIRG.

FORTRAN 77 Interface

Single: CALL LFIRG (N, A, LDA, FACT, LDFACT, IPVT, B, IPATH, X, RES)

Double: The double precision name is DLFIRG.

ScaLAPACK Interface

Generic: CALL LFIRG (A0, FACT0, IPVT0, B0, X0, RES0 [, …])

Specific: The specific interface names are S_LFIRG and D_LFIRG.

See the *ScaLAPACK Usage Notes* below for a description of the arguments for distributed computing.

Description

Routine LFIRG computes the solution of a system of linear algebraic equations having a real general coefficient matrix. Iterative refinement is performed on the solution vector to improve the accuracy. Usually almost all of the digits in the solution are accurate, even if the matrix is somewhat ill-conditioned. The underlying code is based on either LINPACK , LAPACK, or ScaLAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see "*Using ScaLAPACK, LAPACK, LINPACK, and EISPACK*" in the *Introduction* section of this manual.

To compute the solution, the coefficient matrix must first undergo an *LU* factorization. This may be done by calling either LFCRG or LFTRG.

Iterative refinement fails only if the matrix is very ill-conditioned.

Routines LFIRG and LFSRG both solve a linear system given its *LU* factorization. LFIRG generally takes more time and produces a more accurate answer than LFSRG. Each iteration of the iterative refinement algorithm used by LFIRG calls LFSRG.

Comments

Informational error

Type	Code	Description
3	2	The input matrix is too ill-conditioned for iterative refinement to be effective.

ScaLAPACK Usage Notes

The arguments which differ from the standard version of this routine are:

A0 — MXLDA by MXCOL local matrix containing the local portions of the distributed matrix A. A contains the coefficient matrix of the linear system. (Input)

FACT0 — MXLDA by MXCOL local matrix containing the local portions of the distributed matrix FACT as output from routine LFCRG or LFTRG. FACT contains the *LU* factorization of the matrix A. (Input)

IPVT0 — Local vector of length MXLDA containing the local portions of the distributed vector IPVT. IPVT contains the pivoting information for the *LU* factorization as output from subroutine LFCRG or LFTRG. (Input)

B0 — Local vector of length MXLDA containing the local portions of the distributed vector B. B contains the right-hand side of the linear system. (Input)

X0 — Local vector of length MXLDA containing the local portions of the distributed vector X. X contains the solution to the linear system. (Output)
If B is not needed, B and X can share the same storage locations.

RES0 — Local vector of length MXLDA containing the local portions of the distributed vector RES. RES contains the final correction at the improved solution to the linear system. (Output)

All other arguments are global and are the same as described for the standard version of the routine. In the argument descriptions above, MXLDA and MXCOL can be obtained through a call to SCALAPACK_GETDIM (see *Utilities*) after a call to SCALAPACK_SETUP (see *Utilities*) has been made. See the *ScaLAPACK Example* below.

Examples

Example

A set of linear systems is solved successively. The right-hand-side vector is perturbed after solving the system each of the first two times by adding 0.5 to the second element.

```
      USE LFIRG_INT
```

```
      USE LFCRG_INT
      USE UMACH_INT
      USE WRRRN_INT
!                                 Declare variables
      PARAMETER  (LDA=3, LDFACT=3, N=3)
      INTEGER    IPVT(N), NOUT
      REAL       A(LDA,LDA), B(N), FACT(LDFACT,LDFACT), RCOND, RES(N), X(N)
!
!                                 Set values for A and B
!
!                                 A = (  1.0   3.0   3.0)
!                                     (  1.0   3.0   4.0)
!                                     (  1.0   4.0   3.0)
!
!                                 B = ( -0.5  -1.0   1.5)
!
      DATA A/1.0, 1.0, 1.0, 3.0, 3.0, 4.0, 3.0, 4.0, 3.0/
      DATA B/-0.5, -1.0, 1.5/
!
      CALL LFCRG (A, FACT, IPVT, RCOND)
!                                 Print the reciprocal condition number
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) RCOND, 1.0E0/RCOND
!                                 Solve the three systems
      DO 10  J=1, 3
         CALL LFIRG (A, FACT, IPVT, B, X, RES)
!                                 Print results
         CALL WRRRN ('X', X, 1, N, 1)
!                                 Perturb B by adding 0.5 to B(2)
         B(2) = B(2) + 0.5

   10 CONTINUE
!
99999 FORMAT ('  RCOND = ',F5.3,/,'  L1 Condition number = ',F6.3)
      END
```

Output

```
RCOND < 0.02
L1 Condition number < 100.0
            X
     1        2        3
-5.000    2.000   -0.500
            X
     1        2        3
-6.500    2.000    0.000

            X
     1        2        3
-8.000    2.000    0.500
```

ScaLAPACK Example

The same set of linear systems is solved successively as a distributed example. The right-hand side vector is perturbed after solving the system each of the first two times by adding 0.5 to the second element. `SCALAPACK_MAP` and `SCALAPACK_UNMAP` are IMSL utility routines (see *Chapter 11, "Utilities"*) used to map and unmap arrays to and from the processor grid. They are used here for brevity. `DESCINIT` is a ScaLAPACK tools routine which initializes the descriptors for the local arrays.

```
      USE MPI_SETUP_INT
```

```
      USE LFIRG_INT
      USE UMACH_INT
      USE LFCRG_INT
      USE WRRRN_INT
      USE SCALAPACK_SUPPORT
      IMPLICIT NONE
      INCLUDE 'mpif.h'
!                                 Declare variables
      INTEGER     J, LDA, N, DESCA(9), DESCL(9)
      INTEGER     INFO, MXCOL, MXLDA, NOUT
      INTEGER, ALLOCATABLE ::     IPVT0(:)
      REAL, ALLOCATABLE ::        A(:,:), B(:), X(:), X0(:), AINV(:,:)
      REAL, ALLOCATABLE ::        A0(:,:), FACT0(:,:), RES0(:), B0(:)
      REAL        RCOND
      PARAMETER  (LDA=3, N=3)
!                                 Set up for MPI
      MP_NPROCS = MP_SETUP()
      IF(MP_RANK .EQ. 0) THEN
          ALLOCATE (A(LDA,N), AINV(LDA,N), B(N), X(N))
!                                 Set values for A and B
          A(1,:) = (/ 1.0,  3.0,  3.0/)
          A(2,:) = (/ 1.0,  3.0,  4.0/)
          A(3,:) = (/ 1.0,  4.0,  3.0/)
!
          B(:) =   (/-0.5, -1.0,  1.5/)
      ENDIF
!                                  Set up a 1D processor grid and define
!                                  its context id, MP_ICTXT
      CALL SCALAPACK_SETUP(N, N, .TRUE., .TRUE.)
!                                  Get the array descriptor entities MXLDA,
!                                  and MXCOL
      CALL SCALAPACK_GETDIM(N, N, MP_MB, MP_NB, MXLDA, MXCOL)
!                                  Set up the array descriptors
      CALL DESCINIT(DESCA, N, N, MP_MB, MP_NB, 0, 0, MP_ICTXT, MXLDA, INFO)
      CALL DESCINIT(DESCL, N, 1, MP_MB, 1, 0, 0, MP_ICTXT, MXLDA, INFO)
!                                  Allocate space for the local arrays
      ALLOCATE(A0(MXLDA,MXCOL), X0(MXLDA),FACT0(MXLDA,MXCOL), &
                B0(MXLDA), RES0(MXLDA), IPVT0(MXLDA))
!                                  Map input arrays to the processor grid
      CALL SCALAPACK_MAP(A, DESCA, A0)
!                                  Call the factorization routine
      CALL LFCRG (A0, FACT0, IPVT0, RCOND)
!                                 Print the reciprocal condition number
!                                 and the L1 condition number
      IF(MP_RANK .EQ. 0) THEN
         CALL UMACH (2, NOUT)
         WRITE (NOUT,99998) RCOND, 1.0E0/RCOND
      ENDIF
!                                 Solve the three systems
!                                 one at a time in X
      DO 10  J=1, 3
         CALL SCALAPACK_MAP(B, DESCL, B0)
         CALL LFIRG (A0, FACT0, IPVT0, B0, X0, RES0)
         CALL SCALAPACK_UNMAP(X0, DESCL, X)
!                                 Print results
!                                 Only Rank=0 has the solution, X.
         IF(MP_RANK.EQ.0) CALL WRRRN ('X', X, 1, N, 1)
         IF(MP_RANK.EQ.0) B(2) = B(2) + 0.5
   10 CONTINUE
      IF (MP_RANK .EQ. 0) DEALLOCATE(A, AINV, B)
      DEALLOCATE(A0, B0, IPVT0, FACT0, RES0, X0)
!                                 Exit ScaLAPACK usage
      CALL SCALAPACK_EXIT(MP_ICTXT)
!                                 Shut down MPI
      MP_NPROCS = MP_SETUP('FINAL')
99998 FORMAT ('  RCOND = ',F5.3,/,'  L1 Condition number = ',F6.3)
```

```
        END
```

Output

```
RCOND < 0.02
L1 Condition number < 100.0

            X
     1       2       3
-5.000   2.000  -0.500
            X
     1       2       3
-6.500   2.000   0.000

            X
     1       2       3
-8.000   2.000   0.500
```

LFDRG

Computes the determinant of a real general matrix given the *LU* factorization *of the matrix*.

Required Arguments

FACT — N by N matrix containing the *LU* factorization of the matrix A as output from routine LFTRG/DLFTRG or LFCRG/DLFCRG. (Input)

IPVT — Vector of length N containing the pivoting information for the *LU* factorization as output from routine LFTRG/DLFTRG or LFCRG/DLFCRG. (Input).

DET1 — Scalar containing the mantissa of the determinant. (Output)
The value DET1 is normalized so that 1.0 ≤ |DET1| < 10.0 or DET1 = 0.0.

DET2 — Scalar containing the exponent of the determinant. (Output)
The determinant is returned in the form det(*A*) = DET1 * 10^{DET2}.

Optional Arguments

N — Order of the matrix. (Input)
Default: N = size (FACT,2).

LDFACT — Leading dimension of FACT exactly as specified in the dimension statement of the calling program. (Input)
Default: LDFACT = size (FACT,1).

FORTRAN 90 Interface

Generic: CALL LFDRG (FACT, IPVT, DET1, DET2 [, …])

Specific: The specific interface names are S_LFDRG and D_LFDRG.

FORTRAN 77 Interface

Single: CALL LFDRG (N, FACT, LDFACT, IPVT, DET1, DET2)

Double: The double precision name is DLFDRG.

Description

Routine `LFDRG` computes the determinant of a real general coefficient matrix. To compute the determinant, the coefficient matrix must first undergo an *LU* factorization. This may be done by calling either `LFCRG` or `LFTRG`. The formula det A = det L det U is used to compute the determinant. Since the determinant of a triangular matrix is the product of the diagonal elements

$$\det U = \prod_{i=1}^{N} U_{ii}$$

(The matrix U is stored in the upper triangle of `FACT`.) Since L is the product of triangular matrices with unit diagonals and of permutation matrices, det $L = (-1)^k$ where k is the number of pivoting interchanges.

Routine `LFDRG` is based on the LINPACK routine `SGEDI`; see Dongarra et al. (1979)

Example

The determinant is computed for a real general 3 × 3 matrix.

```
      USE LFDRG_INT
      USE LFTRG_INT
      USE UMACH_INT
!                                 Declare variables
      PARAMETER  (LDA=3, LDFACT=3, N=3)
      INTEGER    IPVT(N), NOUT
      REAL       A(LDA,LDA), DET1, DET2, FACT(LDFACT,LDFACT)
!
!                                 Set values for A
!                                 A = ( 33.0  16.0  72.0)
!                                     (-24.0 -10.0 -57.0)
!                                     ( 18.0 -11.0   7.0)
!
      DATA A/33.0, -24.0, 18.0, 16.0, -10.0, -11.0, 72.0, -57.0, 7.0/
!
      CALL LFTRG (A, FACT, IPVT)
!                                 Compute the determinant
      CALL LFDRG (FACT, IPVT, DET1, DET2)
!                                 Print the results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) DET1, DET2
!
99999 FORMAT (' The determinant of A is ', F6.3, ' * 10**', F2.0)
      END
```

Output

```
The determinant of A is -4.761 * 10**3.
```

LINRG

more...

more...

Computes the inverse of a real general matrix.

Required Arguments

A — N by N matrix containing the matrix to be inverted. (Input)

AINV — N by N matrix containing the inverse of A. (Output)
If A is not needed, A and AINV can share the same storage locations.

Optional Arguments

N — Order of the matrix A. (Input)
Default: N = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

LDAINV — Leading dimension of AINV exactly as specified in the dimension statement of the calling program. (Input)
Default: LDAINV = size (AINV,1).

FORTRAN 90 Interface

Generic: CALL LINRG (A, AINV [, …])

Specific: The specific interface names are S_LINRG and D_LINRG.

FORTRAN 77 Interface

Single: CALL LINRG (N, A, LDA, AINV, LDAINV)

Double: The double precision name is DLINRG.

ScaLAPACK Interface

Generic: CALL LINRG (A0, AINV0 [, …])

Specific: The specific interface names are S_LINRG and D_LINRG.

See the ScaLAPACK Usage Notes below for a description of the arguments for distributed computing.

Description

Routine LINRG computes the inverse of a real general matrix. The underlying code is based on either LINPACK , LAPACK, or ScaLAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see "*Using ScaLAPACK, LAPACK, LINPACK, and EISPACK*" in the *Introduction* section of this manual. LINRG first uses the routine LFCRG to compute an LU factorization of the coefficient matrix and to estimate the condition number of the matrix. Routine LFCRG computes U and the information needed to compute L^{-1}. LINRT is then used to compute U^{-1}. Finally, A^{-1} is computed using $A^{-1} = U^{-1}L^{-1}$.

The routine LINRG fails if U, the upper triangular part of the factorization, has a zero diagonal element or if the iterative refinement algorithm fails to converge. This error occurs only if A is singular or very close to a singular matrix.

If the estimated condition number is greater than $1/\varepsilon$ (where ε is machine precision), a warning error is issued. This indicates that very small changes in A can cause very large changes in A^{-1}.

Comments

1. Workspace may be explicitly provided, if desired, by use of L2NRG/DL2NRG. The reference is:

   CALL L2NRG (N, A, LDA, AINV, LDAINV, WK, IWK)

   The additional arguments are as follows:

   WK — Work vector of length N + N(N − 1)/2.

   IWK — Integer work vector of length N.

2. Informational errors

Type	Code	Description
3	1	The input matrix is too ill-conditioned. The inverse might not be accurate.
4	2	The input matrix is singular.

ScaLAPACK Usage Notes

The arguments which differ from the standard version of this routine are:

A0 — MXLDA by MXCOL local matrix containing the local portions of the distributed matrix A. A contains the matrix to be inverted. (Input)

AINV0 — MXLDA by MXCOL local matrix containing the local portions of the distributed matrix AINV. AINV contains the inverse of the matrix A. (Output)
If A is not needed, A and AINV can share the same storage locations.

All other arguments are global and are the same as described for the standard version of the routine. In the argument descriptions above, MXLDA and MXCOL can be obtained through a call to SCALAPACK_GETDIM (see *Utilities*) after a call to SCALAPACK_SETUP (see *Utilities*) has been made. See the ScaLAPACK Example below.

Examples

Example

The inverse is computed for a real general 3 × 3 matrix.

```
      USE LINRG_INT
      USE WRRRN_INT
!                                 Declare variables
      PARAMETER  (LDA=3, LDAINV=3)
      INTEGER    I, J, NOUT
      REAL       A(LDA,LDA), AINV(LDAINV,LDAINV)
!
!                                 Set values for A
!                                 A = (  1.0   3.0   3.0)
!                                     (  1.0   3.0   4.0)
!                                     (  1.0   4.0   3.0)
!
      DATA A/1.0, 1.0, 1.0, 3.0, 3.0, 4.0, 3.0, 4.0, 3.0/
!
      CALL LINRG (A, AINV)
!                                 Print results
      CALL WRRRN ('AINV', AINV)
      END
```

Output

```
            AINV
        1        2        3
1   7.000   -3.000   -3.000
2  -1.000    0.000    1.000
3  -1.000    1.000    0.000
```

ScaLAPACK Example

The inverse of the same 3 × 3 matrix is computed as a distributed example. SCALAPACK_MAP and SCALAPACK_UNMAP are IMSL utility routines (see *Chapter 11, "Utilities"*) used to map and unmap arrays to and from the processor grid. They are used here for brevity. DESCINIT is a ScaLAPACK tools routine which initializes the descriptors for the local arrays.

```
      USE MPI_SETUP_INT
      USE LINRG_INT
      USE WRRRN_INT
      USE SCALAPACK_SUPPORT
      IMPLICIT NONE
      INCLUDE 'mpif.h'
!                                  Declare variables
      INTEGER     LDA, LDAINV, N, DESCA(9)
       INTEGER     INFO, MXCOL, MXLDA
      REAL, ALLOCATABLE ::        A(:,:), AINV(:,:)
      REAL, ALLOCATABLE ::        A0(:,:), AINV0(:,:)
      PARAMETER  (LDA=3, LDAINV=3, N=3)
!                                  Set up for MPI
      MP_NPROCS = MP_SETUP()
      IF(MP_RANK .EQ. 0) THEN
          ALLOCATE (A(LDA,N), AINV(LDAINV,N))
!                                  Set values for A
          A(1,:) = (/ 1.0,  3.0,  3.0/)
          A(2,:) = (/ 1.0,  3.0,  4.0/)
          A(3,:) = (/ 1.0,  4.0,  3.0/)
      ENDIF
!                                   Set up a 1D processor grid and define
!                                   its context ID, MP_ICTXT
      CALL SCALAPACK_SETUP(N, N, .TRUE., .TRUE.)
!                                   Get the array descriptor entities MXLDA,
!                                   and MXCOL
      CALL SCALAPACK_GETDIM(N, N, MP_MB, MP_NB, MXLDA, MXCOL)
!                                   Set up the array descriptors
      CALL DESCINIT(DESCA, N, N, MP_MB, MP_NB, 0, 0, MP_ICTXT, MXLDA, INFO)
!                    Allocate space for the local arrays
      ALLOCATE(A0(MXLDA,MXCOL), AINV0(MXLDA,MXCOL))
!                                   Map input arrays to the processor grid
      CALL SCALAPACK_MAP(A, DESCA, A0)
!                                   Get the inverse
      CALL LINRG (A0, AINV0)
!                                   Unmap the results from the distributed
!                                   arrays back to a non-distributed array.
!                                   After the unmap, only Rank=0 has the full
!                                   array.
      CALL SCALAPACK_UNMAP(AINV0, DESCA, AINV)
!                                   Print results
!                                   Only Rank=0 has the solution, AINV.
      IF(MP_RANK.EQ.0) CALL WRRRN ('AINV', AINV)
      IF (MP_RANK .EQ. 0) DEALLOCATE(A, AINV)
      DEALLOCATE(A0, AINV0)
!                                   Exit ScaLAPACK usage
      CALL SCALAPACK_EXIT(MP_ICTXT)
!                                   Shut down MPI
      MP_NPROCS = MP_SETUP('FINAL')
      END
```

Output

```
          AINV
        1        2        3
```

```
 1   7.000  -3.000  -3.000
 2  -1.000   0.000   1.000
 3  -1.000   1.000   0.000
```

LSACG

more...

more...

Solves a complex general system of linear equations with iterative refinement.

Required Arguments

A — Complex `N` by `N` matrix containing the coefficients of the linear system. (Input)

B — Complex vector of length `N` containing the right-hand side of the linear system. (Input)

X — Complex vector of length `N` containing the solution to the linear system. (Output)

Optional Arguments

N — Number of equations. (Input)
Default: `N` = size (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = size (`A`,1).

IPATH — Path indicator. (Input)
`IPATH` = 1 means the system $AX = B$ is solved.
`IPATH` = 2 means the system $A^H X = B$ is solved.
Default: `IPATH` = 1

FORTRAN 90 Interface

Generic: `CALL LSACG (A, B, X [, …])`

Specific: The specific interface names are `S_LSACG` and `D_LSACG`.

FORTRAN 77 Interface

Single: CALL LSACG (N, A, LDA, B, IPATH, X)

Double: The double precision name is DLSACG.

ScaLAPACK Interface

Generic: CALL LSACG (A0, B0, X0 [, …])

Specific: The specific interface names are S_LSACG and D_LSACG.

See the *ScaLAPACK Usage Notes* below for a description of the arguments for distributed computing.

Description

Routine LSACG solves a system of linear algebraic equations with a complex general coefficient matrix. The underlying code is based on either LINPACK , LAPACK, or ScaLAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see *Using ScaLAPACK, LAPACK, LINPACK, and EISPACK* in the Introduction section of this manual. LSACG first uses the routine LFCCG to compute an *LU* factorization of the coefficient matrix and to estimate the condition number of the matrix. The solution of the linear system is then found using the iterative refinement routine LFICG.

LSACG fails if *U*, the upper triangular part of the factorization, has a zero diagonal element or if the iterative refinement algorithm fails to converge. These errors occur only if *A* is singular or very close to a singular matrix.

If the estimated condition number is greater than $1/\varepsilon$ (where ε is machine precision), a warning error is issued. This indicates that very small changes in *A* can cause very large changes in the solution *x*. Iterative refinement can sometimes find the solution to such a system. LSACG solves the problem that is represented in the computer; however, this problem may differ from the problem whose solution is desired.

Comments

1. Workspace may be explicitly provided, if desired, by use of L2ACG/DL2ACG. The reference is:

   CALL L2ACG (N, A, LDA, B, IPATH, X, FACT, IPVT, WK)

   The additional arguments are as follows:

   FACT — Complex work vector of length N^2 containing the *LU* factorization of A on output.

   IPVT — Integer work vector of length N containing the pivoting information for the *LU* factorization of A on output.

   WK — Complex work vector of length N.

2. Informational errors

Type	Code	Description
3	1	The input matrix is too ill-conditioned. The solution might not be accurate.
4	2	The input matrix is singular.

3. *Integer Options* with *Chapter 11, Options Manager*

16 This option uses four values to solve memory bank conflict (access inefficiency) problems. In routine L2ACG the leading dimension of FACT is increased by IVAL(3) when N is a multiple of IVAL(4). The values IVAL(3) and IVAL(4) are temporarily replaced by IVAL(1) and IVAL(2); respectively, in LSACG. Additional memory allocation for FACT and option value restoration are done automatically in LSACG. Users directly calling L2ACG can allocate additional space for FACT and set IVAL(3) and IVAL(4) so that memory bank conflicts no longer cause inefficiencies. There is no requirement that users change existing applications that use LSACG or L2ACG. Default values for the option are IVAL(*) = 1, 16, 0, 1.

17 This option has two values that determine if the L_1 condition number is to be computed. Routine LSACG temporarily replaces IVAL(2) by IVAL(1). The routine L2CCG computes the condition number if IVAL(2) = 2. Otherwise L2CCG skips this computation. LSACG restores the option. Default values for the option are IVAL(*) = 1, 2.

ScaLAPACK Usage Notes

The arguments which differ from the standard version of this routine are:

A0 — MXLDA by MXCOL complex local matrix containing the local portions of the distributed matrix A. A contains the coefficients of the linear system. (Input)

B0 — Complex local vector of length MXLDA containing the local portions of the distributed vector B. B contains the right-hand side of the linear system. (Input)

X0 — Complex local vector of length MXLDA containing the local portions of the distributed vector X. X contains the solution to the linear system. (Output)

All other arguments are global and are the same as described for the standard version of the routine. In the argument descriptions above, MXLDA and MXCOL can be obtained through a call to SCALAPACK_GETDIM (see *Utilities*) after a call to SCALAPACK_SETUP (see *Utilities*) has been made. See the *ScaLAPACK Example* below.

Examples

Example 1

A system of three linear equations is solved. The coefficient matrix has complex general form and the right-hand-side vector *b* has three elements.

```
      USE LSACG_INT
      USE WRCRN_INT
!                                 Declare variables
      PARAMETER  (LDA=3, N=3)
      COMPLEX    A(LDA,LDA), B(N), X(N)
!                                 Set values for  A and B
!
!                                 A = ( 3.0-2.0i  2.0+4.0i  0.0-3.0i)
!                                     ( 1.0+1.0i  2.0-6.0i  1.0+2.0i)
!                                     ( 4.0+0.0i -5.0+1.0i  3.0-2.0i)
!
!                                 B = (10.0+5.0i  6.0-7.0i -1.0+2.0i)
!
      DATA A/(3.0,-2.0), (1.0,1.0),  (4.0,0.0), (2.0,4.0), (2.0,-6.0), &
             (-5.0,1.0), (0.0,-3.0), (1.0,2.0), (3.0,-2.0)/
      DATA B/(10.0,5.0), (6.0,-7.0), (-1.0,2.0)/
!                                 Solve AX = B     (IPATH = 1)
      CALL LSACG (A, B, X)
!                                 Print results
      CALL WRCRN ('X', X, 1, N, 1)
      END
```

Output

```
                        X
              1                 2                 3
( 1.000,-1.000)   ( 2.000, 1.000)   ( 0.000, 3.000)
```

ScaLAPACK Example

The same system of three linear equations is solved as a distributed computing example. The coefficient matrix has complex general form and the right-hand-side vector *b* has three elements. `SCALAPACK_MAP` and `SCALAPACK_UNMAP` are IMSL utility routines (see *Chapter 11, "Utilities"*) used to map and unmap arrays to and from the processor grid. They are used here for brevity. `DESCINIT` is a ScaLAPACK tools routine which initializes the descriptors for the local arrays.

```
      USE MPI_SETUP_INT
      USE LSACG_INT
      USE WRCRN_INT
      USE SCALAPACK_SUPPORT
      IMPLICIT NONE
      INCLUDE 'mpif.h'
!                                 Declare variables
      INTEGER    LDA, N, DESCA(9), DESCX(9)
      INTEGER       INFO, MXCOL, MXLDA
      COMPLEX, ALLOCATABLE ::       A(:,:), B(:), X(:)
      COMPLEX, ALLOCATABLE ::       A0(:,:), B0(:), X0(:)
      PARAMETER  (LDA=3, N=3)
!                                 Set up for MPI
```

```
      MP_NPROCS = MP_SETUP()
      IF(MP_RANK .EQ. 0) THEN
          ALLOCATE (A(LDA,N), B(N), X(N))
!                                Set values for A and B
          A(1,:) = (/ (3.0, -2.0), (2.0,  4.0), (0.0, -3.0)/)
          A(2,:) = (/ (1.0,  1.0), (2.0, -6.0), (1.0,  2.0)/)
          A(3,:) = (/ (4.0,  0.0), (-5.0, 1.0), (3.0, -2.0)/)
!
          B = (/(10.0, 5.0), (6.0, -7.0), (-1.0, 2.0)/)
      ENDIF
!                                 Set up a 1D processor grid and define
!                                 its context ID, MP_ICTXT
      CALL SCALAPACK_SETUP(N, N, .TRUE., .TRUE.)
!                                 Get the array descriptor entities MXLDA,
!                                 and MXCOL
      CALL SCALAPACK_GETDIM(N, N, MP_MB, MP_NB, MXLDA, MXCOL)
!                                 Set up the array descriptors
      CALL DESCINIT(DESCA, N, N, MP_MB, MP_NB, 0, 0, MP_ICTXT, MXLDA, INFO)
      CALL DESCINIT(DESCX, N, 1, MP_MB, 1, 0, 0, MP_ICTXT, MXLDA, INFO)
!                                 Allocate space for the local arrays
      ALLOCATE (A0(MXLDA,MXCOL), B0(MXLDA), X0(MXLDA))
!                                Map input arrays to the processor grid
      CALL SCALAPACK_MAP(A, DESCA, A0)
      CALL SCALAPACK_MAP(B, DESCX, B0)
!                                Solve the system of equations
      CALL LSACG (A0, B0, X0)
!                                Unmap the results from the distributed
!                                arrays back to a non-distributed array.
!                                After the unmap, only Rank=0 has the full
!                                array.
      CALL SCALAPACK_UNMAP(X0, DESCX, X)
!                               Print results
!                               Only Rank=0 has the solution, X.
      IF(MP_RANK .EQ. 0)CALL WRCRN ('X', X, 1, N, 1)
      IF (MP_RANK .EQ. 0) DEALLOCATE(A, B, X)
      DEALLOCATE(A0, B0, X0)
!                               Exit ScaLAPACK usage
      CALL SCALAPACK_EXIT(MP_ICTXT)
!                               Shut down MPI
      MP_NPROCS = MP_SETUP('FINAL')
      END
```

Output

```
                     X
             1                 2                 3
( 1.000,-1.000)  ( 2.000, 1.000)  ( 0.000, 3.000)
```

LSLCG

more...

more...

Solves a complex general system of linear equations without iterative refinement.

Required Arguments

A — Complex `N` by `N` matrix containing the coefficients of the linear system. (Input)

B — Complex vector of length `N` containing the right-hand side of the linear system. (Input)

X — Complex vector of length `N` containing the solution to the linear system. (Output)
If `B` is not needed, `B` and `X` can share the same storage locations)

Optional Arguments

N — Number of equations. (Input)
Default: `N` = size (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = size (`A`,1).

IPATH — Path indicator. (Input)
`IPATH` = 1 means the system ***AX*** = ***B*** is solved.

`IPATH` = 2 means the system ***AHX*** = ***B*** is solved.

Default: `IPATH` = 1

FORTRAN 90 Interface

Generic: `CALL LSLCG (A, B, X [, …])`

Specific: The specific interface names are `S_LSLCG` and `D_LSLCG`.

FORTRAN 77 Interface

Single: `CALL LSLCG (N, A, LDA, B, IPATH, X)`

Double: The double precision name is `DLSLCG`.

ScaLAPACK Interface

Generic: `CALL LSLCG (A0, B0, X0 [, …])`

Specific: The specific interface names are `S_LSLCG` and `D_LSLCG`.

See the *ScaLAPACK Usage Notes* below for a description of the arguments for distributed computing.

Description

Routine `LSLCG` solves a system of linear algebraic equations with a complex general coefficient matrix. The underlying code is based on either LINPACK , LAPACK, or ScaLAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see *Using ScaLAPACK, LAPACK, LINPACK, and EISPACK* in the Introduction section of this manual. `LSLCG` first uses the routine `LFCCG` to compute an *LU* factorization of the coefficient matrix and to estimate the condition number of the matrix. The solution of the linear system is then found using `LFSCG`.

`LSLCG` fails if *U*, the upper triangular part of the factorization, has a zero diagonal element. This occurs only if *A* either is a singular matrix or is very close to a singular matrix.

If the estimated condition number is greater than $1/\varepsilon$ (where ε is machine precision), a warning error is issued. This indicates that very small changes in *A* can cause very large changes in the solution *x*. If the coefficient matrix is ill-conditioned or poorly scaled, it is recommended that `LSACG` be used.

Comments

1. Workspace may be explicitly provided, if desired, by use of `L2LCG/DL2LCG`. The reference is:

   `CALL L2LCG (N, A, LDA, B, IPATH, X, FACT, IPVT, WK)`

   The additional arguments are as follows:

   FACT — `N` × `N` work array containing the *LU* factorization of A on output. If `A` is not needed, `A` and `FACT` can share the same storage locations.

   IPVT — Integer work vector of length `N` containing the pivoting information for the *LU* factorization of A on output.

   WK — Complex work vector of length `N`.

2. Informational errors

Type	Code	Description
3	1	The input matrix is too ill-conditioned. The solution might not be accurate.
4	2	The input matrix is singular.

3. *Integer Options* with *Chapter 11, Options Manager*

16 This option uses four values to solve memory bank conflict (access inefficiency) problems. In routine L2LCG the leading dimension of FACT is increased by IVAL(3) when N is a multiple of IVAL(4). The values IVAL(3) and IVAL(4) are temporarily replaced by IVAL(1) and IVAL(2); respectively, in LSLCG. Additional memory allocation for FACT and option value restoration are done automatically in LSLCG. Users directly calling L2LCG can allocate additional space for FACT and set IVAL(3) and IVAL(4) so that memory bank conflicts no longer cause inefficiencies. There is no requirement that users change existing applications that use LSLCG or L2LCG. Default values for the option are IVAL(*) = 1, 16, 0, 1.

17 This option has two values that determine if the L_1 condition number is to be computed. Routine LSLCG temporarily replaces IVAL(2) by IVAL(1). The routine L2CCG computes the condition number if IVAL(2) = 2. Otherwise L2CCG skips this computation. LSLCG restores the option. Default values for the option are IVAL(*) = 1, 2.

ScaLAPACK Usage Notes

The arguments which differ from the standard version of this routine are:

A0 — MXLDA by MXCOL complex local matrix containing the local portions of the distributed matrix A. A contains the coefficients of the linear system. (Input)

B0 — Complex local vector of length MXLDA containing the local portions of the distributed vector B. B contains the right-hand side of the linear system. (Input)

X0 — Complex local vector of length MXLDA containing the local portions of the distributed vector X. X contains the solution to the linear system. (Output)

All other arguments are global and are the same as described for the standard version of the routine. In the argument descriptions above, MXLDA and MXCOL can be obtained through a call to SCALAPACK_GETDIM (see *Utilities*) after a call to SCALAPACK_SETUP (see *Utilities*) has been made. See the *ScaLAPACK Example* below.

Examples

Example 1

A system of three linear equations is solved. The coefficient matrix has complex general form and the right-hand-side vector *b* has three elements.

```
      USE LSLCG_INT
      USE WRCRN_INT
!                                 Declare variables
      PARAMETER  (LDA=3, N=3)
      COMPLEX    A(LDA,LDA), B(N), X(N)
!                                 Set values for  A and B
!
!                                 A = ( 3.0-2.0i  2.0+4.0i  0.0-3.0i)
!                                     ( 1.0+1.0i  2.0-6.0i  1.0+2.0i)
!                                     ( 4.0+0.0i -5.0+1.0i  3.0-2.0i)
!
!                                 B = (10.0+5.0i  6.0-7.0i -1.0+2.0i)
!
      DATA A/(3.0,-2.0), (1.0,1.0),  (4.0,0.0), (2.0,4.0), (2.0,-6.0),&
             (-5.0,1.0), (0.0,-3.0), (1.0,2.0), (3.0,-2.0)/
      DATA B/(10.0,5.0), (6.0,-7.0), (-1.0,2.0)/
!                                 Solve AX = B     (IPATH = 1)
      CALL LSLCG (A, B, X)
!                                 Print results
      CALL WRCRN ('X', X, 1, N, 1)
      END
```

Output

```
                         X
             1                 2                 3
( 1.000,-1.000)   ( 2.000, 1.000)   ( 0.000, 3.000)
```

ScaLAPACK Example

The same system of three linear equations is solved as a distributed computing example. The coefficient matrix has complex general form and the right-hand-side vector *b* has three elements. `SCALAPACK_MAP` and `SCALAPACK_UNMAP` are IMSL utility routines (see *Chapter 11, "Utilities"*) used to map and unmap arrays to and from the processor grid. They are used here for brevity. `DESCINIT` is a ScaLAPACK tools routine which initializes the descriptors for the local arrays.

```
      USE MPI_SETUP_INT
      USE LSLCG_INT
      USE WRCRN_INT
      USE SCALAPACK_SUPPORT
      IMPLICIT NONE
      INCLUDE 'mpif.h'
!                                 Declare variables
      INTEGER    LDA, N, DESCA(9), DESCX(9)
      INTEGER       INFO, MXCOL, MXLDA
      COMPLEX, ALLOCATABLE ::       A(:,:), B(:), X(:)
      COMPLEX, ALLOCATABLE ::       A0(:,:), B0(:), X0(:)
      PARAMETER  (LDA=3, N=3)
!                                 Set up for MPI
```

```
      MP_NPROCS = MP_SETUP()
      IF(MP_RANK .EQ. 0) THEN
          ALLOCATE (A(LDA,N), B(N), X(N))
!                                Set values for A and B
          A(1,:) = (/ (3.0, -2.0), (2.0,  4.0), (0.0, -3.0)/)
          A(2,:) = (/ (1.0,  1.0), (2.0, -6.0), (1.0,  2.0)/)
          A(3,:) = (/ (4.0,  0.0), (-5.0, 1.0), (3.0, -2.0)/)
!
          B = (/(10.0, 5.0), (6.0, -7.0), (-1.0, 2.0)/)
      ENDIF
!                                 Set up a 1D processor grid and define
!                                 its context ID, MP_ICTXT
      CALL SCALAPACK_SETUP(N, N, .TRUE., .TRUE.)
!                                 Get the array descriptor entities MXLDA,
!                                 and MXCOL
      CALL SCALAPACK_GETDIM(N, N, MP_MB, MP_NB, MXLDA, MXCOL)
!                                 Set up the array descriptors
      CALL DESCINIT(DESCA, N, N, MP_MB, MP_NB, 0, 0, MP_ICTXT, MXLDA, INFO)
      CALL DESCINIT(DESCX, N, 1, MP_MB, 1, 0, 0, MP_ICTXT, MXLDA, INFO)
!                                Allocate space for the local arrays
      ALLOCATE (A0(MXLDA,MXCOL), B0(MXLDA), X0(MXLDA))
!                                Map input arrays to the processor grid
      CALL SCALAPACK_MAP(A, DESCA, A0)
      CALL SCALAPACK_MAP(B, DESCX, B0)
!                                Solve the system of equations
      CALL LSLCG (A0, B0, X0)
!                                Unmap the results from the distributed
!                                arrays back to a non-distributed array.
!                                After the unmap, only Rank=0 has the full
!                                array.
      CALL SCALAPACK_UNMAP(X0, DESCX, X)
!                                Print results.
!                                Only Rank=0 has the solution, X.
      IF(MP_RANK .EQ. 0)CALL WRCRN ('X', X, 1, N, 1)
      IF (MP_RANK .EQ. 0) DEALLOCATE(A, B, X)
      DEALLOCATE(A0, B0, X0)
!                                Exit ScaLAPACK usage
      CALL SCALAPACK_EXIT(MP_ICTXT)
!                                Shut down MPI
      MP_NPROCS = MP_SETUP('FINAL')
      END
```

Output

```
                         X
              1                 2                  3
( 1.000,-1.000)  ( 2.000, 1.000)  ( 0.000, 3.000)
```

LFCCG

more...

more...

Computes the *LU* factorization of a complex general matrix and estimate its L_1 condition number.

Required Arguments

A — Complex `N` by `N` matrix to be factored. (Input)

FACT — Complex `N` × `N` matrix containing the *LU* factorization of the matrix `A` (Output)
If `A` is not needed, `A` and `FACT` can share the same storage locations

IPVT — Vector of length `N` containing the pivoting information for the *LU* factorization. (Output)

RCOND — Scalar containing an estimate of the reciprocal of the L_1 condition number of `A`. (Output)

Optional Arguments

N — Order of the matrix. (Input)
Default: `N` = size (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = size (`A`,1).

LDFACT — Leading dimension of `FACT` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDFACT` = size (`FACT`,1).

FORTRAN 90 Interface

Generic: `CALL LFCCG (A, FACT, IPVT, RCOND [, …])`

Specific: The specific interface names are `S_LFCCG` and `D_LFCCG`.

FORTRAN 77 Interface

Single: CALL LFCCG (N, A, LDA, FACT, LDFACT, IPVT, RCOND)

Double: The double precision name is DLFCCG.

ScaLAPACK Interface

Generic: CALL LFCCG (A0, FACT0, IPVT0, RCOND [, …])

Specific: The specific interface names are S_LFCCG and D_LFCCG.

See the ScaLAPACK Usage Notes below for a description of the arguments for distributed computing.

Description

Routine LFCCG performs an *LU* factorization of a complex general coefficient matrix. It also estimates the condition number of the matrix. The underlying code is based on either LINPACK, LAPACK, or ScaLAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see *Using ScaLAPACK, LAPACK, LINPACK, and EISPACK* in the Introduction section of this manual. The *LU* factorization is done using scaled partial pivoting. Scaled partial pivoting differs from partial pivoting in that the pivoting strategy is the same as if each row were scaled to have the same ∞-norm.

The L_1 condition number of the matrix *A* is defined to be $\kappa(A) = \|A\|_1 \|A^{-1}\|_1$. Since it is expensive to compute $\|A^{-1}\|_1$, the condition number is only estimated. The estimation algorithm is the same as used by LINPACK and is described by Cline et al. (1979).

If the estimated condition number is greater than $1/\varepsilon$ (where ε is machine precision), a warning error is issued. This indicates that very small changes in *A* can cause very large changes in the solution *x*. Iterative refinement can sometimes find the solution to such a system.

LFCCG fails if *U*, the upper triangular part of the factorization, has a zero diagonal element. This can occur only if *A* either is singular or is very close to a singular matrix.

The *LU* factors are returned in a form that is compatible with routines LFICG, LFSCG and LFDCG. To solve systems of equations with multiple right-hand-side vectors, use LFCCG followed by either LFICG or LFSCG called once for each right-hand side. The routine LFDCG can be called to compute the determinant of the coefficient matrix after LFCCG has performed the factorization.

Let *F* be the matrix FACT and let *p* be the vector IPVT. The triangular matrix *U* is stored in the upper triangle of *F*. The strict lower triangle of *F* contains the information needed to reconstruct *L* using

$$L_{11} = L_{N-1} P_{N-1} \dots L_1 P_1$$

where P_k is the identity matrix with rows k and p_k interchanged and L_k is the identity with F_{ik} for $i = k + 1, \ldots,$ N inserted below the diagonal. The strict lower half of F can also be thought of as containing the negative of the multipliers.

Comments

1. Workspace may be explicitly provided, if desired, by use of L2CCG/DL2CCG. The reference is:

   CALL L2CCG (N, A, LDA, FACT, LDFACT, IPVT, RCOND, WK)

   The additional argument is:

   WK — Complex work vector of length N.

2. Informational errors

Type	Code	Description
3	1	The input matrix is algorithmically singular.
4	2	The input matrix is singular.

ScaLAPACK Usage Notes

The arguments which differ from the standard version of this routine are:

A0 — MXLDA by MXCOL complex local matrix containing the local portions of the distributed matrix A. A contains the matrix to be factored. (Input)

FACT0 — MXLDA by MXCOL complex local matrix containing the local portions of the distributed matrix FACT. FACT contains the *LU* factorization of the matrix A. (Output)

IPVT0 — Local vector of length MXLDA containing the local portions of the distributed vector IPVT. IPVT contains the pivoting information for the *LU* factorization. (Output)

All other arguments are global and are the same as described for the standard version of the routine. In the argument descriptions above, MXLDA and MXCOL can be obtained through a call to SCALAPACK_GETDIM (see *Utilities*) after a call to SCALAPACK_SETUP (see *Utilities*) has been made. See the *ScaLAPACK Example* below.

Examples

Example 1

The inverse of a 3 × 3 matrix is computed. LFCCG is called to factor the matrix and to check for singularity or ill-conditioning. LFICG is called to determine the columns of the inverse.

```
      USE IMSL_LIBRARIES

!                                 Declare variables
      PARAMETER  (LDA=3, LDFACT=3, N=3)
      INTEGER    IPVT(N), NOUT
      REAL       RCOND, THIRD
      COMPLEX    A(LDA,N), AINV(LDA,N), RJ(N), FACT(LDFACT,N), RES(N)
!                                 Declare functions
      COMPLEX    CMPLX
!                                 Set values for  A
!
!                                 A = (  1.0+1.0i  2.0+3.0i  3.0+3.0i)
!                                     (  2.0+1.0i  5.0+3.0i  7.0+4.0i)
!                                     ( -2.0+1.0i -4.0+4.0i -5.0+3.0i)
!
      DATA A/(1.0,1.0), (2.0,1.0), (-2.0,1.0), (2.0,3.0), (5.0,3.0),&
          (-4.0,4.0), (3.0,3.0), (7.0,4.0), (-5.0,3.0)/
!
!                                 Scale A by dividing by three
      THIRD = 1.0/3.0
      DO 10  I=1, N
         CALL CSSCAL (N, THIRD, A(:,I), 1)
   10 CONTINUE
!                                 Factor A
      CALL LFCCG (A, FACT, IPVT, RCOND)
!                                 Print the L1 condition number
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) RCOND, 1.0E0/RCOND
!                                 Set up the columns of the identity
!                                 matrix one at a time in RJ
      CALL CSET (N, (0.0,0.0), RJ, 1)
      DO 20  J=1, N
         RJ(J) = CMPLX(1.0,0.0)
!                                 RJ is the J-th column of the identity
!                                 matrix so the following LFIRG
!                                 reference places the J-th column of
!                                 the inverse of A in the J-th column
!                                 of AINV
         CALL LFICG (A, FACT, IPVT, RJ, AINV(:,J), RES)
         RJ(J) = CMPLX(0.0,0.0)
   20 CONTINUE
!                                 Print results
      CALL WRCRN ('AINV', AINV)
!
99999 FORMAT ('  RCOND = ',F5.3,/,'  L1 Condition number = ',F6.3)
      END
```

Output

```
RCOND < .02
L1 Condition number < 100.0

                         AINV
                 1                 2                 3
1  ( 6.400,-2.800)  (-3.800, 2.600)  (-2.600, 1.200)
2  (-1.600,-1.800)  ( 0.200, 0.600)  ( 0.400,-0.800)
3  (-0.600, 2.200)  ( 1.200,-1.400)  ( 0.400, 0.200)
```

ScaLAPACK Example

The inverse of the same 3 × 3 matrix is computed as a distributed example. LFCCG is called to factor the matrix and to check for singularity or ill-conditioning. LFICG is called to determine the columns of the inverse. SCALAPACK_MAP and SCALAPACK_UNMAP are IMSL utility routines (see *Chapter 11, "Utilities"*) used to map and unmap arrays to and from the processor grid. They are used here for brevity. DESCINIT is a ScaLAPACK tools routine which initializes the descriptors for the local arrays.

```
      USE MPI_SETUP_INT
      USE LFCCG_INT
      USE UMACH_INT
      USE LFICG_INT
      USE WRCRN_INT
      USE SCALAPACK_SUPPORT
      IMPLICIT NONE
      INCLUDE 'mpif.h'
!                                  Declare variables
      INTEGER     J, LDA, N, DESCA(9), DESCL(9)
      INTEGER     INFO, MXCOL, MXLDA, NOUT
      INTEGER, ALLOCATABLE ::     IPVT0(:)
      COMPLEX, ALLOCATABLE ::     A(:,:), AINV(:,:), X0(:), RJ(:)
      COMPLEX, ALLOCATABLE ::     A0(:,:), FACT0(:,:), RES0(:), RJ0(:)
      REAL        RCOND, THIRD
      PARAMETER  (LDA=3, N=3)
!                            Set up for MPI
      MP_NPROCS = MP_SETUP()
      IF(MP_RANK .EQ. 0) THEN
          ALLOCATE (A(LDA,N), AINV(LDA,N))
!                                  Set values for A
          A(1,:) = (/ ( 1.0, 1.0), ( 2.0, 3.0), ( 3.0, 3.0)/)
          A(2,:) = (/ ( 2.0, 1.0), ( 5.0, 3.0), ( 7.0, 4.0)/)
          A(3,:) = (/ (-2.0, 1.0), (-4.0, 4.0), (-5.0, 3.0)/)
!                                  Scale A by dividing by three
          THIRD = 1.0/3.0
          A = A * THIRD
      ENDIF
!                                  Set up a 1D processor grid and define
!                                  its context id, MP_ICTXT
      CALL SCALAPACK_SETUP(N, N, .TRUE., .TRUE.)
!                                  Get the array descriptor entities MXLDA,
!                                  and MXCOL
      CALL SCALAPACK_GETDIM(N, N, MP_MB, MP_NB, MXLDA, MXCOL)
!                                  Set up the array descriptors
      CALL DESCINIT(DESCA, N, N, MP_MB, MP_NB, 0, 0, MP_ICTXT, MXLDA, INFO)
      CALL DESCINIT(DESCL, N, 1, MP_MB, 1, 0, 0, MP_ICTXT, MXLDA, INFO)
!                                 Allocate space for the local arrays
      ALLOCATE(A0(MXLDA,MXCOL), X0(MXLDA),FACT0(MXLDA,MXCOL), RJ(N), &
               RJ0(MXLDA), RES0(MXLDA), IPVT0(MXLDA))
!                                 Map input array to the processor grid
      CALL SCALAPACK_MAP(A, DESCA, A0)
!                                 Factor A
      CALL LFCCG (A0, FACT0, IPVT0, RCOND)
!                                 Print the reciprocal condition number
!                                 and the L1 condition number
      IF(MP_RANK .EQ. 0) THEN
         CALL UMACH (2, NOUT)
         WRITE (NOUT,99998) RCOND, 1.0E0/RCOND
      ENDIF
!                                 Set up the columns of the identity
!                                 matrix one at a time in RJ
      RJ = (0.0, 0.0)
      DO 10  J=1, N
```

```
          RJ(J) = (1.0, 0.0)
          CALL SCALAPACK_MAP(RJ, DESCL, RJ0)
!                                RJ is the J-th column of the identity
!                                matrix so the following LFICG
!                                reference computes the J-th column of
!                                the inverse of A
          CALL LFICG (A0, FACT0, IPVT0, RJ0, X0, RES0)
          RJ(J) = (0.0, 0.0)
          CALL SCALAPACK_UNMAP(X0, DESCL, AINV(:,J))
   10 CONTINUE
!                                Print results
!                                Only Rank=0 has the solution, AINV.
      IF(MP_RANK.EQ.0) CALL WRCRN ('AINV', AINV)
      IF (MP_RANK .EQ. 0) DEALLOCATE(A, AINV)
      DEALLOCATE(A0, FACT0, IPVT0, RJ, RJ0, RES0, X0)
!                                Exit ScaLAPACK usage
      CALL SCALAPACK_EXIT(MP_ICTXT)
!                                Shut down MPI
      MP_NPROCS = MP_SETUP('FINAL')
99998 FORMAT ('  RCOND = ',F5.3,/,'  L1 Condition number = ',F6.3)
      END
```

Output

```
RCOND < .02
L1 Condition number < 100.0

                         AINV
                1                 2                 3
1  ( 6.400,-2.800)  (-3.800, 2.600)  (-2.600, 1.200)
2  (-1.600,-1.800)  ( 0.200, 0.600)  ( 0.400,-0.800)
3  (-0.600, 2.200)  ( 1.200,-1.400)  ( 0.400, 0.200)
```

LFTCG

more... more...

Computes the *LU* factorization of a complex general matrix.

Required Arguments

A — Complex N by N matrix to be factored. (Input)

FACT — Complex N × N matrix containing the *LU* factorization of the matrix A. (Output)
If A is not needed, A and FACT can share the same storage locations.

IPVT — Vector of length N containing the pivoting information for the *LU* factorization. (Output)

Optional Arguments

N — Order of the matrix. (Input)
Default: N = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

LDFACT — Leading dimension of FACT exactly as specified in the dimension statement of the calling program. (Input)
Default: LDFACT = size (FACT,1).

FORTRAN 90 Interface

Generic: CALL LFTCG (A, FACT, IPVT [, …])

Specific: The specific interface names are S_LFTCG and D_LFTCG.

FORTRAN 77 Interface

Single: `CALL LFTCG (N, A, LDA, FACT, LDFACT, IPVT)`

Double: The double precision name is `DLFTCG`.

ScaLAPACK Interface

Generic: `CALL LFTCG (A0, FACT0, IPVT0 [, …])`

Specific: The specific interface names are `S_LFTCG` and `D_LFTCG`.

See the *ScaLAPACK Usage Notes* below for a description of the arguments for distributed computing.

Description

Routine `LFTCG` performs an *LU* factorization of a complex general coefficient matrix. The *LU* factorization is done using scaled partial pivoting. Scaled partial pivoting differs from partial pivoting in that the pivoting strategy is the same as if each row were scaled to have the same $\infty - norm$.

`LFTCG` fails if *U*, the upper triangular part of the factorization, has a zero diagonal element. This can occur only if *A* either is singular or is very close to a singular matrix.

The *LU* factors are returned in a form that is compatible with routines `LFICG`, `LFSCG` and `LFDCG`. To solve systems of equations with multiple right-hand-side vectors, use `LFTCG` followed by either `LFICG` or `LFSCG` called once for each right-hand side. The routine `LFDCG` can be called to compute the determinant of the coefficient matrix after `LFCCG` has performed the factorization.

Let *F* be the matrix `FACT` and let *p* be the vector `IPVT`. The triangular matrix *U* is stored in the upper triangle of *F*. The strict lower triangle of *F* contains the information needed to reconstruct `L` using

$$L = L_{N\text{-}1}P_{N\text{-}1} \ldots L_1P_1$$

where P_k is the identity matrix with rows *k* and P_k interchanged and L_k is the identity with F_{ik} for $i = k + 1, \ldots, N$ inserted below the diagonal. The strict lower half of *F* can also be thought of as containing the negative of the multipliers.

The underlying code is based on either LINPACK , LAPACK, or ScaLAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see "*Using ScaLAPACK, LAPACK, LINPACK, and EISPACK*" in the *Introduction* section of this manual.

Comments

1. Workspace may be explicitly provided, if desired, by use of `L2TCG/DL2TCG`. The reference is:

CALL L2TCG (N, A, LDA, FACT, LDFACT, IPVT, WK)

The additional argument is:

WK — Complex work vector of length N.

2. Informational error

Type	Code	Description
4	2	The input matrix is singular.

ScaLAPACK Usage Notes

The arguments which differ from the standard version of this routine are:

A0 — MXLDA by MXCOL complex local matrix containing the local portions of the distributed matrix A. A contains the matrix to be factored. (Input)

FACT0 — MXLDA by MXCOL complex local matrix containing the local portions of the distributed matrix FACT. FACT contains the *LU* factorization of the matrix A. (Output)
If A is not needed, A and FACT can share the same storage locations.

IPVT0 — Local vector of length MXLDA containing the local portions of the distributed vector IPVT. IPVT contains the pivoting information for the *LU* factorization. (Output)

All other arguments are global and are the same as described for the standard version of the routine. In the argument descriptions above, MXLDA and MXCOL can be obtained through a call to SCALAPACK_GETDIM (see *Utilities*) after a call to SCALAPACK_SETUP (see *Utilities*) has been made. See the ScaLAPACK Example below.

Examples

Example

A linear system with multiple right-hand sides is solved. LFTCG is called to factor the coefficient matrix. LFSCG is called to compute the two solutions for the two right-hand sides. In this case the coefficient matrix is assumed to be well-conditioned and correctly scaled. Otherwise, it would be better to call LFCCG to perform the factorization, and LFICG to compute the solutions.

```
      USE LFTCG_INT
      USE LFSCG_INT
      USE WRCRN_INT
!                                 Declare variables
      PARAMETER  (LDA=3, LDFACT=3, N=3)
      INTEGER    IPVT(N)
      COMPLEX    A(LDA,LDA), B(N,2), X(N,2), FACT(LDFACT,LDFACT)
!                                 Set values for  A
```

```
!                                A = ( 1.0+1.0i  2.0+3.0i  3.0-3.0i)
!                                    ( 2.0+1.0i  5.0+3.0i  7.0-5.0i)
!                                    (-2.0+1.0i -4.0+4.0i  5.0+3.0i)
!
      DATA A/(1.0,1.0), (2.0,1.0), (-2.0,1.0), (2.0,3.0), (5.0,3.0),&
          (-4.0,4.0), (3.0,-3.0), (7.0,-5.0), (5.0,3.0)/
!
!                                Set the right-hand sides, B
!                                B = (  3.0+ 5.0i   9.0+ 0.0i)
!                                    ( 22.0+10.0i 13.0+ 9.0i)
!                                    (-10.0+ 4.0i   6.0+10.0i)
!
      DATA B/(3.0,5.0), (22.0,10.0), (-10.0,4.0), (9.0,0.0),&
          (13.0,9.0), (6.0,10.0)/
!
!                                Factor A
      CALL LFTCG (A, FACT, IPVT)
!                                Solve for the two right-hand sides
      DO 10  J=1, 2
         CALL LFSCG (FACT, IPVT, B(:,J), X(:,J))
   10 CONTINUE
!                                Print results
      CALL WRCRN ('X', X)
      END
```

Output

```
                X
              1                2
1   ( 1.000,-1.000)   ( 0.000, 2.000)
2   ( 2.000, 4.000)   (-2.000,-1.000)
3   ( 3.000, 0.000)   ( 1.000, 3.000)
```

ScaLAPACK Example

The same linear system with multiple right-hand sides is solved as a distributed example. LFTCG is called to factor the matrix. LFSCG is called to compute the two solutions for the two right-hand sides. SCALAPACK_MAP and SCALAPACK_UNMAP are IMSL utility routines (see *Chapter 11, "Utilities"*) used to map and unmap arrays to and from the processor grid. They are used here for brevity. DESCINIT is a ScaLAPACK tools routine which initializes the descriptors for the local arrays.

```
      USE MPI_SETUP_INT
      USE LFTCG_INT
      USE LFSCG_INT
      USE WRCRN_INT
      USE SCALAPACK_SUPPORT
      IMPLICIT NONE
      INCLUDE 'mpif.h'
!                                 Declare variables
      INTEGER     J, LDA, N, DESCA(9), DESCL(9)
      INTEGER     INFO, MXCOL, MXLDA
      INTEGER, ALLOCATABLE ::     IPVT0(:)
      COMPLEX, ALLOCATABLE ::     A(:,:), B(:,:), X(:,:), X0(:)
      COMPLEX, ALLOCATABLE ::     A0(:,:), FACT0(:,:), B0(:)
      PARAMETER  (LDA=3, N=3)
!                           Set up for MPI
      MP_NPROCS = MP_SETUP()
      IF(MP_RANK .EQ. 0) THEN
          ALLOCATE (A(LDA,N), B(N,2), X(N,2))
!                                 Set values for A and B
```

```
         A(1,:) = (/ ( 1.0, 1.0), ( 2.0, 3.0), ( 3.0,-3.0)/)
         A(2,:) = (/ ( 2.0, 1.0), ( 5.0, 3.0), ( 7.0,-5.0)/)
         A(3,:) = (/ (-2.0, 1.0), (-4.0, 4.0), ( 5.0, 3.0)/)
!
         B(1,:) = (/ (  3.0,  5.0), ( 9.0,  0.0)/)
         B(2,:) = (/ ( 22.0, 10.0), (13.0,  9.0)/)
         B(3,:) = (/ (-10.0,  4.0), ( 6.0, 10.0)/)
     ENDIF
!                                Set up a 1D processor grid and define
!                                its context ID, MP_ICTXT
     CALL SCALAPACK_SETUP(N, N, .TRUE., .TRUE.)
!                                Get the array descriptor entities MXLDA,
!                                and MXCOL
     CALL SCALAPACK_GETDIM(N, N, MP_MB, MP_NB, MXLDA, MXCOL)
!                                Set up the array descriptors
     CALL DESCINIT(DESCA, N, N, MP_MB, MP_NB, 0, 0, MP_ICTXT, MXLDA, INFO)
     CALL DESCINIT(DESCL, N, 1, MP_MB, 1, 0, 0, MP_ICTXT, MXLDA, INFO)
!                               Allocate space for the local arrays
     ALLOCATE(A0(MXLDA,MXCOL), X0(MXLDA),FACT0(MXLDA,MXCOL), &
              B0(MXLDA), IPVT0(MXLDA))
!                               Map input array to the processor grid
     CALL SCALAPACK_MAP(A, DESCA, A0)
!                               Factor A
     CALL LFTCG (A0, FACT0, IPVT0)
!                               Solve for the two right-hand sides
     DO 10  J=1, 2
        CALL SCALAPACK_MAP(B(:,J), DESCL, B0)
        CALL LFSCG (FACT0, IPVT0, B0, X0)
        CALL SCALAPACK_UNMAP(X0, DESCL, X(:,J))
  10 CONTINUE
!                               Print results.
!                               Only Rank=0 has the solution, X.
     IF(MP_RANK.EQ.0) CALL WRCRN ('X', X)
     IF (MP_RANK .EQ. 0) DEALLOCATE(A, B, X)
     DEALLOCATE(A0, B0, FACT0, IPVT0, X0)
!                               Exit ScaLAPACK usage
     CALL SCALAPACK_EXIT(MP_ICTXT)
!                               Shut down MPI
     MP_NPROCS = MP_SETUP('FINAL')
     END
```

Output

```
                X
                 1                 2
1  ( 1.000,-1.000)  ( 0.000, 2.000)
2  ( 2.000, 4.000)  (-2.000,-1.000)
3  ( 3.000, 0.000)  ( 1.000, 3.000)
```

LFSCG

more...

more...

Solves a complex general system of linear equations given the *LU* factorization of the coefficient matrix.

Required Arguments

FACT — Complex N by N matrix containing the *LU* factorization of the coefficient matrix A as output from routine LFCCG/DLFCCG or LFTCG/DLFTCG. (Input)

IPVT — Vector of length N containing the pivoting information for the *LU* factorization of A as output from routine LFCCG/DLFCCG or LFTCG/DLFTCG. (Input)

B — Complex vector of length N containing the right-hand side of the linear system. (Input)

X — Complex vector of length N containing the solution to the linear system. (Output)
If B is not needed, B and X can share the same storage locations.

Optional Arguments

N — Number of equations. (Input)
Default: N = size (FACT,2).

LDFACT — Leading dimension of FACT exactly as specified in the dimension statement of the calling program. (Input)
Default: LDFACT = size (FACT,1).

IPATH — Path indicator. (Input)
IPATH = 1 means the system AX = B is solved.
IPATH = 2 means the system $A^H X$ = B is solved.
Default: IPATH = 1.

FORTRAN 90 Interface

Generic: CALL LFSCG (FACT, IPVT, B, X [, …])

Specific: The specific interface names are S_LFSCG and D_LFSCG.

FORTRAN 77 Interface

Single: CALL LFSCG (N, FACT, LDFACT, IPVT, B, IPATH, X)

Double: The double precision name is DLFSCG.

ScaLAPACK Interface

Generic: CALL LFSCG (FACT0, IPVT0, B0, X0 [, …])

Specific: The specific interface names are S_LFSCG and D_LFSCG.

See the ScaLAPACK Usage Notes below for a description of the arguments for distributed computing.

Description

Routine LFSCG computes the solution of a system of linear algebraic equations having a complex general coefficient matrix. To compute the solution, the coefficient matrix must first undergo an *LU* factorization. This may be done by calling either LFCCG or LFTCG. The solution to $Ax = b$ is found by solving the triangular systems $Ly = b$ and $Ux = y$. The forward elimination step consists of solving the system $Ly = b$ by applying the same permutations and elimination operations to b that were applied to the columns of A in the factorization routine. The backward substitution step consists of solving the triangular system $Ux = y$ for x.

Routines LFSCG and LFICG both solve a linear system given its *LU* factorization. LFICG generally takes more time and produces a more accurate answer than LFSCG. Each iteration of the iterative refinement algorithm used by LFICG calls LFSCG.

The underlying code is based on either LINPACK , LAPACK, or ScaLAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see *Using ScaLAPACK, LAPACK, LINPACK, and EISPACK* in the Introduction section of this manual.

ScaLAPACK Usage Notes

The arguments which differ from the standard version of this routine are:

FACT0 — MXLDA by MXCOL complex local matrix containing the local portions of the distributed matrix FACT as output from routine LFCCG/DLFCCG or LFTCG/DLFTCG. FACT contains the *LU* factorization of the matrix A. (Input)

IPVT0 — Local vector of length `MXLDA` containing the local portions of the distributed vector `IPVT`. `IPVT` contains the pivoting information for the *LU* factorization as output from subroutine `LFCCG/DLFCCG` or `LFTCG/DLFTCG`. (Input)

B0 — Complex local vector of length `MXLDA` containing the local portions of the distributed vector `B`. `B` contains the right-hand side of the linear system. (Input)

X0 — Complex local vector of length `MXLDA` containing the local portions of the distributed vector `X`. `X` contains the solution to the linear system. (Output)
If `B` is not needed, `B` and `X` can share the same storage locations.

All other arguments are global and are the same as described for the standard version of the routine. In the argument descriptions above, `MXLDA` and `MXCOL` can be obtained through a call to `SCALAPACK_GETDIM` (see *Utilities*) after a call to `SCALAPACK_SETUP` (see *Utilities*) has been made. See the *ScaLAPACK Example* below.

Examples

Example

The inverse is computed for a complex general 3 × 3 matrix. The input matrix is assumed to be well-conditioned, hence `LFTCG` is used rather than `LFCCG`.

```
      USE IMSL_LIBRARIES
!                                 Declare variables
      PARAMETER  (LDA=3, LDFACT=3, N=3)
      INTEGER    IPVT(N)
      REAL       THIRD
      COMPLEX    A(LDA,LDA), AINV(LDA,LDA), RJ(N), FACT(LDFACT,LDFACT)
!                                 Declare functions
      COMPLEX    CMPLX
!                                 Set values for  A
!
!                                 A = (  1.0+1.0i  2.0+3.0i  3.0+3.0i)
!                                     (  2.0+1.0i  5.0+3.0i  7.0+4.0i)
!                                     ( -2.0+1.0i -4.0+4.0i -5.0+3.0i)
!
      DATA A/(1.0,1.0), (2.0,1.0), (-2.0,1.0), (2.0,3.0), (5.0,3.0),&
          (-4.0,4.0), (3.0,3.0), (7.0,4.0), (-5.0,3.0)/
!
!                                 Scale A by dividing by three
      THIRD = 1.0/3.0
      DO 10  I=1, N
         CALL CSSCAL (N, THIRD, A(:,I), 1)
   10 CONTINUE
!                                 Factor A
      CALL LFTCG (A, FACT, IPVT)
!                                 Set up the columns of the identity
!                                 matrix one at a time in RJ
      CALL CSET (N, (0.0,0.0), RJ, 1)
      DO 20  J=1, N
         RJ(J) = CMPLX(1.0,0.0)
!                                 RJ is the J-th column of the identity
!                                 matrix so the following LFSCG
```

```
!                                 reference places the J-th column of
!                                 the inverse of A in the J-th column
!                                 of AINV
         CALL LFSCG (FACT, IPVT, RJ, AINV(:,J))
         RJ(J) = CMPLX(0.0,0.0)
   20 CONTINUE
!                                 Print results
      CALL WRCRN ('AINV', AINV)
      END
```

Output

```
                         AINV
                  1                  2                  3
1  ( 6.400,-2.800)  (-3.800, 2.600)  (-2.600, 1.200)
2  (-1.600,-1.800)  ( 0.200, 0.600)  ( 0.400,-0.800)
3  (-0.600, 2.200)  ( 1.200,-1.400)  ( 0.400, 0.200)
```

ScaLAPACK Example

The inverse of the same 3 × 3 matrix is computed as a distributed example. The input matrix is assumed to be well-conditioned, hence LFTCG is used rather than LFCCG. LFSCG is called to determine the columns of the inverse. SCALAPACK_MAP and SCALAPACK_UNMAP are IMSL utility routines (see Chapter 11, "Utilities") used to map and unmap arrays to and from the processor grid. They are used here for brevity. DESCINIT is a ScaLAPACK tools routine which initializes the descriptors for the local arrays.

```
      USE MPI_SETUP_INT
      USE LFTCG_INT
      USE LFSCG_INT
      USE WRCRN_INT
      USE SCALAPACK_SUPPORT
      IMPLICIT NONE
      INCLUDE 'mpif.h'
!                                  Declare variables
      INTEGER      J, LDA, N, DESCA(9), DESCL(9)
      INTEGER      INFO, MXCOL, MXLDA
      INTEGER, ALLOCATABLE ::     IPVT0(:)
      COMPLEX, ALLOCATABLE ::     A(:,:), AINV(:,:), X0(:)
      COMPLEX, ALLOCATABLE ::     A0(:,:), FACT0(:,:), RJ(:), RJ0(:)
      REAL         THIRD
      PARAMETER   (LDA=3, N=3)
!                            Set up for MPI
      MP_NPROCS = MP_SETUP()
      IF(MP_RANK .EQ. 0) THEN
          ALLOCATE (A(LDA,N), AINV(LDA,N))
!                                  Set values for A
          A(1,:) = (/ ( 1.0, 1.0), ( 2.0, 3.0), ( 3.0, 3.0)/)
          A(2,:) = (/ ( 2.0, 1.0), ( 5.0, 3.0), ( 7.0, 4.0)/)
          A(3,:) = (/ (-2.0, 1.0), (-4.0, 4.0), (-5.0, 3.0)/)
!                                  Scale A by dividing by three
          THIRD = 1.0/3.0
          A = A * THIRD
      ENDIF
!                                  Set up a 1D processor grid and define
!                                  its context ID, MP_ICTXT
      CALL SCALAPACK_SETUP(N, N, .TRUE., .TRUE.)
!                                  Get the array descriptor entities MXLDA,
!                                  and MXCOL
      CALL SCALAPACK_GETDIM(N, N, MP_MB, MP_NB, MXLDA, MXCOL)
!                                  Set up the array descriptors
```

```
      CALL DESCINIT(DESCA, N, N, MP_MB, MP_NB, 0, 0, MP_ICTXT, MXLDA, INFO)
      CALL DESCINIT(DESCL, N, 1, MP_MB, 1, 0, 0, MP_ICTXT, MXLDA, INFO)
!                                  Allocate space for the local arrays
      ALLOCATE(A0(MXLDA,MXCOL), X0(MXLDA),FACT0(MXLDA,MXCOL), RJ(N), &
               RJ0(MXLDA), IPVT0(MXLDA))
!                                 Map input array to the processor grid
      CALL SCALAPACK_MAP(A, DESCA, A0)
!                                 Factor A
      CALL LFTCG (A0, FACT0, IPVT0)
!                                 Set up the columns of the identity
!                                 matrix one at a time in RJ
      RJ = (0.0, 0.0)
      DO 10  J=1, N
         RJ(J) = (1.0, 0.0)
         CALL SCALAPACK_MAP(RJ, DESCL, RJ0)
!                                 RJ is the J-th column of the identity
!                                 matrix so the following LFICG
!                                 reference computes the J-th column of
!                                 the inverse of A
         CALL LFSCG (FACT0, IPVT0, RJ0, X0)
         RJ(J) = (0.0, 0.0)
         CALL SCALAPACK_UNMAP(X0, DESCL, AINV(:,J))
   10 CONTINUE
!                                 Print results.
!                                 Only Rank=0 has the solution, AINV.
      IF(MP_RANK.EQ.0) CALL WRCRN ('AINV', AINV)
      IF (MP_RANK .EQ. 0) DEALLOCATE(A, AINV)
      DEALLOCATE(A0, FACT0, IPVT0, RJ, RJ0, X0)
!                                 Exit ScaLAPACK usage
      CALL SCALAPACK_EXIT(MP_ICTXT)
!                                 Shut down MPI
      MP_NPROCS = MP_SETUP('FINAL')
      END
```

Output

```
                         AINV
                 1                  2                  3
1  ( 6.400,-2.800)  (-3.800, 2.600)  (-2.600, 1.200)
2  (-1.600,-1.800)  ( 0.200, 0.600)  ( 0.400,-0.800)
3  (-0.600, 2.200)  ( 1.200,-1.400)  ( 0.400, 0.200)
```

LFICG

more... more...

Uses iterative refinement to improve the solution of a complex general system of linear equations.

Required Arguments

A — Complex `N` by `N` matrix containing the coefficient matrix of the linear system. (Input)

FACT — Complex `N` by `N` matrix containing the *LU* factorization of the coefficient matrix `A` as output from routine `LFCCG/DLFCCG` or `LFTCG/DLFTCG`. (Input)

IPVT — Vector of length `N` containing the pivoting information for the *LU* factorization of `A` as output from routine `LFCCG/DLFCCG` or `LFTCG/DLFTCG`. (Input)

B — Complex vector of length `N` containing the right-hand side of the linear system. (Input)

X — Complex vector of length `N` containing the solution to the linear system. (Output)

RES — Complex vector of length `N` containing the residual vector at the improved solution. (Output)

Optional Arguments

N — Number of equations. (Input)
Default: `N` = size (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = size (`A`,1).

LDFACT — Leading dimension of `FACT` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDFACT` = size (`FACT`,1).

IPATH — Path indicator. (Input)
`IPATH` = 1 means the system $AX = B$ is solved.

IPATH = 2 means the system $A^H X = B$ is solved.

Default: IPATH = 1.

FORTRAN 90 Interface

Generic: CALL LFICG (A, FACT, IPVT, B, X, RES [, …])

Specific: The specific interface names are S_LFICG and D_LFICG.

FORTRAN 77 Interface

Single: CALL LFICG (N, A, LDA, FACT, LDFACT, IPVT, B, IPATH, X, RES)

Double: The double precision name is DLFICG.

ScaLAPACK Interface

Generic: CALL LFICG (A0, FACT0, IPVT0, B0, X0, RES0 [, …])

Specific: The specific interface names are S_LFICG and D_LFICG.

See the ScaLAPACK Usage Notes below for a description of the arguments for distributed computing.

Description

Routine LFICG computes the solution of a system of linear algebraic equations having a complex general coefficient matrix. Iterative refinement is performed on the solution vector to improve the accuracy. Usually almost all of the digits in the solution are accurate, even if the matrix is somewhat ill-conditioned.

To compute the solution, the coefficient matrix must first undergo an *LU* factorization. This may be done by calling either LFCCG, or LFTCG.

Iterative refinement fails only if the matrix is very ill-conditioned. Routines LFICG and LFSCG both solve a linear system given its *LU* factorization. LFICG generally takes more time and produces a more accurate answer than LFSCG. Each iteration of the iterative refinement algorithm used by LFICG calls LFSCG.

Comments

Informational error

Type	Code	Description
3	2	The input matrix is too ill-conditioned for iterative refinement to be effective

ScaLAPACK Usage Notes

The arguments which differ from the standard version of this routine are:

A0 — MXLDA by MXCOL complex local matrix containing the local portions of the distributed matrix A. A contains the coefficient matrix of the linear system. (Input)

FACT0 — MXLDA by MXCOL complex local matrix containing the local portions of the distributed matrix FACT as output from routineLFCCG, or LFTCG. FACT contains the *LU* factorization of the matrix A. (Input)

IPVT0 — Local vector of length MXLDA containing the local portions of the distributed vector IPVT. IPVT contains the pivoting information for the *LU* factorization as output from subroutine LFCCG, or LFTCG. (Input)

B0 — Complex local vector of length MXLDA containing the local portions of the distributed vector B. B contains the right-hand side of the linear system. (Input)

X0 — Complex local vector of length MXLDA containing the local portions of the distributed vector X. X contains the solution to the linear system. (Output)

RES0 — Complex local vector of length MXLDA containing the local portions of the distributed vector RES. RES contains the final correction at the improved solution to the linear system. (Output)

All other arguments are global and are the same as described for the standard version of the routine. In the argument descriptions above, MXLDA and MXCOL can be obtained through a call to SCALAPACK_GETDIM (see *Utilities*) after a call to SCALAPACK_SETUP (see *Utilities*) has been made. See the ScaLAPACK Example below.

Examples

Example

A set of linear systems is solved successively. The right-hand-side vector is perturbed after solving the system each of the first two times by adding 0.5 + 0.5*i* to the second element.

```
      USE LFICG_INT
      USE LFCCG_INT
      USE WRCRN_INT
      USE UMACH_INT
```

```
!                                 Declare variables
      PARAMETER  (LDA=3, LDFACT=3, N=3)
      INTEGER    IPVT(N), NOUT
      REAL       RCOND
      COMPLEX    A(LDA,LDA), B(N), X(N), FACT(LDFACT,LDFACT), RES(N)
!                                 Declare functions
      COMPLEX    CMPLX
!                                 Set values for  A
!
!                                 A = (  1.0+1.0i  2.0+3.0i  3.0-3.0i)
!                                     (  2.0+1.0i  5.0+3.0i  7.0-5.0i)
!                                     ( -2.0+1.0i -4.0+4.0i  5.0+3.0i)
!
      DATA A/(1.0,1.0), (2.0,1.0), (-2.0,1.0), (2.0,3.0), (5.0,3.0), &
          (-4.0,4.0), (3.0,-3.0), (7.0,-5.0), (5.0,3.0)/
!
!                                 Set values for B
!                                 B = ( 3.0+5.0i 22.0+10.0i -10.0+4.0i)
!
      DATA B/(3.0,5.0), (22.0,10.0), (-10.0,4.0)/
!                                 Factor A
      CALL LFCCG (A, FACT, IPVT, RCOND)
!                                 Print the L1 condition number
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) RCOND, 1.0E0/RCOND
!                                 Solve the three systems
      DO 10  J=1, 3
      CALL LFICG (A, FACT, IPVT, B, X, RES)
!                                 Print results
         CALL WRCRN ('X', X, 1, N, 1)
!                                 Perturb B by adding 0.5+0.5i to B(2)
         B(2) = B(2) + CMPLX(0.5,0.5)
   10 CONTINUE
!
99999 FORMAT ('  RCOND = ',F5.3,/,'  L1 Condition number = ',F6.3)
      END
```

Output

```
RCOND < 0.025
L1 Condition number < 75.0
                        X
              1                 2                 3
( 1.000,-1.000)  ( 2.000, 4.000)  ( 3.000, 0.000)

                        X
              1                 2                 3
( 0.910,-1.061)  ( 1.986, 4.175)  ( 3.123, 0.071)

                        X
              1                 2                 3
( 0.821,-1.123)  ( 1.972, 4.349)  ( 3.245, 0.142)
```

ScaLAPACK Example

The same set of linear systems is solved successively as a distributed example. The right-hand-side vector is perturbed after solving the system each of the first two times by adding 0.5 + 0.5*i* to the second element. SCALAPACK_MAP and SCALAPACK_UNMAP are IMSL utility routines (see *Chapter 11, "Utilities"*) used to map and unmap arrays to and from the processor grid. They are used here for brevity. DESCINIT is a ScaLAPACK tools routine which initializes the descriptors for the local arrays.

```
      USE MPI_SETUP_INT
      USE LFICG_INT
      USE LFCCG_INT
      USE WRCRN_INT
      USE UMACH_INT
      USE SCALAPACK_SUPPORT
      IMPLICIT NONE
      INCLUDE 'mpif.h'
!                                  Declare variables
      INTEGER     J, LDA, N, DESCA(9), DESCL(9)
      INTEGER     INFO, MXCOL, MXLDA, NOUT
      INTEGER, ALLOCATABLE ::     IPVT0(:)
      COMPLEX, ALLOCATABLE ::     A(:,:), B(:), X(:), X0(:), RES(:)
      COMPLEX, ALLOCATABLE ::     A0(:,:), FACT0(:,:), B0(:), RES0(:)
      REAL        RCOND
      PARAMETER  (LDA=3, N=3)
!                            Set up for MPI
      MP_NPROCS = MP_SETUP()
      IF(MP_RANK .EQ. 0) THEN
          ALLOCATE (A(LDA,N), B(N), X(N), RES(N))
!                                  Set values for A and B
          A(1,:) = (/ ( 1.0, 1.0), ( 2.0, 3.0), ( 3.0, 3.0)/)
          A(2,:) = (/ ( 2.0, 1.0), ( 5.0, 3.0), ( 7.0, 4.0)/)
          A(3,:) = (/ (-2.0, 1.0), (-4.0, 4.0), (-5.0, 3.0)/)
!
          B      = (/ (3.0,  5.0), (22.0, 10.0), (-10.0,  4.0)/)
                ENDIF
!                                  Set up a 1D processor grid and define
!                                  its context ID, MP_ICTXT
      CALL SCALAPACK_SETUP(N, N, .TRUE., .TRUE.)
!                                  Get the array descriptor entities MXLDA,
!                                  and MXCOL
      CALL SCALAPACK_GETDIM(N, N, MP_MB, MP_NB, MXLDA, MXCOL)
!                                  Set up the array descriptors
      CALL DESCINIT(DESCA, N, N, MP_MB, MP_NB, 0, 0, MP_ICTXT, MXLDA, INFO)
      CALL DESCINIT(DESCL, N, 1, MP_MB, 1, 0, 0, MP_ICTXT, MXLDA, INFO)
!                                  Allocate space for the local arrays
      ALLOCATE(A0(MXLDA,MXCOL), X0(MXLDA),FACT0(MXLDA,MXCOL), &
               B0(MXLDA), IPVT0(MXLDA), RES0(MXLDA))
!                                 Map input array to the processor grid
      CALL SCALAPACK_MAP(A, DESCA, A0)
!                                 Factor A
      CALL LFCCG (A0, FACT0, IPVT0, RCOND)
!                                 Print the L1 condition number
      IF (MP_RANK .EQ. 0) THEN
         CALL UMACH (2, NOUT)
         WRITE (NOUT,99999) RCOND, 1.0E0/RCOND
      ENDIF
!                                 Solve the three systems
      DO 10  J=1, 3
         CALL SCALAPACK_MAP(B, DESCL, B0)
         CALL LFICG (A0, FACT0, IPVT0, B0, X0, RES0)
         CALL SCALAPACK_UNMAP(X0, DESCL, X)
!                                 Print results
!                                 Only Rank=0 has the solution, X.
         IF (MP_RANK .EQ. 0) CALL WRCRN ('X', X, 1, N, 1)
!                                 Perturb B by adding 0.5+0.5i to B(2)
         IF(MP_RANK .EQ. 0) B(2) = B(2) + (0.5,0.5)
   10 CONTINUE
      IF (MP_RANK .EQ. 0) DEALLOCATE(A, B, X, RES)
      DEALLOCATE(A0, B0, FACT0, IPVT0, X0, RES0)
!                                 Exit Scalapack usage
      CALL SCALAPACK_EXIT(MP_ICTXT)

!                                 Shut down MPI
```

```
      MP_NPROCS = MP_SETUP(‘FINAL’)
99999 FORMAT (’  RCOND = ’,F5.3,/,’  L1 Condition number = ’,F6.3)
      END
```

Output

```
RCOND < 0.025
L1 Condition number < 75.0
                        X
              1                 2                 3
( 1.000,-1.000)  ( 2.000, 4.000)  ( 3.000, 0.000)

                        X
              1                 2                 3
( 0.910,-1.061)  ( 1.986, 4.175)  ( 3.123, 0.071)

                        X
              1                 2                 3
( 0.821,-1.123)  ( 1.972, 4.349)  ( 3.245, 0.142)
```

LFDCG

Computes the determinant of a complex general matrix given the *LU* factorization of the matrix.

Required Arguments

FACT — Complex N by N matrix containing the *LU* factorization of the coefficient matrix A as output from routine LFCCG/DLFCCG or LFTCG/DLFTCG. (Input)

IPVT — Vector of length N containing the pivoting information for the *LU* factorization of A as output from routine LFCCG/DLFCCG or LFTCG/DLFTCG. (Input)

DET1 — Complex scalar containing the mantissa of the determinant. (Output)
The value DET1 is normalized so that 1.0 ≤ |DET1| < 10.0 or DET1 = 0.0.

DET2 — Scalar containing the exponent of the determinant. (Output)
The determinant is returned in the form det(*A*) = DET1 * 10^{DET}.

Optional Arguments

N — Number of equations. (Input)
Default: N = size (FACT,2).

LDFACT — Leading dimension of FACT exactly as specified in the dimension statement of the calling program. (Input)
Default: LDFACT = size (FACT,1).

FORTRAN 90 Interface

Generic: CALL LFDCG (FACT, IPVT, DET1, DET2 [, …])

Specific: The specific interface names are S_LFDCG and D_LFDCG.

FORTRAN 77 Interface

Single: CALL LFDCG (N, FACT, LDFACT, IPVT, DET1, DET2)

Double: The double precision name is DLFDCG.

Description

Routine LFDCG computes the determinant of a complex general coefficient matrix. To compute the determinant the coefficient matrix must first undergo an *LU* factorization. This may be done by calling either LFCCG or LFTCG. The formula det *A* = det *L* det *U* is used to compute the determinant. Since the determinant of a triangular matrix is the product of the diagonal elements,

$$\det U = \prod_{i=1}^{N} U_{ii}$$

(The matrix *U* is stored in the upper triangle of FACT.) Since *L* is the product of triangular matrices with unit diagonals and of permutation matrices, det $L = (-1)^k$ where *k* is the number of pivoting interchanges.

LFDCG is based on the LINPACK routine CGEDI; see Dongarra et al. (1979).

Example

The determinant is computed for a complex general 3 × 3 matrix.

```
      USE LFDCG_INT
      USE LFTCG_INT
      USE UMACH_INT
!                                 Declare variables
      PARAMETER  (LDA=3, LDFACT=3, N=3)
      INTEGER    IPVT(N), NOUT
      REAL       DET2
      COMPLEX    A(LDA,LDA), FACT(LDFACT,LDFACT), DET1
!                                 Set values for  A
!
!                                 A = (  3.0-2.0i  2.0+4.0i  0.0-3.0i)
!                                     (  1.0+1.0i  2.0-6.0i  1.0+2.0i)
!                                     (  4.0+0.0i -5.0+1.0i  3.0-2.0i)
!
      DATA A/(3.0,-2.0), (1.0,1.0), (4.0,0.0), (2.0,4.0), (2.0,-6.0),&
            (-5.0,1.0), (0.0,-3.0), (1.0,2.0), (3.0,-2.0)/
!
!                                 Factor A
      CALL LFTCG (A, FACT, IPVT)
!                                 Compute the determinant for the
!                                 factored matrix
      CALL LFDCG (FACT, IPVT, DET1, DET2)
!                                 Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) DET1, DET2
!
99999 FORMAT (' The determinant of A is',3X,'(',F6.3,',',F6.3,&
             ') * 10**',F2.0)
      END
```

Output

```
The determinant of A is ( 0.700, 1.100) * 10**1.
```

LINCG

more...

more...

Computes the inverse of a complex general matrix.

Required Arguments

A — Complex `N` by `N` matrix containing the matrix to be inverted. (Input)

AINV — Complex `N` by `N` matrix containing the inverse of `A`. (Output)
If *A* is not needed, `A` and `AINV` can share the same storage locations.

Optional Arguments

N — Number of equations. (Input)
Default: `N` = size (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = size (`A`,1).

LDAINV — Leading dimension of `AINV` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDAINV` = size (`AINV`,1).

FORTRAN 90 Interface

Generic: `CALL LINCG (A, AINV [, …])`

Specific: The specific interface names are `S_LINCG` and `D_LINCG`.

FORTRAN 77 Interface

Single: `CALL LINCG (N, A, LDA, AINV, LDAINV)`

Double: The double precision name is `DLINCG`.

ScaLAPACK Interface

Generic: CALL LINCG (A0, AINV0 [, …])

Specific: The specific interface names are S_LINCG and D_LINCG.

See the *ScaLAPACK Usage Notes* below for a description of the arguments for distributed computing.

Description

Routine LINCG computes the inverse of a complex general matrix. The underlying code is based on either LINPACK , LAPACK, or ScaLAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see *Using ScaLAPACK, LAPACK, LINPACK, and EISPACK* in the Introduction section of this manual.

LINCG first uses the routine LFCCG to compute an *LU* factorization of the coefficient matrix and to estimate the condition number of the matrix. LFCCG computes *U* and the information needed to compute *L*. LINCT is then used to compute U^{-1}, i.e. use the inverse of U. Finally A^{-1} is computed using $A^{-1} = U^{-1}L^{-1}$.

LINCG fails if *U*, the upper triangular part of the factorization, has a zero diagonal element or if the iterative refinement algorithm fails to converge. This errors occurs only if *A* is singular or very close to a singular matrix.

If the estimated condition number is greater than $1/\varepsilon$ (where ε is machine precision), a warning error is issued. This indicates that very small changes in *A* can cause very large changes in A^{-1}.

Comments

1. Workspace may be explicitly provided, if desired, by use of L2NCG/DL2NCG. The reference is:

   CALL L2NCG (N, A, LDA, AINV, LDAINV, WK, IWK)

   The additional arguments are as follows:

   WK — Complex work vector of length N + N(N − 1)/2.

   IWK — Integer work vector of length N.

2. Informational errors

Type	Code	Description
3	1	The input matrix is too ill-conditioned. The inverse might not be accurate.
4	2	The input matrix is singular.

ScaLAPACK Usage Notes

The arguments which differ from the standard version of this routine are:

A0 — `MXLDA` by `MXCOL` `complex` local matrix containing the local portions of the distributed matrix `A`. `A` contains the matrix to be inverted. (Input)

AINV0 — `MXLDA` by `MXCOL` `complex` local matrix containing the local portions of the distributed matrix `AINV`. `AINV` contains the inverse of the matrix `A`. (Output)
If `A` is not needed, `A` and `AINV` can share the same storage locations.

All other arguments are global and are the same as described for the standard version of the routine. In the argument descriptions above, `MXLDA` and `MXCOL` can be obtained through a call to `SCALAPACK_GETDIM` (see *Utilities*) after a call to `SCALAPACK_SETUP` (see *Utilities*) has been made. See the *ScaLAPACK Example* below.

Examples

Example

The inverse is computed for a complex general 3 × 3 matrix.

```
      USE LINCG_INT
      USE WRCRN_INT
      USE CSSCAL_INT
!                                 Declare variables
      PARAMETER  (LDA=3, LDAINV=3, N=3)
      REAL       THIRD
      COMPLEX    A(LDA,LDA), AINV(LDAINV,LDAINV)
!                                 Set values for  A
!
!                                 A = (  1.0+1.0i  2.0+3.0i  3.0+3.0i)
!                                     (  2.0+1.0i  5.0+3.0i  7.0+4.0i)
!                                     ( -2.0+1.0i -4.0+4.0i -5.0+3.0i)
!
      DATA A/(1.0,1.0), (2.0,1.0), (-2.0,1.0), (2.0,3.0), (5.0,3.0),&
          (-4.0,4.0), (3.0,3.0), (7.0,4.0), (-5.0,3.0)/
!
!                                 Scale A by dividing by three
      THIRD = 1.0/3.0
      DO 10  I=1, N
         CALL CSSCAL (N, THIRD, A(:,I), 1)
   10 CONTINUE
!                                 Calculate the inverse of A
      CALL LINCG (A, AINV)
!                                 Print results
      CALL WRCRN ('AINV', AINV)
      END
```

Output

```
                          AINV
                  1                 2                 3
1  ( 6.400,-2.800)  (-3.800, 2.600)  (-2.600, 1.200)
2  (-1.600,-1.800)  ( 0.200, 0.600)  ( 0.400,-0.800)
3  (-0.600, 2.200)  ( 1.200,-1.400)  ( 0.400, 0.200)
```

ScaLAPACK Example

The inverse of the same 3 × 3 matrix is computed as a distributed example. SCALAPACK_MAP and SCALAPACK_UNMAP are IMSL utility routines (see *Chapter 11, "Utilities"*) used to map and unmap arrays to and from the processor grid. They are used here for brevity. DESCINIT is a ScaLAPACK tools routine which initializes the descriptors for the local arrays.

```
      USE MPI_SETUP_INT
      USE LINCG_INT
      USE WRCRN_INT
      USE SCALAPACK_SUPPORT
      IMPLICIT NONE
      INCLUDE 'mpif.h'
!                                 Declare variables
      INTEGER      J, LDA, N, DESCA(9)
      INTEGER      INFO, MXCOL, MXLDA, NPROW, NPCOL
      COMPLEX, ALLOCATABLE ::        A(:,:), AINV(:,:)
      COMPLEX, ALLOCATABLE ::        A0(:,:), AINV0(:,:)
      REAL         THIRD
      PARAMETER   (LDA=3, N=3)
!                           Set up for MPI
      MP_NPROCS = MP_SETUP()
      IF(MP_RANK .EQ. 0) THEN
          ALLOCATE (A(LDA,N), AINV(LDA,N))
!                                 Set values for A
          A(1,:) = (/ ( 1.0, 1.0), ( 2.0, 3.0), ( 3.0, 3.0)/)
          A(2,:) = (/ ( 2.0, 1.0), ( 5.0, 3.0), ( 7.0, 4.0)/)
          A(3,:) = (/ (-2.0, 1.0), (-4.0, 4.0), (-5.0, 3.0)/)
!                                 Scale A by dividing by three
          THIRD = 1.0/3.0
          A = A * THIRD
      ENDIF
!                                 Set up a 1D processor grid and define
!                                 its context ID, MP_ICTXT
      CALL SCALAPACK_SETUP(N, N, .TRUE., .TRUE.)
!                                 Get the array descriptor entities MXLDA,
!                                 and MXCOL
      CALL SCALAPACK_GETDIM(N, N, MP_MB, MP_NB, MXLDA, MXCOL)
!                                 Set up the array descriptors
      CALL DESCINIT(DESCA, N, N, MP_MB, MP_NB, 0, 0, MP_ICTXT, MXLDA, INFO)
!                                Allocate space for the local arrays
      ALLOCATE(A0(MXLDA,MXCOL), AINV0(MXLDA,MXCOL))
!                                Map input array to the processor grid
      CALL SCALAPACK_MAP(A, DESCA, A0)
!                                Factor A
      CALL LINCG (A0, AINV0)
!                                Unmap the results from the distributed
!                                arrays back to a non-distributed array.
!                                After the unmap, only Rank=0 has the full
!                                array.
      CALL SCALAPACK_UNMAP(AINV0, DESCA, AINV)
!                                Print results.
!                                Only Rank=0 has the solution, X.
      IF(MP_RANK.EQ.0) CALL WRCRN ('AINV', AINV)
      IF (MP_RANK .EQ. 0) DEALLOCATE(A, AINV)
      DEALLOCATE(A0, AINV0)
!                                Exit ScaLAPACK usage
      CALL SCALAPACK_EXIT(MP_ICTXT)
!                               Shut down MPI
      MP_NPROCS = MP_SETUP('FINAL')
      END
```

Output

```
                          AINV
                   1                  2                  3
 1  ( 6.400,-2.800)  (-3.800, 2.600)  (-2.600, 1.200)
 2  (-1.600,-1.800)  ( 0.200, 0.600)  ( 0.400,-0.800)
 3  (-0.600, 2.200)  ( 1.200,-1.400)  ( 0.400, 0.200)
```

LSLRT

more...

more...

Solves a real triangular system of linear equations.

Required Arguments

A — N by N matrix containing the coefficient matrix for the triangular linear system. (Input)
For a lower triangular system, only the lower triangular part and diagonal of A are referenced. For an upper triangular system, only the upper triangular part and diagonal of A are referenced.

B — Vector of length N containing the right-hand side of the linear system. (Input)

X — Vector of length N containing the solution to the linear system. (Output)
If B is not needed, B and X can share the same storage locations.

Optional Arguments

N — Number of equations. (Input)
Default: N = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

IPATH — Path indicator. (Input)
IPATH = 1 means solve AX = B, A lower triangular.
IPATH = 2 means solve AX = B, A upper triangular.
IPATH = 3 means solve $A^T X$ = B, A lower triangular.
IPATH = 4 means solve $A^T X$ = B, A upper triangular.
Default: IPATH = 1.

FORTRAN 90 Interface

Generic: `CALL LSLRT (A, B, X [, …])`

Specific: The specific interface names are `S_LSLRT` and `D_LSLRT`.

FORTRAN 77 Interface

Single: `CALL LSLRT (N, A, LDA, B, IPATH, X)`

Double: The double precision name is `DLSLRT`.

ScaLAPACK Interface

Generic: `CALL LSLRT (A0, B0, X0 [, …])`

Specific: The specific interface names are `S_LSLRT` and `D_LSLRT`.

See the *ScaLAPACK Usage Notes* below for a description of the arguments for distributed computing.

Description

Routine `LSLRT` solves a system of linear algebraic equations with a real triangular coefficient matrix. `LSLRT` fails if the matrix `A` has a zero diagonal element, in which case `A` is singular. The underlying code is based on either LINPACK , LAPACK, or ScaLAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see *Using ScaLAPACK, LAPACK, LINPACK, and EISPACK* in the Introduction section of this manual.

ScaLAPACK Usage Notes

The arguments which differ from the standard version of this routine are:

A0 — `MXLDA` by `MXCOL` local matrix containing the local portions of the distributed matrix `A`. `A` contains the coefficients of the linear system. (Input)
For a lower triangular system, only the lower triangular part and diagonal of `A` are referenced. For an upper triangular system, only the upper triangular part and diagonal of `A` are referenced.

B0 — Local vector of length `MXLDA` containing the local portions of the distributed vector `B`. `B` contains the right-hand side of the linear system. (Input)

X0 — Local vector of length `MXLDA` containing the local portions of the distributed vector `X`. `X` contains the solution to the linear system. (Output)
If `B` is not needed, `B` and `X` can share the same storage locations.

All other arguments are global and are the same as described for the standard version of the routine. In the argument descriptions above, MXLDA and MXCOL can be obtained through a call to SCALAPACK_GETDIM (see *Utilities*) after a call to SCALAPACK_SETUP (see *Utilities*) has been made. See the *ScaLAPACK Example* below.

Examples

Example

A system of three linear equations is solved. The coefficient matrix has lower triangular form and the right-hand-side vector, *b*, has three elements.

```
      USE LSLRT_INT
      USE WRRRN_INT
!                                 Declare variables
      PARAMETER  (LDA=3)
      REAL       A(LDA,LDA), B(LDA), X(LDA)
!                                 Set values for A and B
!
!                                 A = (  2.0              )
!                                     (  2.0    -1.0      )
!                                     ( -4.0     2.0    5.0)
!
!                                 B = (  2.0     5.0    0.0)
!
      DATA A/2.0, 2.0, -4.0, 0.0, -1.0, 2.0, 0.0, 0.0, 5.0/
      DATA B/2.0, 5.0, 0.0/
!
!                                 Solve AX = B     (IPATH = 1)
      CALL LSLRT (A, B, X)
!                                 Print results
      CALL WRRRN ('X', X, 1, 3, 1)
      END
```

Output

```
           X
    1        2        3
1.000   -3.000    2.000
```

ScaLAPACK Example

The same system of three linear equations is solved as a distributed computing example. The coefficient matrix has lower triangular form and the right-hand-side vector *b* has three elements. SCALAPACK_MAP and SCALAPACK_UNMAP are IMSL utility routines (see *Chapter 11, "Utilities"*) used to map and unmap arrays to and from the processor grid. They are used here for brevity. DESCINIT is a ScaLAPACK tools routine which initializes the descriptors for the local arrays.

```
      USE MPI_SETUP_INT
      USE LSLRT_INT
      USE WRRRN_INT
      USE SCALAPACK_SUPPORT
      IMPLICIT NONE
```

```
      INCLUDE 'mpif.h'
!                                   Declare variables
      INTEGER    LDA, N, DESCA(9), DESCX(9)
      INTEGER       INFO, MXCOL, MXLDA
      REAL, ALLOCATABLE ::          A(:,:), B(:), X(:)
      REAL, ALLOCATABLE ::          A0(:,:), B0(:), X0(:)
      PARAMETER  (LDA=3, N=3)
!                                   Set up for MPI
      MP_NPROCS = MP_SETUP()
      IF(MP_RANK .EQ. 0) THEN
          ALLOCATE (A(LDA,N), B(N), X(N))
!                                   Set values for A and B
          A(1,:) = (/ 2.0,  0.0,  0.0/)
          A(2,:) = (/ 2.0, -1.0,  0.0/)
          A(3,:) = (/-4.0,  2.0,  5.0/)
!
          B =      (/ 2.0,  5.0,  0.0/)
      ENDIF
!                                    Set up a 1D processor grid and define
!                                    its context ID, MP_ICTXT
      CALL SCALAPACK_SETUP(N, N, .TRUE., .TRUE.)
!                                    Get the array descriptor entities MXLDA,
!                                    and MXCOL
      CALL SCALAPACK_GETDIM(N, N, MP_MB, MP_NB, MXLDA, MXCOL)
!                                    Set up the array descriptors
      CALL DESCINIT(DESCA, N, N, MP_MB, MP_NB, 0, 0, MP_ICTXT, MXLDA, INFO)
      CALL DESCINIT(DESCX, N, 1, MP_MB, 1, 0, 0, MP_ICTXT, MXLDA, INFO)
!                                   Allocate space for the local arrays
      ALLOCATE (A0(MXLDA,MXCOL), B0(MXLDA), X0(MXLDA))
!                                   Map input arrays to the processor grid
      CALL SCALAPACK_MAP(A, DESCA, A0)
      CALL SCALAPACK_MAP(B, DESCX, B0)
!                                   Solve AX = B   (IPATH = 1)
      CALL LSLRT (A0, B0, X0)
!                                   Unmap the results from the distributed
!                                   arrays back to a non-distributed array.
!                                   After the unmap, only Rank=0 has the full
!                                   array.
      CALL SCALAPACK_UNMAP(X0, DESCX, X)
!                                   Print results.
!                                   Only Rank=0 has the solution, X.
      IF(MP_RANK .EQ. 0)CALL WRRRN ('X', X, 1, N, 1)
      IF (MP_RANK .EQ. 0) DEALLOCATE(A, B, X)
      DEALLOCATE(A0, B0, X0)
!                                   Exit Scalapack usage
      CALL SCALAPACK_EXIT(MP_ICTXT)
!                                   Shut down MPI
      MP_NPROCS = MP_SETUP('FINAL')
      END
```

Output

```
            X
     1        2        3
 1.000   -3.000    2.000
```

LFCRT

more...

more...

Estimates the condition number of a real triangular matrix.

Required Arguments

A — N by N matrix containing the coefficient matrix for the triangular linear system. (Input)
For a lower triangular system, only the lower triangular part and diagonal of A are referenced. For an upper triangular system, only the upper triangular part and diagonal of A are referenced.

RCOND — Scalar containing an estimate of the reciprocal of the L_1 condition number of A. (Output)

Optional Arguments

N — Number of equations. (Input)
Default: N = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

IPATH — Path indicator. (Input)
IPATH = 1 means A is lower triangular. IPATH = 2 means A is upper triangular.
Default: IPATH =1.

FORTRAN 90 Interface

Generic: CALL LFCRT (A, RCOND [, …])

Specific: The specific interface names are S_LFCRT and D_LFCRT.

FORTRAN 77 Interface

Single: `CALL LFCRT (N, A, LDA, IPATH, RCOND)`

Double: The double precision name is `DLFCRT`.

ScaLAPACK Interface

Generic: `CALL LFCRT (A0, RCOND [, …])`

Specific: The specific interface names are `S_LFCRT` and `D_LFCRT`.

See the ScaLAPACK Usage Notes below for a description of the arguments for distributed computing.

Description

Routine `LFCRT` estimates the condition number of a real triangular matrix. The L_1 condition number of the matrix A is defined to be $\kappa(A) = \|A\|_1 \|A^{-1}\|_1$. Since it is expensive to compute $\|A^{-1}\|_1$, the condition number is only estimated. The estimation algorithm is the same as used by LINPACK and is described by Cline et al. (1979).

If the estimated condition number is greater than $1/\varepsilon$ (where ε is machine precision), a warning error is issued. This indicates that very small changes in `A` can cause very large changes in the solution x.

The underlying code is based on either LINPACK , LAPACK, or ScaLAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see *Using ScaLAPACK, LAPACK, LINPACK, and EISPACK* in the Introduction section of this manual.

Comments

1. Workspace may be explicitly provided, if desired, by use of `L2CRT`/ `DL2CRT`. The reference is:

   `CALL L2CRT (N, A, LDA, IPATH, RCOND, WK)`

   The additional argument is:

   WK — Work vector of length `N`.

2. Informational error

Type	Code	Description
3	1	The input triangular matrix is algorithmically singular.

ScaLAPACK Usage Notes

The arguments which differ from the standard version of this routine are:

A0 — MXLDA by MXCOL local matrix containing the local portions of the distributed matrix A. A contains the coefficient matrix for the triangular linear system. (Input)
For a lower triangular system, only the lower triangular part and diagonal of A are referenced. For an upper triangular system, only the upper triangular part and diagonal of A are referenced.

All other arguments are global and are the same as described for the standard version of the routine. In the argument descriptions above, MXLDA and MXCOL can be obtained through a call to SCALAPACK_GETDIM (see *Utilities*) after a call to SCALAPACK_SETUP (see *Utilities*) has been made. See the *ScaLAPACK Example* below.

Examples

Example

An estimate of the reciprocal condition number is computed for a 3 × 3 lower triangular coefficient matrix.

```
      USE LFCRT_INT
      USE UMACH_INT
!                                 Declare variables
      PARAMETER  (LDA=3)
      REAL       A(LDA,LDA), RCOND
      INTEGER    NOUT
!                                 Set values for A and B
!                                 A = (  2.0              )
!                                     (  2.0    -1.0      )
!                                     ( -4.0     2.0   5.0)
!
      DATA A/2.0, 2.0, -4.0, 0.0, -1.0, 2.0, 0.0, 0.0, 5.0/
!
!                                 Compute the reciprocal condition
!                                 number  (IPATH=1)
      CALL LFCRT (A, RCOND)
!                                 Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) RCOND, 1.0E0/RCOND
99999 FORMAT ('  RCOND = ',F5.3,/,'  L1 Condition number = ',F6.3)
      END
```

Output

```
RCOND < 0.1
L1 Condition number < 15.0
```

ScaLAPACK Example

The same lower triangular matrix as in the example above is used in this distributed computing example. An estimate of the reciprocal condition number is computed for the 3 × 3 lower triangular coefficient matrix. SCALAPACK_MAP is an IMSL utility routine (see *Chapter 11, "Utilities"*) used to map an array to the processor grid. It is used here for brevity. DESCINIT is a ScaLAPACK tools routine which initializes the descriptors for the local arrays.

```
      USE MPI_SETUP_INT
      USE LFCRT_INT
      USE SCALAPACK_SUPPORT
      IMPLICIT NONE
      INCLUDE 'mpif.h'
!                                  Declare variables
      INTEGER    LDA, N, NOUT, DESCA(9)
      INTEGER       INFO, MXCOL, MXLDA
      REAL          RCOND
      REAL, ALLOCATABLE ::         A(:,:)
      REAL, ALLOCATABLE ::         A0(:,:)
      PARAMETER  (LDA=3, N=3)
!                                  Set up for MPI
      MP_NPROCS = MP_SETUP()
      IF(MP_RANK .EQ. 0) THEN
          ALLOCATE (A(LDA,N))
!                                  Set values for A
          A(1,:) = (/ 2.0,  0.0,  0.0/)
          A(2,:) = (/ 2.0, -1.0,  0.0/)
          A(3,:) = (/-4.0,  2.0,  5.0/)
      ENDIF
!                                   Set up a 1D processor grid and define
!                                   its context ID, MP_ICTXT
      CALL SCALAPACK_SETUP(N, N, .TRUE., .TRUE.)
!                                   Get the array descriptor entities MXLDA,
!                                   and MXCOL
      CALL SCALAPACK_GETDIM(N, N, MP_MB, MP_NB, MXLDA, MXCOL)
!                                   Set up the array descriptor
      CALL DESCINIT(DESCA, N, N, MP_MB, MP_NB, 0, 0, MP_ICTXT, MXLDA, INFO)
!                                   Allocate space for the local arrays
      ALLOCATE (A0(MXLDA,MXCOL))
!                                  Map input array to the processor grid
      CALL SCALAPACK_MAP(A, DESCA, A0)
!                                  Compute the reciprocal condition
!                                  number  (IPATH=1)
      CALL LFCRT (A0, RCOND)
!                                  Print results.
!                                  Only Rank=0 has the solution, RCOND.
      IF(MP_RANK .EQ. 0) THEN
         CALL UMACH (2, NOUT)
         WRITE (NOUT,99999) RCOND, 1.0E0/RCOND
      ENDIF
      IF (MP_RANK .EQ. 0) DEALLOCATE(A)
      DEALLOCATE(A0)
!                                  Exit Scalapack usage
      CALL SCALAPACK_EXIT(MP_ICTXT)
!                                  Shut down MPI
      MP_NPROCS = MP_SETUP('FINAL')
99999 FORMAT ('  RCOND = ',F5.3,/,'  L1 Condition number = ',F6.3)
      END
```

Output

```
RCOND < 0.1
L1 Condition number < 15.0
```

LFDRT

Computes the determinant of a real triangular matrix.

Required Arguments

A — N by N matrix containing the triangular matrix. (Input)
The matrix can be either upper or lower triangular.

DET1 — Scalar containing the mantissa of the determinant. (Output)
The value DET1 is normalized so that 1.0 ≤ |DET1| < 10.0 or DET1 = 0.0.

DET2 — Scalar containing the exponent of the determinant. (Output)
The determinant is returned in the form det(A) = DET1 * 10^{DET2}.

Optional Arguments

N — Number of equations. (Input)
Default: N = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

FORTRAN 90 Interface

Generic: CALL LFDRT (A, DET1, DET2 [, …])

Specific: The specific interface names are S_LFDRT and D_LFDRT.

FORTRAN 77 Interface

Single: CALL LFDRT (N, A, LDA, DET1, DET2)

Double: The double precision name is DLFDRT.

Description

Routine LFDRT computes the determinant of a real triangular coefficient matrix. The determinant of a triangular matrix is the product of the diagonal elements

$$\det A = \prod_{i=1}^{N} A_{ii}$$

`LFDRT` is based on the LINPACK routine `STRDI`; see Dongarra et al. (1979).

Comments

Informational error

Type	Code	Description
3	1	The input triangular matrix is singular.

Example

The determinant is computed for a 3×3 lower triangular matrix.

```
      USE LFDRT_INT
      USE UMACH_INT
!                                 Declare variables
      PARAMETER  (LDA=3)
      REAL       A(LDA,LDA), DET1, DET2
      INTEGER    NOUT
!                                 Set values for  A
!                                 A = (  2.0                )
!                                     (  2.0    -1.0        )
!                                     ( -4.0     2.0    5.0)
!
      DATA A/2.0, 2.0, -4.0, 0.0, -1.0, 2.0, 0.0, 0.0, 5.0/
!
!                                 Compute the determinant of A
      CALL LFDRT (A, DET1, DET2)
!                                 Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) DET1, DET2
99999 FORMAT (' The determinant of A is ', F6.3, ' * 10**', F2.0)
      END
```

Output

```
The determinant of A is -1.000 * 10**1.
```

LINRT

Computes the inverse of a real triangular matrix.

Required Arguments

A — N by N matrix containing the triangular matrix to be inverted. (Input)
For a lower triangular matrix, only the lower triangular part and diagonal of A are referenced. For an upper triangular matrix, only the upper triangular part and diagonal of A are referenced.

AINV — N by N matrix containing the inverse of A. (Output)
If A is lower triangular, AINV is also lower triangular. If A is upper triangular, AINV is also upper triangular. If A is not needed, A and AINV can share the same storage locations.

Optional Arguments

N — Number of equations. (Input)
Default: N = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

IPATH — Path indicator. (Input)
IPATH = 1 means A is lower triangular. IPATH = 2 means A is upper triangular.
Default: IPATH = 1.

LDAINV — Leading dimension of AINV exactly as specified in the dimension statement of the calling program. (Input)
Default: LDAINV = size (AINV,1).

FORTRAN 90 Interface

Generic: CALL LINRT (A, AINV [, …])

Specific: The specific interface names are S_LINRT and D_LINRT.

FORTRAN 77 Interface

Single: CALL LINRT (N, A, LDA, IPATH, AINV, LDAINV)

Double: The double precision name is DLINRT.

Description

Routine LINRT computes the inverse of a real triangular matrix. It fails if A has a zero diagonal element.

Example

The inverse is computed for a 3 × 3 lower triangular matrix.

```
      USE LINRT_INT
      USE WRRRN_INT
!                                 Declare variables
      PARAMETER  (LDA=3)
      REAL       A(LDA,LDA), AINV(LDA,LDA)
!                                 Set values for  A
!                                 A = (  2.0             )
!                                     (  2.0    -1.0      )
!                                     ( -4.0     2.0    5.0)
!
      DATA A/2.0, 2.0, -4.0, 0.0, -1.0, 2.0, 0.0, 0.0, 5.0/
!
!                                 Compute the inverse of A
      CALL LINRT (A, AINV)
!                                 Print results
      CALL WRRRN ('AINV', AINV)
      END
```

Output

```
          AINV
       1       2       3
1   0.500   0.000   0.000
2   1.000  -1.000   0.000
3   0.000   0.400   0.200
```

LSLCT

more... more...

Solves a complex triangular system of linear equations.

Required Arguments

A — Complex N by N matrix containing the coefficient matrix of the triangular linear system. (Input)
For a lower triangular system, only the lower triangle of A is referenced. For an upper triangular system, only the upper triangle of A is referenced.

B — Complex vector of length N containing the right-hand side of the linear system. (Input)

X — Complex vector of length N containing the solution to the linear system. (Output)
If B is not needed, B and X can share the same storage locations.

Optional Arguments

N — Number of equations. (Input)
Default: N = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

IPATH — Path indicator. (Input)
IPATH = 1 means solve $AX = B$, A lower triangular
IPATH = 2 means solve $AX = B$, A upper triangular
IPATH = 3 means solve $A^H X = B$, A lower triangular
IPATH = 4 means solve $A^H X = B$, A upper triangular
Default: IPATH = 1.

FORTRAN 90 Interface

Generic: `CALL LSLCT (A, B, X [, …])`

Specific: The specific interface names are `S_LSLCT` and `D_LSLCT`.

FORTRAN 77 Interface

Single: `CALL LSLCT (N, A, LDA, B, IPATH, X)`

Double: The double precision name is `DLSLCT`.

ScaLAPACK Interface

Generic: `CALL LSLCT (A0, B0, X0 [, …])`

Specific: The specific interface names are `S_LSLCT` and `D_LSLCT`.

See the *ScaLAPACK Usage Notes* below for a description of the arguments for distributed computing.

Description

Routine `LSLCT` solves a system of linear algebraic equations with a complex triangular coefficient matrix. `LSLCT` fails if the matrix `A` has a zero diagonal element, in which case `A` is singular. The underlying code is based on either LINPACK , LAPACK, or ScaLAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see *Using ScaLAPACK, LAPACK, LINPACK, and EISPACK* in the Introduction section of this manual.

Comments

Informational error

Type	**Code**	**Description**
4	1	The input triangular matrix is singular. Some of its diagonal elements are near zero.

ScaLAPACK Usage Notes

The arguments which differ from the standard version of this routine are:

A0 — `MXLDA` by `MXCOL` complex local matrix containing the local portions of the distributed matrix `A`. `A` contains the coefficient matrix of the triangular linear system. (Input)
For a lower triangular system, only the lower triangular part and diagonal of `A` are referenced. For an upper triangular system, only the upper triangular part and diagonal of `A` are referenced.

B0 — Local complex vector of length `MXLDA` containing the local portions of the distributed vector `B`. `B` contains the right-hand side of the linear system. (Input)

X0 — Local complex vector of length `MXLDA` containing the local portions of the distributed vector `X`. `X` contains the solution to the linear system. (Output)
If `B` is not needed, `B` and `X` can share the same storage locations.

All other arguments are global and are the same as described for the standard version of the routine. In the argument descriptions above, `MXLDA` and `MXCOL` can be obtained through a call to `SCALAPACK_GETDIM` (see *Utilities*) after a call to `SCALAPACK_SETUP` (see *Utilities*) has been made. See the *ScaLAPACK Example* below.

Examples

Example

A system of three linear equations is solved. The coefficient matrix has lower triangular form and the right-hand-side vector, *b*, has three elements.

```
      USE LSLCT_INT
      USE WRCRN_INT
!                                 Declare variables
      INTEGER      LDA
      PARAMETER    (LDA=3)
      COMPLEX      A(LDA,LDA), B(LDA), X(LDA)
!                                Set values for A and B
!
!                                A = ( -3.0+2.0i                     )
!                                    ( -2.0-1.0i  0.0+6.0i           )
!                                    ( -1.0+3.0i  1.0-5.0i -4.0+0.0i )
!
!                                B = (-13.0+0.0i -10.0-1.0i -11.0+3.0i)
!
      DATA A/(-3.0,2.0), (-2.0,-1.0), (-1.0, 3.0), (0.0,0.0), (0.0,6.0),&
             (1.0,-5.0), (0.0,0.0), (0.0,0.0), (-4.0,0.0)/
      DATA B/(-13.0,0.0), (-10.0,-1.0), (-11.0,3.0)/
!
!                                 Solve AX = B
      CALL LSLCT (A, B, X)
!                                 Print results
      CALL WRCRN ('X', X, 1, 3, 1)
      END
```

Output

```
                          X
              1                 2                 3
 ( 3.000, 2.000)  ( 1.000, 1.000)  ( 2.000, 0.000)
```

ScaLAPACK Example

The same lower triangular matrix as in the example above is used in this distributed computing example. The system of three linear equations is solved. SCALAPACK_MAP and SCALAPACK_UNMAP are IMSL utility routines (see *Chapter 11, "Utilities"*) used to map and unmap arrays to and from the processor grid. They are used here for brevity. DESCINIT is a ScaLAPACK tools routine which initializes the descriptors for the local arrays.

```
      USE MPI_SETUP_INT
      USE LSLCT_INT
      USE WRCRN_INT
      USE SCALAPACK_SUPPORT
      IMPLICIT NONE
      INCLUDE 'mpif.h'
!                                  Declare variables
      INTEGER    LDA, N, DESCA(9), DESCX(9)
      INTEGER       INFO, MXCOL, MXLDA
      COMPLEX, ALLOCATABLE ::        A(:,:), B(:), X(:)
      COMPLEX, ALLOCATABLE ::        A0(:,:), B0(:), X0(:)
      PARAMETER  (LDA=3, N=3)
!                                  Set up for MPI
      MP_NPROCS = MP_SETUP()
      IF(MP_RANK .EQ. 0) THEN
          ALLOCATE (A(LDA,N), B(N), X(N))
!                                  Set values for A
          A(1,:) = (/ (-3.0,  2.0), (0.0,  0.0), ( 0.0, 0.0)/)
          A(2,:) = (/ (-2.0, -1.0), (0.0,  6.0), ( 0.0, 0.0)/)
          A(3,:) = (/ (-1.0,  3.0), (1.0, -5.0), (-4.0, 0.0)/)
!
          B      = (/ (-13.0, 0.0), (-10.0, -1.0), (-11.0, 3.0)
      ENDIF
!                                   Set up a 1D processor grid and define
!                                   its context ID, MP_ICTXT
      CALL SCALAPACK_SETUP(N, N, .TRUE., .TRUE.)
!                                   Get the array descriptor entities MXLDA,
!                                   and MXCOL
      CALL SCALAPACK_GETDIM(N, N, MP_MB, MP_NB, MXLDA, MXCOL)
!                                   Set up the array descriptor
      CALL DESCINIT(DESCA, N, N, MP_MB, MP_NB, 0, 0, MP_ICTXT, MXLDA, INFO)
      CALL DESCINIT(DESCX, N, 1, MP_MB, 1, 0, 0, MP_ICTXT, MXLDA, INFO)
!                                   Allocate space for the local arrays
      ALLOCATE (A0(MXLDA,MXCOL), B0(MXLDA), X0(MXLDA))
!                                  Map input arrays to the processor grid
      CALL SCALAPACK_MAP(A, DESCA, A0)
      CALL SCALAPACK_MAP(B, DESCX, B0)
!                                  Solve AX = B
      CALL LSLCT (A0, B0, X0)
!                                  Unmap the results from the distributed
!                                  arrays back to a non-distributed array.
!                                  After the unmap, only Rank=0 has the full
!                                  array.
      CALL SCALAPACK_UNMAP(X0, DESCX, X)
!                                  Print results.
!                                  Only Rank=0 has the solution, X.
      IF(MP_RANK .EQ. 0) CALL WRCRN ('X', X, 1, 3, 1)
      IF (MP_RANK .EQ. 0) DEALLOCATE(A, B, X)
      DEALLOCATE(A0, B0, X0)
!                                  Exit ScaLAPACK usage
      CALL SCALAPACK_EXIT(MP_ICTXT)
!                                  Shut down MPI
      MP_NPROCS = MP_SETUP('FINAL')
      END
```

Output

```
                               X
               1                   2                   3
  ( 3.000, 2.000)  ( 1.000, 1.000)  ( 2.000, 0.000)
```

LFCCT

more...

more...

Estimates the condition number of a complex triangular matrix.

Required Arguments

A — Complex `N` by `N` matrix containing the triangular matrix. (Input)
For a lower triangular system, only the lower triangle of `A` is referenced. For an upper triangular system, only the upper triangle of `A` is referenced.

RCOND — Scalar containing an estimate of the reciprocal of the L_1 condition number of `A`. (Output)

Optional Arguments

N — Number of equations. (Input)
Default: `N` = size (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = size (`A`,1).

IPATH — Path indicator. (Input)
`IPATH` = 1 means `A` is lower triangular.
`IPATH` = 2 means `A` is upper triangular.
Default: `IPATH` =1.

FORTRAN 90 Interface

Generic: `CALL LFCCT (A, RCOND [,…])`

Specific: The specific interface names are `S_LFCCT` and `D_LFCCT`.

FORTRAN 77 Interface

Single: `CALL LFCCT (N, A, LDA, IPATH, RCOND)`

Double: The double precision name is `DLFCCT`.

ScaLAPACK Interface

Generic: `CALL LFCCT (A0, RCOND [,…])`

Specific: The specific interface names are `S_LFCCT` and `D_LFCCT`.

See the *ScaLAPACK Usage Notes* below for a description of the arguments for distributed computing.

Description

Routine `LFCCT` estimates the condition number of a complex triangular matrix. The L_1 condition number of the matrix A is defined to be $\kappa(A) = \|A\|_1 \|A^{-1}\|_1$. Since it is expensive to compute $\|A^{-1}\|_1$, the condition number is only estimated. The estimation algorithm is the same as used by LINPACK and is described by Cline et al. (1979). If the estimated condition number is greater than $1/\varepsilon$ (where ε is machine precision), a warning error is issued. This indicates that very small changes in A can cause very large changes in the solution x. The underlying code is based on either LINPACK , LAPACK, or ScaLAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see *Using ScaLAPACK, LAPACK, LINPACK, and EISPACK* in the Introduction section of this manual.

Comments

1. Workspace may be explicitly provided, if desired, by use of `L2CCT/DL2CCT`. The reference is:

   `CALL L2CCT (N, A, LDA, IPATH, RCOND, CWK)`

   The additional argument is:

   CWK — Complex work vector of length `N`.

2. Informational error

Type	Code	Description
3	1	The input triangular matrix is algorithmically singular.

ScaLAPACK Usage Notes

The arguments which differ from the standard version of this routine are:

A0 — MXLDA by MXCOL complex local matrix containing the local portions of the distributed matrix A. A contains the coefficient matrix of the triangular linear system. (Input)
For a lower triangular system, only the lower triangular part and diagonal of A are referenced. For an upper triangular system, only the upper triangular part and diagonal of A are referenced.

All other arguments are global and are the same as described for the standard version of the routine. In the argument descriptions above, MXLDA and MXCOL can be obtained through a call to SCALAPACK_GETDIM (see *Utilities*) after a call to SCALAPACK_SETUP (see *Utilities*) has been made. See the *ScaLAPACK Example* below.

Examples

Example

An estimate of the reciprocal condition number is computed for a 3 × 3 lower triangular coefficient matrix.

```
      USE LFCCT_INT
      USE UMACH_INT
!                                 Declare variables
      INTEGER    LDA, N
      PARAMETER  (LDA=3)
      INTEGER    NOUT
      REAL       RCOND
      COMPLEX    A(LDA,LDA)
!                                Set values for A
!
!                                A = ( -3.0+2.0i                     )
!                                    ( -2.0-1.0i  0.0+6.0i           )
!                                    ( -1.0+3.0i  1.0-5.0i -4.0+0.0i )
!
      DATA A/(-3.0,2.0), (-2.0,-1.0), (-1.0, 3.0), (0.0,0.0), (0.0,6.0),&
            (1.0,-5.0), (0.0,0.0), (0.0,0.0), (-4.0,0.0)/
!
!                                 Compute the reciprocal condition
!                                 number
      CALL LFCCT (A, RCOND)
!                                 Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) RCOND, 1.0E0/RCOND
99999 FORMAT ('  RCOND = ',F5.3,/,'  L1 Condition number = ',F6.3)
      END
```

Output

```
RCOND < 0.2
L1 Condition number < 10.0
```

ScaLAPACK Example

The same lower triangular matrix as in the example above is used in this distributed computing example. An estimate of the reciprocal condition number is computed for a 3 × 3 lower triangular coefficient matrix. SCALAPACK_MAP and SCALAPACK_UNMAP are IMSL utility routines (see Chapter 11, "Utilities") used to map and unmap arrays to and from the processor grid. They are used here for brevity. DESCINIT is a ScaLAPACK tools routine which initializes the descriptors for the local arrays.

```
      USE MPI_SETUP_INT
      USE LFCCT_INT
      USE UMACH_INT
      USE SCALAPACK_SUPPORT
      IMPLICIT NONE
      INCLUDE 'mpif.h'
!                                  Declare variables
      INTEGER    LDA, N, NOUT, DESCA(9)
      INTEGER       INFO, MXCOL, MXLDA
      REAL          RCOND
      COMPLEX, ALLOCATABLE ::        A(:,:)
      COMPLEX, ALLOCATABLE ::        A0(:,:)
      PARAMETER  (LDA=3, N=3)
!                                  Set up for MPI
      MP_NPROCS = MP_SETUP()
      IF(MP_RANK .EQ. 0) THEN
          ALLOCATE (A(LDA,N))
!                                  Set values for A
          A(1,:) = (/ (-3.0,  2.0), (0.0,  0.0), ( 0.0, 0.0)/)
          A(2,:) = (/ (-2.0, -1.0), (0.0,  6.0), ( 0.0, 0.0)/)
          A(3,:) = (/ (-1.0,  3.0), (1.0, -5.0), (-4.0, 0.0)/)
      ENDIF
!                                   Set up a 1D processor grid and define
!                                   its context ID, MP_ICTXT
      CALL SCALAPACK_SETUP(N, N, .TRUE., .TRUE.)
!                                   Get the array descriptor entities MXLDA,
!                                   and MXCOL
      CALL SCALAPACK_GETDIM(N, N, MP_MB, MP_NB, MXLDA, MXCOL)
!                                   Set up the array descriptor
      CALL DESCINIT(DESCA, N, N, MP_MB, MP_NB, 0, 0, MP_ICTXT, MXLDA, INFO)
!                                   Allocate space for the local arrays
      ALLOCATE (A0(MXLDA,MXCOL))
!                                  Map input arrays to the processor grid
      CALL SCALAPACK_MAP(A, DESCA, A0)
!                                  Compute the reciprocal condition
!                                  number
      CALL LFCCT (A0, RCOND)
!                                  Print results.
!                                  Only Rank=0 has the solution, RCOND.
      IF (MP_RANK .EQ. 0) THEN
         CALL UMACH (2, NOUT)
         WRITE (NOUT,99999) RCOND, 1.0E0/RCOND
      ENDIF
      IF (MP_RANK .EQ. 0) DEALLOCATE(A)
      DEALLOCATE(A0)
!                                 Exit ScaLAPACK usage
      CALL SCALAPACK_EXIT(MP_ICTXT)
!                                 Shut down MPI
      MP_NPROCS = MP_SETUP('FINAL')
99999 FORMAT ('  RCOND = ',F5.3,/,'  L1 Condition number = ',F6.3)
      END
```

Output

```
RCOND < 0.2
L1 Condition number < 10.0
```

LFDCT

Computes the determinant of a complex triangular matrix.

Required Arguments

A — Complex `N` by `N` matrix containing the triangular matrix.(Input)

DET1 — Complex scalar containing the mantissa of the determinant. (Output)
The value `DET1` is normalized so that 1.0 ≤ |`DET1`| < 10.0 or `DET1` = 0.0.

DET2 — Scalar containing the exponent of the determinant. (Output)
The determinant is returned in the form `det(A)` = `DET1 * 10`^{DET2}.

Optional Arguments

N — Number of equations. (Input)
Default: `N` = `size` (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = `size` (`A`,1).

FORTRAN 90 Interface

Generic: `CALL LFDCT` (`A`, `DET1`, `DET2` `[,…]`)

Specific: The specific interface names are `S_LFDCT` and `D_LFDCT`.

FORTRAN 77 Interface

Single: `CALL LFDCT` (`N`, `A`, `LDA`, `DET1`, `DET2`)

Double: The double precision name is `DLFDCT`.

Description

Routine `LFDCT` computes the determinant of a complex triangular coefficient matrix. The determinant of a triangular matrix is the product of the diagonal elements

$$\det A = \prod_{i=1}^{N} A_{ii}$$

LFDCT is based on the LINPACK routine CTRDI; see Dongarra et al. (1979).

Comments

Informational error

Type	Code	Description
3	1	The input triangular matrix is singular.

Example

The determinant is computed for a 3 × 3 complex lower triangular matrix.

```
      USE LFDCT_INT
      USE UMACH_INT
!                                 Declare variables
      INTEGER    LDA, N
      PARAMETER  (LDA=3, N=3)
      INTEGER    NOUT
      REAL       DET2
      COMPLEX    A(LDA,LDA), DET1
!                                Set values for A
!
!                                A = ( -3.0+2.0i                    )
!                                    ( -2.0-1.0i  0.0+6.0i          )
!                                    ( -1.0+3.0i  1.0-5.0i -4.0+0.0i )
!
      DATA A/(-3.0,2.0), (-2.0,-1.0), (-1.0, 3.0), (0.0,0.0), (0.0,6.0),&
            (1.0,-5.0), (0.0,0.0), (0.0,0.0), (-4.0,0.0)/
!
!                                 Compute the determinant of A
      CALL LFDCT (A, DET1, DET2)
!                                 Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) DET1, DET2
99999 FORMAT (’ The determinant of A is (’,F4.1,’,’,F4.1,’) * 10**’,&
             F2.0)
      END
```

Output

```
The determinant of A is ( 0.5, 0.7) * 10**2.
```

LINCT

Computes the inverse of a complex triangular matrixs.

Required Arguments

A — Complex N by N matrix containing the triangular matrix to be inverted. (Input)
For a lower triangular matrix, only the lower triangle of A is referenced. For an upper triangular matrix, only the upper triangle of A is referenced.

AINV — Complex N by N matrix containing the inverse of A. (Output)
If A is lower triangular, AINV is also lower triangular. If A is upper triangular, AINV is also upper triangular. If A is not needed, A and AINV can share the same storage locations.

Optional Arguments

N — Number of equations. (Input)
Default: N = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

IPATH — Path indicator. (Input)
IPATH = 1 means ***A*** is lower triangular.
IPATH = 2 means ***A*** is upper triangular.
Default: IPATH = 1.

LDAINV — Leading dimension of AINV exactly as specified in the dimension statement of the calling program. (Input)
Default: LDAINV = size (AINV,1).

FORTRAN 90 Interface

Generic: CALL LINCT (A, AINV [,…])

Specific: The specific interface names are S_LINCT and D_LINCT.

FORTRAN 77 Interface

Single: `CALL LINCT (N, A, LDA, IPATH, AINV, LDAINV)`

Double: The double precision name is `DLINCT`.

Description

Routine `LINCT` computes the inverse of a complex triangular matrix. It fails if `A` has a zero diagonal element.

Comments

Informational error

Type	Code	Description
4	1	The input triangular matrix is singular. Some of its diagonal elements are close to zero.

Example

The inverse is computed for a 3 × 3 lower triangular matrix.

```
      USE LINCT_INT
      USE WRCRN_INT
!                                 Declare variables
      INTEGER    LDA
      PARAMETER  (LDA=3)
      COMPLEX    A(LDA,LDA), AINV(LDA,LDA)
!                                Set values for A
!
!                                A = ( -3.0+2.0i                   )
!                                    ( -2.0-1.0i  0.0+6.0i          )
!                                    ( -1.0+3.0i  1.0-5.0i -4.0+0.0i )
!
      DATA A/(-3.0,2.0), (-2.0,-1.0), (-1.0, 3.0), (0.0,0.0), (0.0,6.0),&
            (1.0,-5.0), (0.0,0.0), (0.0,0.0), (-4.0,0.0)/
!
!                                 Compute the inverse of A
      CALL LINCT (A, AINV)
!                                 Print results
      CALL WRCRN ('AINV', AINV)
      END
```

Output

```
                            AINV
                   1                   2                   3
1  (-0.2308,-0.1538)  ( 0.0000, 0.0000)  ( 0.0000, 0.0000)
2  (-0.0897, 0.0513)  ( 0.0000,-0.1667)  ( 0.0000, 0.0000)
3  ( 0.2147,-0.0096)  (-0.2083,-0.0417)  (-0.2500, 0.0000)
```

LSADS

more...

more...

Solves a real symmetric positive definite system of linear equations with iterative refinement.

Required Arguments

A — `N` by `N` matrix containing the coefficient matrix of the symmetric positive definite linear system. (Input)
Only the upper triangle of `A` is referenced.

B — Vector of length `N` containing the right-hand side of the linear system. (Input)

X — Vector of length `N` containing the solution to the linear system. (Output)

Optional Arguments

N — Number of equations. (Input)
Default: `N` = size (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = size (`A`,1).

FORTRAN 90 Interface

Generic: `CALL LSADS (A, B, X [,…])`

Specific: The specific interface names are `S_LSADS` and `D_LSADS`.

FORTRAN 77 Interface

Single: `CALL LSADS (N, A, LDA, B, X)`

Double: The double precision name is `DLSADS`.

ScaLAPACK Interface

Generic: `CALL LSADS (A0, B0, X0 [,…])`

Specific: The specific interface names are `S_LSADS` and `D_LSADS`.

See the *ScaLAPACK Usage Notes* below for a description of the arguments for distributed computing.

Description

Routine `LSADS` solves a system of linear algebraic equations having a real symmetric positive definite coefficient matrix. The underlying code is based on either LINPACK , LAPACK, or ScaLAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see *Using ScaLAPACK, LAPACK, LINPACK, and EISPACK* in the Introduction section of this manual. `LSADS` first uses the routine `LFCDS` to compute an R^TR Cholesky factorization of the coefficient matrix and to estimate the condition number of the matrix. The matrix R is upper triangular. The solution of the linear system is then found using the iterative refinement routine `LFIDS`. `LSADS` fails if any submatrix of R is not positive definite, if R has a zero diagonal element or if the iterative refinement algorithm fails to converge. These errors occur only if A is either very close to a singular matrix or a matrix which is not positive definite. If the estimated condition number is greater than $1/\varepsilon$ (where ε is machine precision), a warning error is issued. This indicates that very small changes in A can cause very large changes in the solution x. Iterative refinement can sometimes find the solution to such a system. `LSADS` solves the problem that is represented in the computer; however, this problem may differ from the problem whose solution is desired.

Comments

1. Workspace may be explicitly provided, if desired, by use of `L2ADS/DL2ADS`. The reference is:

   `CALL L2ADS (N, A, LDA, B, X, FACT, WK)`

   The additional arguments are as follows:

   FACT— Work vector of length N^2 containing the R^TR factorization of `A` on output.

   WK — Work vector of length `N`.

2. Informational errors

Type	Code	Description
3	1	The input matrix is too ill-conditioned. The solution might not be accurate.
4	2	The input matrix is not positive definite.

3. *Integer Options* with *Chapter 11* Options Manager

16 This option uses four values to solve memory bank conflict (access inefficiency) problems. In routine L2ADS the leading dimension of FACT is increased by IVAL(3) when N is a multiple of IVAL(4). The values IVAL(3) and IVAL(4) are temporarily replaced by IVAL(1) and IVAL(2), respectively, in LSADS. Additional memory allocation for FACT and option value restoration are done automatically in LSADS. Users directly calling L2ADS can allocate additional space for FACT and set IVAL(3) and IVAL(4) so that memory bank conflicts no longer cause inefficiencies. There is no requirement that users change existing applications that use LSADS or L2ADS. Default values for the option are IVAL(*) = 1, 16, 0, 1.

17 This option has two values that determine if the L_1 condition number is to be computed. Routine LSADS temporarily replaces IVAL(2) by IVAL(1). The routine L2CDS computes the condition number if IVAL(2) = 2. Otherwise L2CDS skips this computation. LSADS restores the option. Default values for the option are IVAL(*) = 1, 2.

ScaLAPACK Usage Notes

The arguments which differ from the standard version of this routine are:

A0 — MXLDA by MXCOL local matrix containing the local portions of the distributed matrix A. A contains the coefficient matrix of the symmetric positive definite linear system. (Input)

B0 — Local vector of length MXLDA containing the local portions of the distributed vector B. B contains the right-hand side of the linear system. (Input)

X0 — Local vector of length MXLDA containing the local portions of the distributed vector X. X contains the solution to the linear system. (Output)

All other arguments are global and are the same as described for the standard version of the routine. In the argument descriptions above, MXLDA and MXCOL can be obtained through a call to SCALAPACK_GETDIM (see *Utilities*) after a call to SCALAPACK_SETUP (see *Utilities*) has been made. See the *ScaLAPACK Example* below.

Examples

Example

A system of three linear equations is solved. The coefficient matrix has real positive definite form and the right-hand-side vector *b* has three elements.

```
      USE LSADS_INT
      USE WRRRN_INT
!                                  Declare variables
      INTEGER    LDA, N
      PARAMETER  (LDA=3, N=3)
      REAL       A(LDA,LDA), B(N), X(N)
!
!                                  Set values for A and B
!
```

```
!                                 A = (  1.0  -3.0   2.0)
!                                     ( -3.0  10.0  -5.0)
!                                     (  2.0  -5.0   6.0)
!
!                                 B = ( 27.0 -78.0  64.0)
!
      DATA A/1.0, -3.0, 2.0, -3.0, 10.0, -5.0, 2.0, -5.0, 6.0/
      DATA B/27.0, -78.0, 64.0/
!
      CALL LSADS (A, B, X)
!                                 Print results
      CALL WRRRN ('X', X, 1, N, 1)
!
      END
```

Output

```
          X
    1        2        3
1.000   -4.000    7.000
```

ScaLAPACK Example

The same system of three linear equations is solved as a distributed computing example. The coefficient matrix has real positive definite form and the right-hand-side vector *b* has three elements. `SCALAPACK_MAP` and `SCALAPACK_UNMAP` are IMSL utility routines (see *Chapter 11, "Utilities"*) used to map and unmap arrays to and from the processor grid. They are used here for brevity. `DESCINIT` is a ScaLAPACK tools routine which initializes the descriptors for the local arrays.

```
      USE MPI_SETUP_INT
      USE LSADS_INT
      USE WRRRN_INT
      USE SCALAPACK_SUPPORT
      IMPLICIT NONE
      INCLUDE 'mpif.h'
!                                 Declare variables
      INTEGER    LDA, N, DESCA(9), DESCX(9)
      INTEGER       INFO, MXCOL, MXLDA
      REAL, ALLOCATABLE ::        A(:,:), B(:), X(:)
      REAL, ALLOCATABLE ::        A0(:,:), B0(:), X0(:)
      PARAMETER  (LDA=3, N=3)
!                                 Set up for MPI
      MP_NPROCS = MP_SETUP()
      IF(MP_RANK .EQ. 0) THEN
          ALLOCATE (A(LDA,N), B(N), X(N))
!                                 Set values for A and B
          A(1,:) = (/  1.0,  -3.0,  2.0/)
          A(2,:) = (/ -3.0,  10.0, -5.0/)
          A(3,:) = (/  2.0,  -5.0,  6.0/)
!
          B = (/27.0, -78.0,  64.0/)
      ENDIF
!                                  Set up a 1D processor grid and define
!                                  its context ID, MP_ICTXT
      CALL SCALAPACK_SETUP(N, N, .TRUE., .TRUE.)
!                                  Get the array descriptor entities MXLDA,
!                                  and MXCOL
      CALL SCALAPACK_GETDIM(N, N, MP_MB, MP_NB, MXLDA, MXCOL)
!                                  Set up the array descriptors
      CALL DESCINIT(DESCA, N, N, MP_MB, MP_NB, 0, 0, MP_ICTXT, MXLDA, INFO)
```

```
      CALL DESCINIT(DESCX, N, 1, MP_MB, 1, 0, 0, MP_ICTXT, MXLDA, INFO)
!                               Allocate space for the local arrays
      ALLOCATE (A0(MXLDA,MXCOL), B0(MXLDA), X0(MXLDA))
!                                Map input arrays to the processor grid
      CALL SCALAPACK_MAP(A, DESCA, A0)
      CALL SCALAPACK_MAP(B, DESCX, B0)
!                                Solve the system of equations
      CALL LSADS (A0, B0, X0)
!                                Unmap the results from the distributed
!                                arrays back to a non-distributed array.
!                                After the unmap, only Rank=0 has the full
!                                array.
      CALL SCALAPACK_UNMAP(X0, DESCX, X)
!                                Print results.
!                                Only Rank=0 has the solution, X.
      IF(MP_RANK .EQ. 0)CALL WRRRN ('X', X, 1, N, 1)
      IF (MP_RANK .EQ. 0) DEALLOCATE(A, B, X)
      DEALLOCATE(A0, B0, X0)
!                                Exit ScaLAPACK usage
      CALL SCALAPACK_EXIT(MP_ICTXT)
!                                Shut down MPI
      MP_NPROCS = MP_SETUP('FINAL')
      END
```

Output

```
          X
    1       2       3
1.000   -4.000   7.000
```

LSLDS

more...

more...

Solves a real symmetric positive definite system of linear equations without iterative refinement .

Required Arguments

A — N by N matrix containing the coefficient matrix of the symmetric positive definite linear system. (Input)
Only the upper triangle of A is referenced.

B — Vector of length N containing the right-hand side of the linear system. (Input)

X — Vector of length N containing the solution to the linear system. (Output)

Optional Arguments

N — Number of equations. (Input)
Default: N = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

FORTRAN 90 Interface

Generic: CALL LSLDS (A, B, X [, …])

Specific: The specific interface names are S_LSLDS and D_LSLDS.

FORTRAN 77 Interface

Single: CALL LSLDS (N, A, LDA, B, X)

Double: The double precision name is DLSLDS.

ScaLAPACK Interface

Generic: `CALL LSLDS (A0, B0, X0 [, …])`

Specific: The specific interface names are `S_LSLDS` and `D_LSLDS`.

See the *ScaLAPACK Usage Notes* below for a description of the arguments for distributed computing.

Description

Routine `LSLDS` solves a system of linear algebraic equations having a real symmetric positive definite coefficient matrix. The underlying code is based on either LINPACK , LAPACK, or ScaLAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see *Using ScaLAPACK, LAPACK, LINPACK, and EISPACK* in the Introduction section of this manual. `LSLDS` first uses the routine `LFCDS` to compute an $R^T R$ Cholesky factorization of the coefficient matrix and to estimate the condition number of the matrix. The matrix R is upper triangular. The solution of the linear system is then found using the routine `LFSDS`. `LSLDS` fails if any submatrix of R is not positive definite or if R has a zero diagonal element. These errors occur only if A either is very close to a singular matrix or to a matrix which is not positive definite. If the estimated condition number is greater than $1/\varepsilon$ (where ε is machine precision), a warning error is issued. This indicates that very small changes in A can cause very large changes in the solution x. If the coefficient matrix is ill-conditioned, it is recommended that `LSADS` be used.

Comments

1. Workspace may be explicitly provided, if desired, by use of `L2LDS/DL2LDS`. The reference is:

   `CALL L2LDS (N, A, LDA, B, X, FACT, WK)`

   The additional arguments are as follows:

   FACT — `N` × `N` work array containing the $R^T R$ factorization of `A` on output. If `A` is not needed, `A` can share the same storage locations as `FACT`.

   WK — Work vector of length `N`.

2. Informational errors

Type	Code	Description
3	1	The input matrix is too ill-conditioned. The solution might not be accurate.
4	2	The input matrix is not positive definite.

3. *Integer Options* with *Chapter 11* Options Manager

16 This option uses four values to solve memory bank conflict (access inefficiency) problems. In routine `L2LDS` the leading dimension of `FACT` is increased by `IVAL`(3) when `N` is a multiple of `IVAL`(4). The values `IVAL`(3) and `IVAL`(4) are temporarily replaced by `IVAL`(1) and `IVAL`(2), respectively, in `LSLDS`. Additional memory allocation for `FACT` and option value restoration are done automatically in `LSLDS`. Users directly calling `L2LDS` can allocate additional space for `FACT` and set `IVAL`(3) and `IVAL`(4) so that memory bank conflicts no longer cause inefficiencies. There is no requirement that users change existing applications that use `LSLDS` or `L2LDS`. Default values for the option are `IVAL(*)` = 1, 16, 0, 1.

17 This option has two values that determine if the L_1 condition number is to be computed. Routine `LSLDS` temporarily replaces `IVAL`(2) by `IVAL`(1). The routine `L2CDS` computes the condition number if `IVAL`(2) = 2. Otherwise `L2CDS` skips this computation. `LSLDS` restores the option. Default values for the option are `IVAL(*)` = 1, 2.

ScaLAPACK Usage Notes

The arguments which differ from the standard version of this routine are:

A0 — `MXLDA` by `MXCOL` local matrix containing the local portions of the distributed matrix `A`. `A` contains the coefficient matrix of the symmetric positive definite linear system. (Input)

B0 — Local vector of length `MXLDA` containing the local portions of the distributed vector `B`. `B` contains the right-hand side of the linear system. (Input)

X0 — Local vector of length `MXLDA` containing the local portions of the distributed vector `X`. `X` contains the solution to the linear system. (Output)

All other arguments are global and are the same as described for the standard version of the routine. In the argument descriptions above, `MXLDA` and `MXCOL` can be obtained through a call to `SCALAPACK_GETDIM` (see *Utilities*) after a call to `SCALAPACK_SETUP` (see *Utilities*) has been made. See the *ScaLAPACK Example* below.

Examples

Example

A system of three linear equations is solved. The coefficient matrix has real positive definite form and the right-hand-side vector *b* has three elements.

```
      USE LSLDS_INT
      USE WRRRN_INT
!                                 Declare variables
      INTEGER    LDA, N
      PARAMETER  (LDA=3, N=3)
      REAL       A(LDA,LDA), B(N), X(N)
!
!                                 Set values for A and B
!
```

```
!                                 A = (  1.0  -3.0   2.0)
!                                     ( -3.0  10.0  -5.0)
!                                     (  2.0  -5.0   6.0)
!
!                                 B = ( 27.0 -78.0  64.0)
!
      DATA A/1.0, -3.0, 2.0, -3.0, 10.0, -5.0, 2.0, -5.0, 6.0/
      DATA B/27.0, -78.0, 64.0/
!
      CALL LSLDS (A, B, X)

!                                 Print results
      CALL WRRRN ('X', X, 1, N, 1)
!
      END
```

Output

```
          X
    1        2        3
1.000   -4.000    7.000
```

ScaLAPACK Example

The same system of three linear equations is solved as a distributed computing example. The coefficient matrix has real positive definite form and the right-hand-side vector *b* has three elements. `SCALAPACK_MAP` and `SCALAPACK_UNMAP` are IMSL utility routines (see *Chapter 11, “Utilities”*) used to map and unmap arrays to and from the processor grid. They are used here for brevity. `DESCINIT` is a ScaLAPACK tools routine which initializes the descriptors for the local arrays.

```
      USE MPI_SETUP_INT
      USE LSLDS_INT
      USE WRRRN_INT
      USE SCALAPACK_SUPPORT
      IMPLICIT NONE
      INCLUDE 'mpif.h'
!                                 Declare variables
      INTEGER    LDA, N, DESCA(9), DESCX(9)
      INTEGER       INFO, MXCOL, MXLDA
      REAL, ALLOCATABLE ::        A(:,:), B(:), X(:)
      REAL, ALLOCATABLE ::        A0(:,:), B0(:), X0(:)
      PARAMETER  (LDA=3, N=3)
!                                 Set up for MPI
      MP_NPROCS = MP_SETUP()
      IF(MP_RANK .EQ. 0) THEN
          ALLOCATE (A(LDA,N), B(N), X(N))
!                                 Set values for A and B
          A(1,:) = (/  1.0,  -3.0,   2.0/)
          A(2,:) = (/ -3.0,  10.0, -5.0/)
          A(3,:) = (/  2.0,  -5.0,   6.0/)
!
          B = (/27.0, -78.0,  64.0/)
      ENDIF
!                                  Set up a 1D processor grid and define
!                                  its context ID, MP_ICTXT
      CALL SCALAPACK_SETUP(N, N, .TRUE., .TRUE.)
!                                  Get the array descriptor entities MXLDA,
!                                  and MXCOL
      CALL SCALAPACK_GETDIM(N, N, MP_MB, MP_NB, MXLDA, MXCOL)
!                                  Set up the array descriptors
```

```
      CALL DESCINIT(DESCA, N, N, MP_MB, MP_NB, 0, 0, MP_ICTXT, MXLDA, INFO)
      CALL DESCINIT(DESCX, N, 1, MP_MB, 1, 0, 0, MP_ICTXT, MXLDA, INFO)
!                                Allocate space for the local arrays
      ALLOCATE (A0(MXLDA,MXCOL), B0(MXLDA), X0(MXLDA))
!                                Map input arrays to the processor grid
      CALL SCALAPACK_MAP(A, DESCA, A0)
      CALL SCALAPACK_MAP(B, DESCX, B0)
!                                Solve the system of equations
      CALL LSLDS (A0, B0, X0)
!                                Unmap the results from the distributed
!                                arrays back to a non-distributed array.
!                                After the unmap, only Rank=0 has the full
!                                array.
      CALL SCALAPACK_UNMAP(X0, DESCX, X)
!                                Print results.
!                                Only Rank=0 has the solution, X.
      IF(MP_RANK .EQ. 0)CALL WRRRN ('X', X, 1, N, 1)
!                                Exit ScaLAPACK usage
      CALL SCALAPACK_EXIT(MP_ICTXT)
!                                Shut down MPI
      MP_NPROCS = MP_SETUP('FINAL')
      END
```

Output

```
            X
    1        2        3
1.000   -4.000    7.000
```

LFCDS

more...

more...

Computes the $R^T R$ Cholesky factorization of a real symmetric positive definite matrix and estimate its L_1 condition number.

Required Arguments

A — `N` by `N` symmetric positive definite matrix to be factored. (Input)
Only the upper triangle of `A` is referenced.

FACT — `N` by `N` matrix containing the upper triangular matrix *R* of the factorization of `A` in the upper triangular part. (Output)
Only the upper triangle of `FACT` will be used. If `A` is not needed, `A` and `FACT` can share the same storage locations.

RCOND — Scalar containing an estimate of the reciprocal of the L_1 condition number of `A`. (Output)

Optional Arguments

N — Order of the matrix. (Input)
Default: `N` = size (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = size (`A`,1).

LDFACT — Leading dimension of `FACT` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDFACT` = size (`FACT`,1).

FORTRAN 90 Interface

Generic: `CALL LFCDS (A, FACT, RCOND [, …])`

Specific: The specific interface names are `S_LFCDS` and `D_LFCDS`.

FORTRAN 77 Interface

Single: `CALL LFCDS (N, A, LDA, FACT, LDFACT, RCOND)`

Double: The double precision name is `DLFCDS`.

ScaLAPACK Interface

Generic: `CALL LFCDS (A0, FACT0, RCOND [, …])`

Specific: The specific interface names are `S_LFCDS` and `D_LFCDS`.

See the *ScaLAPACK Usage Notes* below for a description of the arguments for distributed computing.

Description

Routine `LFCDS` computes an $R^T R$ Cholesky factorization and estimates the condition number of a real symmetric positive definite coefficient matrix. The matrix R is upper triangular.

The L_1condition number of the matrix A is defined to be $\kappa(A) = \|A\|_1 \|A^{-1}\|_1$. Since it is expensive to compute $\|A^{-1}\|_1$, the condition number is only estimated. The estimation algorithm is the same as used by LINPACK and is described by Cline et al. (1979).

If the estimated condition number is greater than $1/\varepsilon$ (where ε is machine precision), a warning error is issued. This indicates that very small changes in A can cause very large changes in the solution x. Iterative refinement can sometimes find the solution to such a system.

`LFCDS` fails if any submatrix of R is not positive definite or if R has a zero diagonal element. These errors occur only if A is very close to a singular matrix or to a matrix which is not positive definite.

The $R^T R$ factors are returned in a form that is compatible with routines `LFIDS`, `LFSDS` and `LFDDS`. To solve systems of equations with multiple right-hand-side vectors, use `LFCDS` followed by either `LFIDS` or `LFSDS` called once for each right-hand side. The routine `LFDDS` can be called to compute the determinant of the coefficient matrix after `LFCDS` has performed the factorization.

Comments

1. Workspace may be explicitly provided, if desired, by use of `L2CDS/DL2CDS`. The reference is:

CALL L2CDS (N, A, LDA, FACT, LDFACT, RCOND, WK)

The additional argument is:

WK — Work vector of length N.

2. Informational errors

Type	Code	Description
3	1	The input matrix is algorithmically singular.
4	2	The input matrix is not positive definite.

ScaLAPACK Usage Notes

The arguments which differ from the standard version of this routine are:

A0 — MXLDA by MXCOL local matrix containing the local portions of the distributed matrix A. A contains the symmetric positive definite matrix to be factored. (Input)

FACT0 — MXLDA by MXCOL local matrix containing the local portions of the distributed matrix FACT. FACT contains the upper triangular matrix *R* of the factorization of A in the upper triangular part. (Output)
Only the upper triangle of FACT will be used. If A is not needed, A and FACT can share the same storage locations.

All other arguments are global and are the same as described for the standard version of the routine. In the argument descriptions above, MXLDA and MXCOL can be obtained through a call to SCALAPACK_GETDIM (see *Utilities*) after a call to SCALAPACK_SETUP (see *Utilities*) has been made. See the *ScaLAPACK Example* below.

Examples

Example

The inverse of a 3 × 3 matrix is computed. LFCDS is called to factor the matrix and to check for nonpositive definiteness or ill-conditioning. LFIDS is called to determine the columns of the inverse.

```
      USE LFCDS_INT
      USE UMACH_INT
      USE WRRRN_INT
      USE LFIDS_INT
!                                 Declare variables
      INTEGER    LDA, LDFACT, N, NOUT
      PARAMETER  (LDA=3, LDFACT=3, N=3)
      REAL       A(LDA,LDA), AINV(LDA,LDA), RCOND, FACT(LDFACT,LDFACT),&
                 RES(N), RJ(N)
!
!                                 Set values for A
```

```
!                                 A = (  1.0  -3.0   2.0)
!                                     ( -3.0  10.0  -5.0)
!                                     (  2.0  -5.0   6.0)
!
      DATA A/1.0, -3.0, 2.0, -3.0, 10.0, -5.0, 2.0, -5.0, 6.0/
!                                 Factor the matrix A
      CALL LFCDS (A, FACT, RCOND)
!                                 Set up the columns of the identity
!                                 matrix one at a time in RJ
      RJ = 0.0E0
      DO 10  J=1, N
         RJ(J) = 1.0E0
!                                 RJ is the J-th column of the identity
!                                 matrix so the following LFIDS
!                                 reference places the J-th column of
!                                 the inverse of A in the J-th column
!                                 of AINV
         CALL LFIDS (A, FACT, RJ, AINV(:,J), RES)
         RJ(J) = 0.0E0
   10 CONTINUE
!                                 Print the results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) RCOND, 1.0E0/RCOND
      CALL WRRRN ('AINV', AINV)
99999 FORMAT ('  RCOND = ',F5.3,/,'  L1 Condition number = ',F9.3)
      END
```

Output

```
RCOND < 0.005
L1 Condition number < 875.0

          AINV
        1        2        3
1   35.00     8.00    -5.00
2    8.00     2.00    -1.00
3   -5.00    -1.00     1.00
```

ScaLAPACK Example

The inverse of the same 3 × 3 matrix is computed as a distributed example. `LFCDS` is called to factor the matrix and to check for singularity or ill-conditioning. `LFIDS` is called to determine the columns of the inverse. `SCALAPACK_MAP` and `SCALAPACK_UNMAP` are IMSL utility routines (see *Chapter 11, "Utilities"*) used to map and unmap arrays to and from the processor grid. They are used here for brevity. `DESCINIT` is a ScaLAPACK tools routine which initializes the descriptors for the local arrays.

```
      USE MPI_SETUP_INT
      USE LFCDS_INT
      USE UMACH_INT
      USE LFIDS_INT
      USE WRRRN_INT
      USE SCALAPACK_SUPPORT
      IMPLICIT NONE
      INCLUDE 'mpif.h'
!                                 Declare variables
      INTEGER     J, LDA, N, NOUT, DESCA(9), DESCL(9)
      INTEGER     INFO, MXCOL, MXLDA
      REAL, ALLOCATABLE ::        A(:,:), AINV(:,:), X0(:), RJ(:)
      REAL, ALLOCATABLE ::        A0(:,:), FACT0(:,:), RES0(:), RJ0(:)
      REAL        RCOND
```

```
      PARAMETER  (LDA=3, N=3)
!                                Set up for MPI
      MP_NPROCS = MP_SETUP()
      IF(MP_RANK .EQ. 0) THEN
          ALLOCATE (A(LDA,N), AINV(LDA,N))
!                                Set values for A
          A(1,:) = (/  1.0,  -3.0,  2.0/)
          A(2,:) = (/ -3.0,  10.0, -5.0/)
          A(3,:) = (/  2.0,  -5.0,  6.0/)

      ENDIF
!                                 Set up a 1D processor grid and define
!                                 its context ID, MP_ICTXT
      CALL SCALAPACK_SETUP(N, N, .TRUE., .TRUE.)
!                                 Get the array descriptor entities MXLDA,
!                                 and MXCOL
      CALL SCALAPACK_GETDIM(N, N, MP_MB, MP_NB, MXLDA, MXCOL)
!                                 Set up the array descriptors
      CALL DESCINIT(DESCA, N, N, MP_MB, MP_NB, 0, 0, MP_ICTXT, MXLDA, INFO)
      CALL DESCINIT(DESCL, N, 1, MP_MB, 1, 0, 0, MP_ICTXT, MXLDA, INFO)
!                                 Allocate space for the local arrays
      ALLOCATE(A0(MXLDA,MXCOL), X0(MXLDA),FACT0(MXLDA,MXCOL), RJ(N), &
               RJ0(MXLDA), RES0(MXLDA))
!                                 Map input array to the processor grid
      CALL SCALAPACK_MAP(A, DESCA, A0)
!                                 Call the factorization routine
      CALL LFCDS (A0, FACT0, RCOND)
!                                Print the reciprocal condition number
!                                and the L1 condition number
      IF(MP_RANK .EQ. 0) THEN
         CALL UMACH (2, NOUT)
         WRITE (NOUT,99998) RCOND, 1.0E0/RCOND
      ENDIF
!                                Set up the columns of the identity
!                                matrix one at a time in RJ
      RJ = 0.0E0
      DO 10  J=1, N
         RJ(J) = 1.0
!                                Map input array to the processor grid
         CALL SCALAPACK_MAP(RJ, DESCL, RJ0)
!                                RJ is the J-th column of the identity
!                                matrix so the following LFIDS
!                                reference computes the J-th column of
!                                the inverse of A
         CALL LFIDS (A0, FACT0, RJ0, X0, RES0)
         RJ(J) = 0.0
         CALL SCALAPACK_UNMAP(X0, DESCL, AINV(:,J))
   10 CONTINUE
!                                Print results.
!                                Only Rank=0 has the solution, AINV.
      IF(MP_RANK.EQ.0) CALL WRRRN ('AINV', AINV)
      IF (MP_RANK .EQ. 0) DEALLOCATE(A, AINV)
      DEALLOCATE(A0, FACT0, RJ, RJ0, RES0, X0)
!                               Exit ScaLAPACK usage
      CALL SCALAPACK_EXIT(MP_ICTXT)
!                               Shut down MPI
      MP_NPROCS = MP_SETUP('FINAL')
99998 FORMAT ('  RCOND = ',F5.3,/,'  L1 Condition number = ',F9.3)
      END
```

Output

```
RCOND < 0.005
L1 Condition number < 875.0
```

```
            AINV
          1        2        3
1   35.00     8.00    -5.00
2    8.00     2.00    -1.00
3   -5.00    -1.00     1.00
```

LFTDS

more...

more...

Computes the $R^T R$ Cholesky factorization of a real symmetric positive definite matrix.

Required Arguments

A — N by N symmetric positive definite matrix to be factored. (Input)
Only the upper triangle of A is referenced.

FACT — N by N matrix containing the upper triangular matrix *R* of the factorization of A in the upper triangle, and the lower triangular matrix R^T in the lower triangle. (Output)
If A is not needed, A and FACT can share the same storage location.

Optional Arguments

N — Order of the matrix. (Input)
Default: N = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

LDFACT — Leading dimension of FACT exactly as specified in the dimension statement of the calling program. (Input)
Default: LDFACT = size (FACT,1).

FORTRAN 90 Interface

Generic: CALL LFTDS (A, FACT [, …])

Specific: The specific interface names are S_LFTDS and D_LFTDS.

FORTRAN 77 Interface

Single: CALL LFTDS (N, A, LDA, FACT, LDFACT)

Double: The double precision name is DLFTDS.

ScaLAPACK Interface

Generic: CALL LFTDS (A0, FACT0 [, …])

Specific: The specific interface names are S_LFTDS and D_LFTDS.

See the *ScaLAPACK Usage Notes* below for a description of the arguments for distributed computing.

Description

Routine LFTDS computes an $R^T R$ Cholesky factorization of a real symmetric positive definite coefficient matrix. The matrix R is upper triangular.

LFTDS fails if any submatrix of R is not positive definite or if R has a zero diagonal element. These errors occur only if A is very close to a singular matrix or to a matrix which is not positive definite.

The $R^T R$ factors are returned in a form that is compatible with routines LFIDS, LFSDS and LFDDS. To solve systems of equations with multiple right-hand-side vectors, use LFTDS followed by either LFIDS or LFSDS called once for each right-hand side. The routine LFDDS can be called to compute the determinant of the coefficient matrix after LFTDS has performed the factorization.

The underlying code is based on either LINPACK , LAPACK, or ScaLAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see *Using ScaLAPACK, LAPACK, LINPACK, and EISPACK* in the Introduction section of this manual.

Comments

Informational error

Type	Code	Description
4	2	The input matrix is not positive definite.

ScaLAPACK Usage Notes

The arguments which differ from the standard version of this routine are:

A0 — MXLDA by MXCOL local matrix containing the local portions of the distributed matrix A. A contains the symmetric positive definite matrix to be factored. (Input)

FACT0 — MXLDA by MXCOL local matrix containing the local portions of the distributed matrix FACT. FACT contains the upper triangular matrix *R* of the factorization of A in the upper triangular part. (Output)
Only the upper triangle of FACT will be used. If A is not needed, A and FACT can share the same storage locations.

All other arguments are global and are the same as described for the standard version of the routine. In the argument descriptions above, MXLDA and MXCOL can be obtained through a call to SCALAPACK_GETDIM (see *Utilities*) after a call to SCALAPACK_SETUP (see *Utilities*) has been made. See the ScaLAPACK Example below.

Examples

Example

The inverse of a 3 × 3 matrix is computed. LFTDS is called to factor the matrix and to check for nonpositive definiteness. LFSDS is called to determine the columns of the inverse.

```
      USE LFTDS_INT
      USE LFSDS_INT
      USE WRRRN_INT
!                                 Declare variables
      INTEGER    LDA, LDFACT, N
      PARAMETER  (LDA=3, LDFACT=3, N=3)
      REAL       A(LDA,LDA), AINV(LDA,LDA), FACT(LDFACT,LDFACT), RJ(N)
!
!                                 Set values for A
!                                 A = (  1.0  -3.0   2.0)
!                                     ( -3.0  10.0  -5.0)
!                                     (  2.0  -5.0   6.0)
!
      DATA A/1.0, -3.0, 2.0, -3.0, 10.0, -5.0, 2.0, -5.0, 6.0/
!                                 Factor the matrix A
      CALL LFTDS (A, FACT)
!                                 Set up the columns of the identity
!                                 matrix one at a time in RJ
      RJ = 0.0E0
      DO 10  J=1, N
         RJ(J) = 1.0E0
!                                 RJ is the J-th column of the identity
!                                 matrix so the following LFSDS
!                                 reference places the J-th column of
!                                 the inverse of A in the J-th column
!                                 of AINV
         CALL LFSDS (FACT, RJ, AINV(:,J))
         RJ(J) = 0.0E0
   10 CONTINUE
!                                 Print the results
      CALL WRRRN ('AINV', AINV)
!
      END
```

Output

```
           AINV
        1          2          3
1   35.00     8.00    -5.00
2    8.00     2.00    -1.00
3   -5.00    -1.00     1.00
```

ScaLAPACK Example

The inverse of the same 3 × 3 matrix is computed as a distributed example. `LFTDS` is called to factor the matrix and to check for nonpositive definiteness. `LFSDS` is called to determine the columns of the inverse. `SCALAPACK_MAP` and `SCALAPACK_UNMAP` are IMSL utility routines (see *Chapter 11, "Utilities"*) used to map and unmap arrays to and from the processor grid. They are used here for brevity. `DESCINIT` is a ScaLAPACK tools routine which initializes the descriptors for the local arrays.

```
      USE MPI_SETUP_INT
      USE LFTDS_INT
      USE UMACH_INT
      USE LFSDS_INT
      USE WRRRN_INT
      USE SCALAPACK_SUPPORT
      IMPLICIT NONE
      INCLUDE 'mpif.h'
!                                  Declare variables
      INTEGER     J, LDA, N, DESCA(9), DESCL(9)
      INTEGER     INFO, MXCOL, MXLDA
      REAL, ALLOCATABLE ::        A(:,:), AINV(:,:), X0(:)
      REAL, ALLOCATABLE ::        A0(:,:), FACT0(:,:), RES0(:), RJ0(:)
      PARAMETER  (LDA=3, N=3)
!                                  Set up for MPI
      MP_NPROCS = MP_SETUP()
      IF(MP_RANK .EQ. 0) THEN
          ALLOCATE (A(LDA,N), AINV(LDA,N))
!                                  Set values for A
          A(1,:) = (/  1.0,  -3.0,   2.0/)
          A(2,:) = (/ -3.0,  10.0,  -5.0/)
          A(3,:) = (/  2.0,  -5.0,   6.0/)

      ENDIF
!                                   Set up a 1D processor grid and define
!                                   its context ID, MP_ICTXT
      CALL SCALAPACK_SETUP(N, N, .TRUE., .TRUE.)
!                                   Get the array descriptor entities MXLDA,
!                                   and MXCOL
      CALL SCALAPACK_GETDIM(N, N, MP_MB, MP_NB, MXLDA, MXCOL)
!                                   Set up the array descriptors
      CALL DESCINIT(DESCA, N, N, MP_MB, MP_NB, 0, 0, MP_ICTXT, MXLDA, INFO)
      CALL DESCINIT(DESCL, N, 1, MP_MB, 1, 0, 0, MP_ICTXT, MXLDA, INFO)
!                                   Allocate space for the local arrays
      ALLOCATE(A0(MXLDA,MXCOL), X0(MXLDA),FACT0(MXLDA,MXCOL), RJ(N), &
               RJ0(MXLDA), RES0(MXLDA), IPVT0(MXLDA))
!                                   Map input arrays to the processor grid
      CALL SCALAPACK_MAP(A, DESCA, A0)
!                                   Call the factorization routine
      CALL LFTDS (A0, FACT0)
!                                  Set up the columns of the identity
!                                  matrix one at a time in RJ
      RJ = 0.0E0
      DO 10  J=1, N
         RJ(J) = 1.0
```

```
          CALL SCALAPACK_MAP(RJ, DESCL, RJ0)
!                                RJ is the J-th column of the identity
!                                matrix so the following LFSDS
!                                reference computes the J-th column of
!                                the inverse of A
          CALL LFSDS (FACT0, RJ0, X0)
          RJ(J) = 0.0
          CALL SCALAPACK_UNMAP(X0, DESCL, AINV(:,J))
   10 CONTINUE
!                                Print results.
!                                Only Rank=0 has the solution, AINV.
      IF(MP_RANK.EQ.0) CALL WRRRN ('AINV', AINV)
      IF (MP_RANK .EQ. 0) DEALLOCATE(A, AINV)
      DEALLOCATE(A0, FACT0, IPVT0, RJ, RJ0, RES0, X0)
!                               Exit ScaLAPACK usage
      CALL SCALAPACK_EXIT(MP_ICTXT)
!                               Shut down MPI
      MP_NPROCS = MP_SETUP('FINAL')
      END
```

Output

```
RCOND < 0.005
L1 Condition number < 875.0

          AINV
        1       2       3
1   35.00    8.00   -5.00
2    8.00    2.00   -1.00
3   -5.00   -1.00    1.00
```

LFSDS

more...

more...

Solves a real symmetric positive definite system of linear equations given the $R^T R$ Cholesky factorization of the coefficient matrix.

Required Arguments

FACT — N by N matrix containing the $R^T R$ factorization of the coefficient matrix A as output from routine LFCDS/DLFCDS or LFTDS/DLFTDS. (Input)

B — Vector of length N containing the right-hand side of the linear system. (Input)

X — Vector of length N containing the solution to the linear system. (Output)
If B is not needed, B and X can share the same storage locations.

Optional Arguments

N — Number of equations. (Input)
Default: N = size (FACT,2).

LDFACT — Leading dimension of FACT exactly as specified in the dimension statement of the calling program. (Input)
Default: LDFACT = size (FACT,1).

FORTRAN 90 Interface

Generic: CALL LFSDS (FACT, B, X [, …])

Specific: The specific interface names are S_LFSDS and D_LFSDS.

FORTRAN 77 Interface

Single: CALL LFSDS (N, FACT, LDFACT, B, X)

Double: The double precision name is DLFSDS.

ScaLAPACK Interface

Generic: CALL LFSDS (FACT0, B0, X0 [, …])

Specific: The specific interface names are S_LFSDS and D_LFSDS.

See the *ScaLAPACK Usage Notes* below for a description of the arguments for distributed computing.

Description

Routine LFSDS computes the solution for a system of linear algebraic equations having a real symmetric positive definite coefficient matrix. To compute the solution, the coefficient matrix must first undergo an $R^T R$ factorization. This may be done by calling either LFCDS or LFTDS. R is an upper triangular matrix.

The solution to $Ax = b$ is found by solving the triangular systems $R^T y = b$ and $Rx = y$.

LFSDS and LFIDS both solve a linear system given its $R^T R$ factorization. LFIDS generally takes more time and produces a more accurate answer than LFSDS. Each iteration of the iterative refinement algorithm used by LFIDS calls LFSDS.

The underlying code is based on either LINPACK, LAPACK, or ScaLAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see *Using ScaLAPACK, LAPACK, LINPACK, and EISPACK* in the Introduction section of this manual.

Comments

Informational error

Type	Code	Description
4	1	The input matrix is singular.

ScaLAPACK Usage Notes

The arguments which differ from the standard version of this routine are:

FACT0 — MXLDA by MXCOL local matrix containing the local portions of the distributed matrix FACT. FACT contains the $R^T R$ factorization of the coefficient matrix A as output from routine LFCDS/DLFCDS or LFTDS/DLFTDS. (Input)

B0 — Local vector of length MXLDA containing the local portions of the distributed vector B. B contains the right-hand side of the linear system. (Input)

X0 — Local vector of length MXLDA containing the local portions of the distributed vector X. X contains the solution to the linear system. (Output)
If B is not needed, B and X can share the same storage locations.

All other arguments are global and are the same as described for the standard version of the routine. In the argument descriptions above, MXLDA and MXCOL can be obtained through a call to SCALAPACK_GETDIM (see *Utilities*) after a call to SCALAPACK_SETUP (see *Utilities*) has been made. See the *ScaLAPACK Example* below.

Examples

Example

A set of linear systems is solved successively. LFTDS is called to factor the coefficient matrix. LFSDS is called to compute the four solutions for the four right-hand sides. In this case the coefficient matrix is assumed to be well-conditioned and correctly scaled. Otherwise, it would be better to call LFCDS to perform the factorization, and LFIDS to compute the solutions.

```
      USE LFSDS_INT
      USE LFTDS_INT
      USE WRRRN_INT
!                                 Declare variables
      INTEGER    LDA, LDFACT, N
      PARAMETER  (LDA=3, LDFACT=3, N=3)
      REAL       A(LDA,LDA), B(N,4), FACT(LDFACT,LDFACT), X(N,4)
!
!                                 Set values for A and B
!
!                                 A = (  1.0  -3.0   2.0)
!                                     ( -3.0  10.0  -5.0)
!                                     (  2.0  -5.0   6.0)
!
!                                 B = ( -1.0   3.6  -8.0  -9.4)
!                                     ( -3.0  -4.2  11.0  17.6)
!                                     ( -3.0  -5.2  -6.0 -23.4)
!
      DATA A/1.0, -3.0, 2.0, -3.0, 10.0, -5.0, 2.0, -5.0, 6.0/
      DATA B/-1.0, -3.0, -3.0, 3.6, -4.2, -5.2, -8.0, 11.0, -6.0,&
          -9.4, 17.6, -23.4/
!                                 Factor the matrix A
      CALL LFTDS (A, FACT)
!                                 Compute the solutions
      DO 10  I=1, 4
         CALL LFSDS (FACT, B(:,I), X(:,I))
   10 CONTINUE
!                                 Print solutions
      CALL WRRRN ('The solution vectors are', X)
!
      END
```

Output

```
     The solution vectors are
        1        2        3        4
1   -44.0    118.4   -162.0    -71.2
2   -11.0     25.6    -36.0    -16.6
3     5.0    -19.0     23.0      6.0
```

ScaLAPACK Example

The same set of linear systems is solved successively as a distributed example. Routine LFTDS is called to factor the coefficient matrix. The routine LFSDS is called to compute the four solutions for the four right-hand sides. In this case, the coefficient matrix is assumed to be well-conditioned and correctly scaled. Otherwise, it would be better to call LFCDS to perform the factorization, and LFIDS to compute the solutions. SCALAPACK_MAP and SCALAPACK_UNMAP are IMSL utility routines (see *Chapter 11, "Utilities"*) used to map and unmap arrays to and from the processor grid. They are used here for brevity. DESCINIT is a ScaLAPACK tools routine which initializes the descriptors for the local arrays.

```
      USE MPI_SETUP_INT
      USE LFSDS_INT
      USE LFTDS_INT
      USE WRRRN_INT
      USE SCALAPACK_SUPPORT
      IMPLICIT NONE
      INCLUDE 'mpif.h'
!                                  Declare variables
      INTEGER     J, LDA, N, DESCA(9), DESCL(9)
      INTEGER     INFO, MXCOL, MXLDA
      REAL, ALLOCATABLE ::         A(:,:), B(:,:), X(:,:), X0(:)
      REAL, ALLOCATABLE ::         A0(:,:), FACT0(:,:), B0(:)
      PARAMETER  (LDA=3, N=3)
!                                  Set up for MPI
      MP_NPROCS = MP_SETUP()
      IF(MP_RANK .EQ. 0) THEN
          ALLOCATE (A(LDA,N), B(N,4), X(N,4))
!                                  Set values for A and B
          A(1,:) = (/  1.0,  -3.0,  2.0/)
          A(2,:) = (/ -3.0,  10.0, -5.0/)
          A(3,:) = (/  2.0,  -5.0,  6.0/)
!
          B(1,:) = (/ -1.0,  3.6, -8.0,  -9.4/)
          B(2,:) = (/ -3.0, -4.2, 11.0,  17.6/)
          B(3,:) = (/ -3.0, -5.2, -6.0, -23.4/)
      ENDIF
!                                   Set up a 1D processor grid and define
!                                   its context ID, MP_ICTXT
      CALL SCALAPACK_SETUP(N, N, .TRUE., .TRUE.)
!                                   Get the array descriptor entities MXLDA,
!                                   and MXCOL
      CALL SCALAPACK_GETDIM(N, N, MP_MB, MP_NB, MXLDA, MXCOL)
!                                   Set up the array descriptors
      CALL DESCINIT(DESCA, N, N, MP_MB, MP_NB, 0, 0, MP_ICTXT, MXLDA, INFO)
      CALL DESCINIT(DESCL, N, 1, MP_MB, 1, 0, 0, MP_ICTXT, MXLDA, INFO)
!                                   Allocate space for the local arrays
      ALLOCATE(A0(MXLDA,MXCOL), X0(MXLDA),FACT0(MXLDA,MXCOL), B0(MXLDA))
!                                   Map input arrays to the processor grid
      CALL SCALAPACK_MAP(A, DESCA, A0)
!                                   Call the factorization routine
      CALL LFTDS (A0, FACT0)
```

```
!                                   Set up the columns of the B
!                                   matrix one at a time in X0
      DO 10  J=1, 4
         CALL SCALAPACK_MAP(B(:,j), DESCL, B0)
!                                   Solve for the J-th column of X
         CALL LFSDS (FACT0, B0, X0)
         CALL SCALAPACK_UNMAP(X0, DESCL, X(:,J))
   10 CONTINUE
!                                   Print results.
!                                   Only Rank=0 has the solution, X.
      IF(MP_RANK.EQ.0) CALL WRRRN ('The solution vectors are', X)
      IF (MP_RANK .EQ. 0) DEALLOCATE(A, B, X)
      DEALLOCATE(A0, FACT0, B0, X0)
!                                   Exit Scalapack usage
      CALL SCALAPACK_EXIT(MP_ICTXT)
!                                   Shut down MPI
      MP_NPROCS = MP_SETUP('FINAL')
      END
```

Output

```
     The solution vectors are
        1        2        3        4
1   -44.0    118.4   -162.0    -71.2
2   -11.0     25.6    -36.0    -16.6
3     5.0    -19.0     23.0      6.0
```

LFIDS

more...

more...

Uses iterative refinement to improve the solution of a real symmetric positive definite system of linear equations.

Required Arguments

A — N by N matrix containing the symmetric positive definite coefficient matrix of the linear system. (Input)
Only the upper triangle of A is referenced.

FACT — N by N matrix containing the $R^T R$ factorization of the coefficient matrix A as output from routine LFCDS/DLFCDS or LFTDS/DLFTDS. (Input)

B — Vector of length N containing the right-hand side of the linear system. (Input)

X — Vector of length N containing the solution to the linear system. (Output)
If B is not needed, B and X can share the same storage locations.

RES — Vector of length N containing the residual vector at the improved solution. (Output)

Optional Arguments

N — Number of equations. (Input)
Default: N = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimesion statement of the calling program. (Input)
Default: LDA = size (A,1).

LDFACT — Leading dimension of FACT exactly as specified in the dimension statement of the calling program. (Input)
Default: LDFACT = size (FACT,1).

FORTRAN 90 Interface

Generic: `CALL LFIDS (A, FACT, B, X, RES [, …])`

Specific: The specific interface names are `S_LFIDS` and `D_LFIDS`.

FORTRAN 77 Interface

Single: `CALL LFIDS (N, A, LDA, FACT, LDFACT, B, X, RES)`

Double: The double precision name is `DLFIDS`.

ScaLAPACK Interface

Generic: `CALL LFIDS (A0, FACT0, B0, X0, RES0 [, …])`

Specific: The specific interface names are `S_LFIDS` and `D_LFIDS`.

See the *ScaLAPACK Usage Notes* below for a description of the arguments for distributed computing.

Description

Routine `LFIDS` computes the solution of a system of linear algebraic equations having a real symmetric positive definite coefficient matrix. Iterative refinement is performed on the solution vector to improve the accuracy. Usually almost all of the digits in the solution are accurate, even if the matrix is somewhat ill-conditioned. The underlying code is based on either LINPACK , LAPACK, or ScaLAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see *Using ScaLAPACK, LAPACK, LINPACK, and EISPACK* in the Introduction section of this manual.

To compute the solution, the coefficient matrix must first undergo an $R^T R$ factorization. This may be done by calling either `LFCDS` or `LFTDS`.

Iterative refinement fails only if the matrix is very ill-conditioned.

`LFIDS` and `LFSDS` both solve a linear system given its $R^T R$ factorization. `LFIDS` generally takes more time and produces a more accurate answer than `LFSDS`. Each iteration of the iterative refinement algorithm used by `LFIDS` calls `LFSDS`.

Comments

Informational error

Type	Code	Description
3	2	The input matrix is too ill-conditioned for iterative refinement to be effective.

ScaLAPACK Usage Notes

The arguments which differ from the standard version of this routine are:

A0 — MXLDA by MXCOL local matrix containing the local portions of the distributed matrix A. A contains the symmetric positive definite coefficient matrix of the linear system. (Input)

FACT0 — MXLDA by MXCOL local matrix containing the local portions of the distributed matrix FACT. FACT contains the $R^T R$ factorization of the coefficient matrix A as output from routine LFCDS/DLFCDS or LFTDS/DLFTDS. (Input)

B0 — Local vector of length MXLDA containing the local portions of the distributed vector B. B contains the right-hand side of the linear system. (Input)

X0 — Local vector of length MXLDA containing the local portions of the distributed vector X. X contains the solution to the linear system. (Output)
If B is not needed, B and X can share the same storage locations.

RES0 — Local vector of length MXLDA containing the local portions of the distributed vector RES. RES contains the residual vector at the improved solution to the linear system. (Output)

All other arguments are global and are the same as described for the standard version of the routine. In the argument descriptions above, MXLDA and MXCOL can be obtained through a call to SCALAPACK_GETDIM (see *Utilities*) after a call to SCALAPACK_SETUP (see *Utilities*) has been made. See the *ScaLAPACK Example* below.

Examples

Example

A set of linear systems is solved successively. The right-hand-side vector is perturbed after solving the system each of the first two times by adding 0.2 to the second element.

```
      USE LFIDS_INT
      USE LFCDS_INT
      USE UMACH_INT
      USE WRRRN_INT
!                                 Declare variables
      INTEGER    LDA, LDFACT, N
      PARAMETER  (LDA=3, LDFACT=3, N=3)
      REAL       A(LDA,LDA), B(N), RCOND, FACT(LDFACT,LDFACT), RES(N,3),&
                X(N,3)
```

```
!
!                                 Set values for A and B
!
!                                 A = (  1.0  -3.0   2.0)
!                                     ( -3.0  10.0  -5.0)
!                                     (  2.0  -5.0   6.0)
!
!                                 B = (  1.0  -3.0   2.0)
!
      DATA A/1.0, -3.0, 2.0, -3.0, 10.0, -5.0, 2.0, -5.0, 6.0/
      DATA B/1.0, -3.0, 2.0/
!                                 Factor the matrix A
      CALL LFCDS (A, FACT, RCOND)
!                                 Print the estimated condition number
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) RCOND, 1.0E0/RCOND
!                                 Compute the solutions
      DO 10  I=1, 3
         CALL LFIDS (A, FACT, B, X(:,I), RES(:,I))
         B(2) = B(2) + .2E0
   10 CONTINUE
!                                 Print solutions and residuals
      CALL WRRRN ('The solution vectors are', X)
      CALL WRRRN ('The residual vectors are', RES)
!
99999 FORMAT ('  RCOND = ',F5.3,/,'  L1 Condition number = ',F9.3)
      END
```

Output

```
RCOND = 0.001
L1 Condition number =   674.727

The solution vectors are
        1       2       3
1   1.000   2.600   4.200
2   0.000   0.400   0.800
3   0.000  -0.200  -0.400

The residual vectors are
         1         2         3
1   0.0000    0.0000    0.0000
2   0.0000    0.0000    0.0000
3   0.0000    0.0000    0.0000
```

ScaLAPACK Example

The same set of linear systems is solved successively as a distributed example. The right-hand-side vector is perturbed after solving the system each of the first two times by adding 0.2 to the second element. SCALAPACK_MAP and SCALAPACK_UNMAP are IMSL utility routines (see Chapter 11, "Utilities") used to map and unmap arrays to and from the processor grid. They are used here for brevity. DESCINIT is a ScaLAPACK tools routine which initializes the descriptors for the local arrays.

```
      USE MPI_SETUP_INT
      USE LFIDS_INT
      USE LFCDS_INT
      USE UMACH_INT
      USE WRRRN_INT
      USE SCALAPACK_SUPPORT
      IMPLICIT NONE
```

```
      INCLUDE 'mpif.h'
!                                 Declare variables
      INTEGER     J, LDA, N, NOUT, DESCA(9), DESCL(9)
      INTEGER     INFO, MXCOL, MXLDA
      REAL        RCOND
      REAL, ALLOCATABLE ::        A(:,:), B(:), X(:,:), RES(:,:), X0(:)
      REAL, ALLOCATABLE ::        A0(:,:), FACT0(:,:), B0(:), RES0(:)
      PARAMETER  (LDA=3, N=3)
!                                 Set up for MPI
      MP_NPROCS = MP_SETUP()
      IF(MP_RANK .EQ. 0) THEN
          ALLOCATE (A(LDA,N), B(N), X(N,3), RES(N,3))
!                                 Set values for A and B
          A(1,:) = (/ 1.0,  -3.0,  2.0/)
          A(2,:) = (/-3.0,  10.0, -5.0/)
          A(3,:) = (/ 2.0,  -5.0,  6.0/)
!
          B      = (/ 1.0,  -3.0,  2.0/)
      ENDIF
!                                  Set up a 1D processor grid and define
!                                  its context ID, MP_ICTXT
      CALL SCALAPACK_SETUP(N, N, .TRUE., .TRUE.)
!                                  Get the array descriptor entities MXLDA,
!                                  and MXCOL
      CALL SCALAPACK_GETDIM(N, N, MP_MB, MP_NB, MXLDA, MXCOL)
!                                  Set up the array descriptors
      CALL DESCINIT(DESCA, N, N, MP_MB, MP_NB, 0, 0, MP_ICTXT, MXLDA, INFO)
      CALL DESCINIT(DESCL, N, 1, MP_MB, 1, 0, 0, MP_ICTXT, MXLDA, INFO)
!                                  Allocate space for the local arrays
      ALLOCATE(A0(MXLDA,MXCOL), X0(MXLDA), FACT0(MXLDA,MXCOL), B0(MXLDA), &
               RES0(MXLDA))
!                                  Map input arrays to the processor grid
      CALL SCALAPACK_MAP(A, DESCA, A0)
!                                  Call the factorization routine
      CALL LFCDS (A0, FACT0, RCOND)
!                                  Print the estimated condition number
      CALL UMACH (2, NOUT)
      IF(MP_RANK .EQ. 0) WRITE (NOUT,99999) RCOND, 1.0E0/RCOND
!                                  Set up the columns of the B
!                                  matrix one at a time in X0
      DO 10  J=1, 3
         CALL SCALAPACK_MAP(B, DESCL, B0)
!                                  Solve for the J-th column of X
         CALL LFIDS (A0, FACT0, B0, X0, RES0)
         CALL SCALAPACK_UNMAP(X0, DESCL, X(:,J))
         CALL SCALAPACK_UNMAP(RES0, DESCL, RES(:,J))
         IF(MP_RANK .EQ. 0) B(2) = B(2) + .2E0
   10 CONTINUE
!                                 Print results.
!                                 Only Rank=0 has the full arrays
      IF(MP_RANK.EQ.0) CALL WRRRN ('The solution vectors are', X)
      IF(MP_RANK.EQ.0) CALL WRRRN ('The residual vectors are', RES)
      IF (MP_RANK .EQ. 0) DEALLOCATE(A, B, X, RES)
      DEALLOCATE(A0, B0, FACT0, RES0, X0)
!                                Exit ScaLAPACK usage
      CALL SCALAPACK_EXIT(MP_ICTXT)
!                                Shut down MPI
      MP_NPROCS = MP_SETUP('FINAL')
99999 FORMAT ('  RCOND = ',F5.3,/,'  L1 Condition number = ',F9.3)
      END
```

Output

```
RCOND = 0.001
L1 Condition number =   674.727
```

```
The solution vectors are
        1       2       3
1   1.000   2.600   4.200
2   0.000   0.400   0.800
3   0.000  -0.200  -0.400

The residual vectors are
         1        2        3
1   0.0000   0.0000   0.0000
2   0.0000   0.0000   0.0000
3   0.0000   0.0000   0.0000
```

LFDDS

Computes the determinant of a real symmetric positive definite matrix given the $R^T R$ Cholesky factorization of the matrix .

Required Arguments

FACT — N by N matrix containing the $R^T R$ factorization of the coefficient matrix A as output from routine LFCDS/DLFCDS or LFTDS/DLFTDS. (Input)

DET1 — Scalar containing the mantissa of the determinant. (Output)
The value DET1 is normalized so that, 1.0 ≤ |DET1| < 10.0 or DET1 = 0.0.

DET2 — Scalar containing the exponent of the determinant. (Output)
The determinant is returned in the form, det(A) = DET1 * 10DET2.

Optional Arguments

N — Number of equations. (Input)
Default: N = size (FACT,2).

LDFACT — Leading dimension of FACT exactly as specified in the dimension statement of the calling program. (Input)
Default: LDFACT = size (FACT,1).

FORTRAN 90 Interface

Generic: CALL LFDDS (FACT, DET1, DET2 [, …])

Specific: The specific interface names are S_LFDDS and D_LFDDS.

FORTRAN 77 Interface

Single: CALL LFDDS (N, FACT, LDFACT, DET1, DET2)

Double: The double precision name is DLFDDS.

Description

Routine LFDDS computes the determinant of a real symmetric positive definite coefficient matrix. To compute the determinant, the coefficient matrix must first undergo an $R^T R$ factorization. This may be done by calling either LFCDS or LFTDS. The formula det A = det R^T det R = (det R)^2 is used to compute the determinant. Since the determinant of a triangular matrix is the product of the diagonal elements,

$$\det R = \prod_{i=1}^{N} R_{ii}$$

(The matrix R is stored in the upper triangle of FACT.)

LFDDS is based on the LINPACK routine SPODI; see Dongarra et al. (1979).

Example

The determinant is computed for a real positive definite 3 × 3 matrix.

```
      USE LFDDS_INT
      USE LFTDS_INT
      USE UMACH_INT
!                                 Declare variables
      INTEGER    LDA, LDFACT, NOUT
      PARAMETER  (LDA=3, LDFACT=3)
      REAL       A(LDA,LDA), DET1, DET2, FACT(LDFACT,LDFACT)
!
!                                 Set values for A
!                                 A = (  1.0  -3.0   2.0)
!                                     ( -3.0  20.0  -5.0)
!                                     (  2.0  -5.0   6.0)
!
      DATA A/1.0, -3.0, 2.0, -3.0, 20.0, -5.0, 2.0, -5.0, 6.0/
!                                 Factor the matrix
      CALL LFTDS (A, FACT)
!                                 Compute the determinant
      CALL LFDDS (FACT, DET1, DET2)
!                                 Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) DET1, DET2
!
99999 FORMAT (' The determinant of A is ',F6.3,' * 10**',F2.0)
      END
```

Output

```
The determinant of A is 2.100 * 10**1.
```

LINDS

more...

more...

Computes the inverse of a real symmetric positive definite matrix.

Required Arguments

A — `N` by `N` matrix containing the symmetric positive definite matrix to be inverted. (Input)
Only the upper triangle of `A` is referenced.

AINV — `N` by `N` matrix containing the inverse of `A`. (Output)
If `A` is not needed, `A` and `AINV` can share the same storage locations.

Optional Arguments

N — Order of the matrix `A`. (Input)
Default: `N` = size (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = size (`A`,1).

LDAINV — Leading dimension of `AINV` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDAINV` = size (`AINV`,1).

FORTRAN 90 Interface

Generic: `CALL LINDS (A, AINV [, …])`

Specific: The specific interface names are `S_LINDS` and `D_LINDS`.

FORTRAN 77 Interface

Single: `CALL LINDS (N, A, LDA, AINV, LDAINV)`

Double: The double precision name is DLINDS.

ScaLAPACK Interface

Generic: CALL LINDS (A0, AINV0 [, …])

Specific: The specific interface names are S_LINDS and D_LINDS.

See the *ScaLAPACK Usage Notes* below for a description of the arguments for distributed computing.

Description

Routine LINDS computes the inverse of a real symmetric positive definite matrix. The underlying code is based on either LINPACK , LAPACK, or ScaLAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see *Using ScaLAPACK, LAPACK, LINPACK, and EISPACK* in the Introduction section of this manual. LINDS first uses the routine LFCDS to compute an $R^T R$ factorization of the coefficient matrix and to estimate the condition number of the matrix. LINRT is then used to compute R^{-1}. Finally A^{-1} is computed using $A^{-1} = R^{-1} R^{-T}$.

LINDS fails if any submatrix of *R* is not positive definite or if *R* has a zero diagonal element. These errors occur only if *A* is very close to a singular matrix or to a matrix which is not positive definite.

If the estimated condition number is greater than $1/\varepsilon$ (where ε is machine precision), a warning error is issued. This indicates that very small changes in *A* can cause very large changes in *A*.

Comments

1. Workspace may be explicitly provided, if desired, by use of L2NDS/DL2NDS. The reference is:

   CALL L2NDS (N, A, LDA, AINV, LDAINV, WK)

   The additional argument is:

   WK — Work vector of length N.

2. Informational errors

Type	Code	Description
3	1	The input matrix is too ill-conditioned. The solution might not be accurate.
4	2	The input matrix is not positive definite.

ScaLAPACK Usage Notes

The arguments which differ from the standard version of this routine are:

A0 — MXLDA by MXCOL local matrix containing the local portions of the distributed matrix A. A contains the symmetric positive definite matrix to be inverted. (Input)

AINV0 — MXLDA by MXCOL local matrix containing the local portions of the distributed matrix AINV. AINV contains the inverse of the matrix A. (Output)
If A is not needed, A and AINV can share the same storage locations.

All other arguments are global and are the same as described for the standard version of the routine. In the argument descriptions above, MXLDA and MXCOL can be obtained through a call to SCALAPACK_GETDIM (see *Utilities*) after a call to SCALAPACK_SETUP (see *Utilities*) has been made. See the *ScaLAPACK Example* below.

Examples

Example

The inverse is computed for a real positive definite 3×3 matrix.

```
      USE LINDS_INT
      USE WRRRN_INT
!                                 Declare variables
      INTEGER    LDA, LDAINV
      PARAMETER  (LDA=3, LDAINV=3)
      REAL       A(LDA,LDA), AINV(LDAINV,LDAINV)
!
!                                 Set values for A
!                                 A = (  1.0  -3.0   2.0)
!                                     ( -3.0  10.0  -5.0)
!                                     (  2.0  -5.0   6.0)
!
      DATA A/1.0, -3.0, 2.0, -3.0, 10.0, -5.0, 2.0, -5.0, 6.0/
!
      CALL LINDS (A, AINV)
!                                 Print results
      CALL WRRRN ('AINV', AINV)
!
      END
```

Output

```
           AINV
        1       2       3
1   35.00    8.00   -5.00
2    8.00    2.00   -1.00
3   -5.00   -1.00    1.00
```

ScaLAPACK Example

The inverse of the same 3 × 3 matrix is computed as a distributed example. SCALAPACK_MAP and SCALAPACK_UNMAP are IMSL utility routines (see *Chapter 11, "Utilities"*) used to map and unmap arrays to and from the processor grid. They are used here for brevity. DESCINIT is a ScaLAPACK tools routine which initializes the descriptors for the local arrays.

```
      USE MPI_SETUP_INT
      USE LINDS_INT
      USE WRRRN_INT
      USE SCALAPACK_SUPPORT
      IMPLICIT NONE
      INCLUDE 'mpif.h'
!                                  Declare variables
      INTEGER     J, LDA, LDFACT, N, DESCA(9)
      INTEGER     INFO, MXCOL, MXLDA
      REAL, ALLOCATABLE ::         A(:,:), AINV(:,:)
      REAL, ALLOCATABLE ::         A0(:,:), AINV0(:,:)
      PARAMETER  (LDA=3, N=3)
!                                  Set up for MPI
      MP_NPROCS = MP_SETUP()
      IF(MP_RANK .EQ. 0) THEN
          ALLOCATE (A(LDA,N), AINV(LDA,N))
!                                  Set values for A
          A(1,:) = (/  1.0,  -3.0,   2.0/)
          A(2,:) = (/ -3.0,  10.0,  -5.0/)
          A(3,:) = (/  2.0,  -5.0,   6.0/)

      ENDIF

!                                   Set up a 1D processor grid and define
!                                   its context ID, MP_ICTXT
      CALL SCALAPACK_SETUP(N, N, .TRUE., .TRUE.)
!                                   Get the array descriptor entities MXLDA,
!                                   and MXCOL
      CALL SCALAPACK_GETDIM(N, N, MP_MB, MP_NB, MXLDA, MXCOL)
!                                   Set up the array descriptors
      CALL DESCINIT(DESCA, N, N, MP_MB, MP_NB, 0, 0, MP_ICTXT, MXLDA, INFO)
!                                   Allocate space for the local arrays
      ALLOCATE(A0(MXLDA,MXCOL), AINV0(MXLDA,MXCOL))
!                                   Map input arrays to the processor grid
      CALL SCALAPACK_MAP(A, DESCA, A0)
!                                   Call the routine to get the inverse
      CALL LINDS (A0, AINV0)
!                                   Unmap the results from the distributed
!                                   arrays back to a nondistributed array.
!                                   After the unmap, only Rank=0 has the full
!                                   array.
      CALL SCALAPACK_UNMAP(AINV0, DESCA, AINV)
!                                   Print results.
!                                   Only Rank=0 has the solution, AINV.
      IF(MP_RANK.EQ.0) CALL WRRRN ('AINV', AINV)
      IF (MP_RANK .EQ. 0) DEALLOCATE(A, AINV)
      DEALLOCATE(A0, AINV0)
!                                   Exit ScaLAPACK usage
      CALL SCALAPACK_EXIT(MP_ICTXT)
!                                   Shut down MPI
      MP_NPROCS = MP_SETUP('FINAL')
      END
```

Output

```
            AINV
          1        2        3
1   35.00     8.00    -5.00
2    8.00     2.00    -1.00
3   -5.00    -1.00     1.00
```

LSASF

more...

Solves a real symmetric system of linear equations with iterative refinement.

Required Arguments

A — N by N matrix containing the coefficient matrix of the symmetric linear system. (Input)
Only the upper triangle of A is referenced.

B — Vector of length N containing the right-hand side of the linear system. (Input)

X — Vector of length N containing the solution to the linear system. (Output)

Optional Arguments

N — Number of equations. (Input)
Default: N = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

FORTRAN 90 Interface

Generic: CALL LSASF (A, B, X [, …])

Specific: The specific interface names are S_LSASF and D_LSASF.

FORTRAN 77 Interface

Single: CALL LSASF (N, A, LDA, B, X)

Double: The double precision name is DLSASF.

Description

Routine LSASF solves systems of linear algebraic equations having a real symmetric indefinite coefficient matrix. It first uses the routine LFCSF to compute a UDU^T factorization of the coefficient matrix and to estimate the condition number of the matrix. D is a block diagonal matrix with blocks of order 1 or 2, and U is a matrix composed of the product of a permutation matrix and a unit upper triangular matrix. The solution of the linear system is then found using the iterative refinement routine LFISF.

LSASF fails if a block in D is singular or if the iterative refinement algorithm fails to converge. These errors occur only if A is singular or very close to a singular matrix.

If the estimated condition number is greater than $1/\varepsilon$ (where ε is machine precision), a warning error is issued. This indicates that very small changes in A can cause very large changes in the solution x. Iterative refinement can sometimes find the solution to such a system. LSASF solves the problem that is represented in the computer; however, this problem may differ from the problem whose solution is desired.

Comments

1. Workspace may be explicitly provided, if desired, by use of L2ASF/DL2ASF. The reference is

   CALL L2ASF (N, A, LDA, B, X, FACT, IPVT, WK)

   The additional arguments are as follows:

   FACT — N × N work array containing information about the UDU^T factorization of A on output. If A is not needed, A and FACT can share the same storage location.

   IPVT — Integer work vector of length N containing the pivoting information for the factorization of A on output.

   WK — Work vector of length N.

2. Informational errors

Type	Code	Description
3	1	The input matrix is too ill-conditioned. The solution might not be accurate.
4	2	The input matrix is singular.

3. *Integer Options* with *Chapter 11* Options Manager

   16 This option uses four values to solve memory bank conflict (access inefficiency) problems. In routine L2ASF the leading dimension of FACT is increased by IVAL(3) when N is a multiple of IVAL(4). The values IVAL(3) and IVAL(4) are temporarily replaced by IVAL(1) and IVAL(2), respectively, in LSASF. Additional memory allocation for FACT and option value restoration are done automatically in LSASF. Users directly calling L2ASF can allocate additional space for FACT and set IVAL(3) and IVAL(4) so that memory bank conflicts no longer cause inefficiencies. There is no requirement that users change existing applications that use LSASF or L2ASF. Default values for the option are IVAL(*) = 1, 16, 0, 1.

17 This option has two values that determine if the L_1 condition number is to be computed. Routine LSASF temporarily replaces IVAL(2) by IVAL(1). The routine L2CSF computes the condition number if IVAL(2) = 2. Otherwise L2CSF skips this computation. LSASF restores the option. Default values for the option are IVAL(*) = 1, 2.

Example

A system of three linear equations is solved. The coefficient matrix has real symmetric form and the right-hand-side vector *b* has three elements.

```
      USE LSASF_INT
      USE WRRRN_INT
!                                 Declare variables
      PARAMETER  (LDA=3, N=3)
      REAL       A(LDA,LDA), B(N), X(N)
!
!                                 Set values for A and B
!
!                                 A = (  1.0  -2.0   1.0)
!                                     ( -2.0   3.0  -2.0)
!                                     (  1.0  -2.0   3.0)
!
!                                 B = (  4.1  -4.7   6.5)
!
      DATA A/1.0, -2.0, 1.0, -2.0, 3.0, -2.0, 1.0, -2.0, 3.0/
      DATA B/4.1, -4.7, 6.5/
!
      CALL LSASF (A, B, X)
!                                 Print results
      CALL WRRRN ('X', X, 1, N, 1)
      END
```

Output

```
            X
     1        2        3
-4.100   -3.500    1.200
```

LSLSF

more...

Solves a real symmetric system of linear equations without iterative refinement .

Required Arguments

A — N by N matrix containing the coefficient matrix of the symmetric linear system. (Input)
Only the upper triangle of A is referenced.

B — Vector of length N containing the right-hand side of the linear system. (Input)

X — Vector of length N containing the solution to the linear system. (Output)

Optional Arguments

N — Number of equations. (Input)
Default: N = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

FORTRAN 90 Interface

Generic: CALL LSLSF (A, B, X [, …])

Specific: The specific interface names are S_LSLSF and D_LSLSF.

FORTRAN 77 Interface

Single: CALL LSLSF (N, A, LDA, B, X)

Double: The double precision name is DLSLSF.

Description

Routine `LSLSF` solves systems of linear algebraic equations having a real symmetric indefinite coefficient matrix. It first uses the routine `LFCSF` to compute a UDU^T factorization of the coefficient matrix. D is a block diagonal matrix with blocks of order 1 or 2, and U is a matrix composed of the product of a permutation matrix and a unit upper triangular matrix.

The solution of the linear system is then found using the routine `LFSSF`.

`LSLSF` fails if a block in D is singular. This occurs only if A either is singular or is very close to a singular matrix.

Comments

1. Workspace may be explicitly provided, if desired, by use of `L2LSF`/`DL2LSF`. The reference is:

   `CALL L2LSF (N, A, LDA, B, X, FACT, IPVT, WK)`

   The additional arguments are as follows:

   FACT — `N` × `N` work array containing information about the UDU^T factorization of `A` on output. If `A` is not needed, `A` and `FACT` can share the same storage locations.

   IPVT — Integer work vector of length `N` containing the pivoting information for the factorization of `A` on output.

   WK — Work vector of length `N`.

2. Informational errors

Type	Code	Description
3	1	The input matrix is too ill-conditioned. The solution might not be accurate.
4	2	The input matrix is singular.

3. *Integer Options* with *Chapter 11* Options Manager

   16 This option uses four values to solve memory bank conflict (access inefficiency) problems. In routine `LSLSF` the leading dimension of `FACT` is increased by `IVAL`(3) when `N` is a multiple of `IVAL`(4). The values `IVAL`(3) and `IVAL`(4) are temporarily replaced by `IVAL`(1) and `IVAL`(2), respectively, in `LSLSF`. Additional memory allocation for `FACT` and option value restoration are done automatically in `LSLSF`. Users directly calling `LSLSF` can allocate additional space for `FACT` and set `IVAL`(3) and `IVAL`(4) so that memory bank conflicts no longer cause inefficiencies. There is no requirement that users change existing applications that use `LSLSF` or `LSLSF`. Default values for the option are `IVAL(*)` = 1, 16, 0, 1.

   17 This option has two values that determine if the L_1 condition number is to be computed. Routine `LSLSF` temporarily replaces `IVAL`(2) by `IVAL`(1). The routine `L2CSF` computes the condition number if `IVAL`(2) = 2. Otherwise `L2CSF` skips this computation. `LSLSF` restores the option. Default values for the option are `IVAL(*)` = 1, 2.

Example

A system of three linear equations is solved. The coefficient matrix has real symmetric form and the right-hand-side vector *b* has three elements.

```
      USE LSLSF_INT
      USE WRRRN_INT
!                                 Declare variables
      PARAMETER  (LDA=3, N=3)
      REAL       A(LDA,LDA), B(N), X(N)
!
!                                 Set values for A and B
!
!                                 A = (  1.0  -2.0   1.0)
!                                     ( -2.0   3.0  -2.0)
!                                     (  1.0  -2.0   3.0)
!
!                                 B = (  4.1  -4.7   6.5)
!
      DATA A/1.0, -2.0, 1.0, -2.0, 3.0, -2.0, 1.0, -2.0, 3.0/
      DATA B/4.1, -4.7, 6.5/
!
      CALL LSLSF (A, B, X)
!                                 Print results
      CALL WRRRN ('X', X, 1, N, 1)
      END
```

Output

```
            X
     1        2        3
-4.100   -3.500   1.200
```

LFCSF

more...

Computes the $U\,DU^T$ factorization of a real symmetric matrix and estimate its L_1 condition number.

Required Arguments

A — `N` by `N` symmetric matrix to be factored. (Input)
Only the upper triangle of `A` is referenced.

FACT — `N` by `N` matrix containing information about the factorization of the symmetric matrix `A`. (Output)
Only the upper triangle of `FACT` is used. If `A` is not needed, `A` and `FACT` can share the same storage locations.

IPVT — Vector of length `N` containing the pivoting information for the factorization. (Output)

RCOND — Scalar containing an estimate of the reciprocal of the L_1 condition number of `A`. (Output)

Optional Arguments

N — Order of the matrix. (Input)
Default: `N` = size (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = size (`A`,1).

LDFACT — Leading dimension of `FACT` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDFACT` = size (`FACT`,1).

FORTRAN 90 Interface

Generic: `CALL LFCSF (A, FACT, IPVT, RCOND [, …])`

Specific: The specific interface names are `S_LFCSF` and `D_LFCSF`.

FORTRAN 77 Interface

Single: `CALL LFCSF (N, A, LDA, FACT, LDFACT, IPVT, RCOND)`

Double: The double precision name is `DLFCSF`.

Description

Routine `LFCSF` performs a UDU^T factorization of a real symmetric indefinite coefficient matrix. It also estimates the condition number of the matrix. The UDU^T factorization is called the diagonal pivoting factorization.

The L_1 condition number of the matrix A is defined to be $\kappa(A) = \|A\|_1 \|A^{-1}\|_1$. Since it is expensive to compute $\|A^{-1}\|_1$, the condition number is only estimated. The estimation algorithm is the same as used by LINPACK and is described by Cline et al. (1979).

If the estimated condition number is greater than $1/\varepsilon$ (where ε is machine precision), a warning error is issued. This indicates that very small changes in `A` can cause very large changes in the solution x. Iterative refinement can sometimes find the solution to such a system.

`LFCSF` fails if `A` is singular or very close to a singular matrix.

The UDU^T factors are returned in a form that is compatible with routines `LFISF`, `LFSSF` and `LFDSF`. To solve systems of equations with multiple right-hand-side vectors, use `LFCSF` followed by either `LFISF` or `LFSSF` called once for each right-hand side. The routine `LFDSF` can be called to compute the determinant of the coefficient matrix after `LFCSF` has performed the factorization.

The underlying code is based on either LINPACK or LAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see "*Using ScaLAPACK, LAPACK, LINPACK, and EISPACK*" in the *Introduction* section of this manual.

Comments

1. Workspace may be explicitly provided, if desired, by use of `L2CSF/DL2CSF`. The reference is:

   `CALL L2CSF (N, A, LDA, FACT, LDFACT, IPVT, RCOND, WK)`

   The additional argument is:

   WK — Work vector of length `N`.

2. Informational errors

Type	Code	Description
3	1	The input matrix is algorithmically singular.
4	2	The input matrix is singular.

Example

The inverse of a 3 × 3 matrix is computed. LFCSF is called to factor the matrix and to check for singularity or ill-conditioning. LFISF is called to determine the columns of the inverse.

```
      USE LFCSF_INT
      USE UMACH_INT
      USE LFISF_INT
      USE WRRRN_INT
!                                 Declare variables
      PARAMETER  (LDA=3, N=3)
      INTEGER    IPVT(N), NOUT
      REAL       A(LDA,LDA), AINV(N,N), FACT(LDA,LDA), RJ(N), RES(N),&
                 RCOND
!
!                                 Set values for A
!
!                                 A = (  1.0  -2.0   1.0)
!                                     ( -2.0   3.0  -2.0)
!                                     (  1.0  -2.0   3.0)
!
      DATA A/1.0, -2.0, 1.0, -2.0, 3.0, -2.0, 1.0, -2.0, 3.0/
!                                 Factor A and return the reciprocal
!                                 condition number estimate
      CALL LFCSF (A, FACT, IPVT, RCOND)
!                                 Print the estimate of the condition
!                                 number
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) RCOND, 1.0E0/RCOND
!
!                                 matrix one at a time in RJ
      RJ = 0.E0
      DO 10  J=1, N
         RJ(J) = 1.0E0
!                                 RJ is the J-th column of the identity
!                                 matrix so the following LFISF
!                                 reference places the J-th column of
!                                 the inverse of A in the J-th column
!                                 of AINV
         CALL LFISF (A, FACT, IPVT, RJ, AINV(:,J), RES)
         RJ(J) = 0.0E0
   10 CONTINUE
!                                 Print the inverse
      CALL WRRRN ('AINV', AINV)
99999 FORMAT ('  RCOND = ',F5.3,/,'  L1 Condition number = ',F6.3)
      END
```

Output

```
RCOND < 0.05
L1 Condition number < 40.0
```

```
            AINV
         1        2        3
 1  -2.500  -2.000  -0.500
 2  -2.000  -1.000   0.000
 3  -0.500   0.000   0.500
```

LFTSF

more...

Computes the UDU^T factorization of a real symmetric matrix.

Required Arguments

A — `N` by `N` symmetric matrix to be factored. (Input)
Only the upper triangle of `A` is referenced.

FACT — `N` by `N` matrix containing information about the factorization of the symmetric matrix `A`. (Output)
Only the upper triangle of `FACT` is used. If `A` is not needed, `A` and `FACT` can share the same storage locations.

IPVT — Vector of length `N` containing the pivoting information for the factorization. (Output)

Optional Arguments

N — Order of the matrix. (Input)
Default: `N` = size (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = size (`A`,1).

LDFACT — Leading dimension of `FACT` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDFACT` = size (`FACT`,1).

FORTRAN 90 Interface

Generic: `CALL LFTSF (A, FACT, IPVT [, …])`

Specific: The specific interface names are `S_LFTSF` and `D_LFTSF`.

FORTRAN 77 Interface

Single:	`CALL LFTSF (N, A, LDA, FACT, LDFACT, IPVT)`
Double:	The double precision name is `DLFTSF`.

Description

Routine `LFTSF` performs a UDU^T factorization of a real symmetric indefinite coefficient matrix. The UDU^T factorization is called the diagonal pivoting factorization.

`LFTSF` fails if A is singular or very close to a singular matrix.

The UDU^T factors are returned in a form that is compatible with routines `LFISF`, `LFSSF` and `LFDSF`. To solve systems of equations with multiple right-hand-side vectors, use `LFTSF` followed by either `LFISF` or `LFSSF` called once for each right-hand side. The routine `LFDSF` can be called to compute the determinant of the coefficient matrix after `LFTSF` has performed the factorization.

The underlying code is based on either LINPACK or LAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see *Using ScaLAPACK, LAPACK, LINPACK, and EISPACK* in the Introduction section of this manual.

Comments

Informational error

Type	Code	Description
4	2	The input matrix is singular.

Example

The inverse of a 3×3 matrix is computed. `LFTSF` is called to factor the matrix and to check for singularity. `LFSSF` is called to determine the columns of the inverse.

```
      USE LFTSF_INT
      USE LFSSF_INT
      USE WRRRN_INT
!                                 Declare variables
      PARAMETER  (LDA=3, N=3)
      INTEGER    IPVT(N)
      REAL       A(LDA,LDA), AINV(N,N), FACT(LDA,LDA), RJ(N)
!
!                                 Set values for A
!                                 A = (  1.0  -2.0   1.0)
!                                     ( -2.0   3.0  -2.0)
!                                     (  1.0  -2.0   3.0)
```

```
!
      DATA A/1.0, -2.0, 1.0, -2.0, 3.0, -2.0, 1.0, -2.0, 3.0/
!                                   Factor A
      CALL LFTSF (A, FACT, IPVT)
!                                   Set up the columns of the identity
!                                   matrix one at a time in RJ
      RJ = 0.0E0
      DO 10  J=1, N
         RJ(J) = 1.0E0
!                                   RJ is the J-th column of the identity
!                                   matrix so the following LFSSF
!                                   reference places the J-th column of
!                                   the inverse of A in the J-th column
!                                   of AINV
         CALL LFSSF (FACT, IPVT, RJ, AINV(:,J))
         RJ(J) = 0.0E0
   10 CONTINUE
!                                   Print the inverse
      CALL WRRRN ('AINV', AINV)
      END
```

Output

```
             AINV
        1        2        3
1  -2.500  -2.000  -0.500
2  -2.000  -1.000   0.000
3  -0.500   0.000   0.500
```

LFSSF

more...

Solves a real symmetric system of linear equations given the $U D U^T$ factorization of the coefficient matrix.

Required Arguments

FACT — N by N matrix containing the factorization of the coefficient matrix A as output from routine LFCSF/DLFCSF or LFTSF/DLFTSF. (Input)
Only the upper triangle of FACT is used.

IPVT — Vector of length N containing the pivoting information for the factorization of A as output from routine LFCSF/DLFCSF or LFTSF/DLFTSF. (Input)

B — Vector of length N containing the right-hand side of the linear system. (Input)

X — Vector of length N containing the solution to the linear system. (Output)
If B is not needed, B and X can share the same storage locations.

Optional Arguments

N — Number of equations. (Input)
Default: N = size (FACT,2).

LDFACT — Leading dimension of FACT exactly as specified in the dimension statement of the calling program. (Input)
Default: LDFACT = size (FACT,1).

FORTRAN 90 Interface

Generic:	CALL LFSSF (FACT, IPVT, B, X [, …])
Specific:	The specific interface names are S_LFSSF and D_LFSSF.

FORTRAN 77 Interface

Single: CALL LFSSF (N, FACT, LDFACT, IPVT, B, X)

Double: The double precision name is DLFSSF.

Description

Routine LFSSF computes the solution of a system of linear algebraic equations having a real symmetric indefinite coefficient matrix.

To compute the solution, the coefficient matrix must first undergo a UDU^T factorization. This may be done by calling either LFCSF or LFTSF.

LFSSF and LFISF both solve a linear system given its UDU^T factorization. LFISF generally takes more time and produces a more accurate answer than LFSSF. Each iteration of the iterative refinement algorithm used by LFISF calls LFSSF.

The underlying code is based on either LINPACK or LAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see "*Using ScaLAPACK, LAPACK, LINPACK, and EISPACK*" in the *Introduction* section of this manual.

Example

A set of linear systems is solved successively. LFTSF is called to factor the coefficient matrix. LFSSF is called to compute the four solutions for the four right-hand sides. In this case the coefficient matrix is assumed to be well-conditioned and correctly scaled. Otherwise, it would be better to call LFCSF to perform the factorization, and LFISF to compute the solutions.

```
      USE LFSSF_INT
      USE LFTSF_INT
      USE WRRRN_INT
!                                 Declare variables
      PARAMETER  (LDA=3, N=3)
      INTEGER    IPVT(N)
      REAL       A(LDA,LDA), B(N,4), X(N,4), FACT(LDA,LDA)
!
!                                 Set values for A and B
!
!                                 A = (  1.0  -2.0   1.0)
!                                     ( -2.0   3.0  -2.0)
!                                     (  1.0  -2.0   3.0)
!
!                                 B = ( -1.0   3.6  -8.0  -9.4)
!                                     ( -3.0  -4.2  11.0  17.6)
!                                     ( -3.0  -5.2  -6.0 -23.4)
!
      DATA A/1.0, -2.0, 1.0, -2.0, 3.0, -2.0, 1.0, -2.0, 3.0/
      DATA B/-1.0, -3.0, -3.0, 3.6, -4.2, -5.2, -8.0, 11.0, -6.0,&
          -9.4, 17.6, -23.4/
```

```
!                                  Factor A
      CALL LFTSF (A, FACT, IPVT)
!                                  Solve for the four right-hand sides
      DO 10  I=1, 4
         CALL LFSSF (FACT, IPVT, B(:,I), X(:,I))
   10 CONTINUE

!                                  Print results
      CALL WRRRN ('X', X)
      END
```

Output

```
                    X
         1        2        3        4
1   10.00     2.00     1.00     0.00
2    5.00    -3.00     5.00     1.20
3   -1.00    -4.40     1.00    -7.00
```

LFISF

more...

Uses iterative refinement to improve the solution of a real symmetric system of linear equations.

Required Arguments

A — N by N matrix containing the coefficient matrix of the symmetric linear system. (Input)
Only the upper triangle of A is referenced

FACT — N by N matrix containing the factorization of the coefficient matrix A as output from routine LFCSF/DLFCSF or LFTSF/DLFTSF. (Input)
Only the upper triangle of FACT is used.

IPVT — Vector of length N containing the pivoting information for the factorization of A as output from routine LFCSF/DLFCSF or LFTSF/DLFTSF. (Input)

B — Vector of length N containing the right-hand side of the linear system. (Input)

X — Vector of length N containing the solution to the linear system. (Output)
If B is not needed, B and X can share the same storage locations.

RES — Vector of length N containing the residual vector at the improved solution. (Output)

Optional Arguments

N — Number of equations. (Input)
Default: N = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

LDFACT — Leading dimension of FACT exactly as specified in the dimension statement of the calling program. (Input)
Default: LDFACT = size (FACT,1).

FORTRAN 90 Interface

Generic: `CALL LFISF (A, FACT, IPVT, B, X, RES [, …])`

Specific: The specific interface names are `S_LFISF` and `D_LFISF`.

FORTRAN 77 Interface

Single: `CALL LFISF (N, A, LDA, FACT, LDFACT, IPVT, B, X, RES)`

Double: The double precision name is `DLFISF`.

Description

Routine `LFISF` computes the solution of a system of linear algebraic equations having a real symmetric indefinite coefficient matrix. Iterative refinement is performed on the solution vector to improve the accuracy. Usually almost all of the digits in the solution are accurate, even if the matrix is somewhat ill-conditioned.

To compute the solution, the coefficient matrix must first undergo a $U\,DU^T$ factorization. This may be done by calling either `LFCSF` or `LFTSF`.

Iterative refinement fails only if the matrix is very ill-conditioned.

`LFISF` and `LFSSF` both solve a linear system given its $U\,DU^T$ factorization. `LFISF` generally takes more time and produces a more accurate answer than `LFSSF`. Each iteration of the iterative refinement algorithm used by `LFISF` calls `LFSSF`.

Comments

Informational error

Type	Code	Description
3	2	The input matrix is too ill-conditioned for iterative refinement to be effective.

Example

A set of linear systems is solved successively. The right-hand-side vector is perturbed after solving the system each of the first two times by adding 0.2 to the second element.

```
      USE LFISF_INT
      USE UMACH_INT
```

```
      USE LFCSF_INT
      USE WRRRN_INT
!                                 Declare variables
      PARAMETER  (LDA=3, N=3)
      INTEGER    IPVT(N), NOUT
      REAL       A(LDA,LDA), B(N), X(N), FACT(LDA,LDA), RES(N), RCOND
!
!                                 Set values for A and B
!                                 A = (  1.0  -2.0   1.0)
!                                     ( -2.0   3.0  -2.0)
!                                     (  1.0  -2.0   3.0)
!
!                                 B = (  4.1  -4.7   6.5)
!
      DATA A/1.0, -2.0, 1.0, -2.0, 3.0, -2.0, 1.0, -2.0, 3.0/
      DATA B/4.1, -4.7, 6.5/
!                                 Factor A and compute the estimate
!                                 of the reciprocal condition number
      CALL LFCSF (A, FACT, IPVT, RCOND)
!                                 Print condition number
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) RCOND, 1.0E0/RCOND
!                                 Solve, then perturb right-hand side
      DO 10  I=1, 3
         CALL LFISF (A, FACT, IPVT, B, X, RES)
!                                 Print results
         CALL WRRRN ('X', X, 1, N, 1)
         CALL WRRRN ('RES', RES, 1, N, 1)
         B(2) = B(2) + .20E0
   10 CONTINUE
!
99999 FORMAT ('  RCOND = ',F5.3,/,'  L1 Condition number = ',F6.3)
      END
```

Output

```
RCOND < 0.035
L1 Condition number < 40.0

           X
     1       2       3
-4.100  -3.500   1.200
               RES
         1           2           3
-2.384E-07  -2.384E-07   0.000E+00
            X
     1       2       3
-4.500  -3.700   1.200
               RES
         1           2           3
-2.384E-07  -2.384E-07   0.000E+00
            X
     1       2       3
-4.900  -3.900   1.200
               RES
         1           2           3
-2.384E-07  -2.384E-07   0.000E+00
```

LFDSF

Computes the determinant of a real symmetric matrix given the UDU^T factorization of the matrix.

Required Arguments

FACT — N by N matrix containing the factored matrix *A* as output from subroutine LFTSF/DLFTSF or LFCSF/DLFCSF. (Input)

IPVT — Vector of length N containing the pivoting information for the UDU^T factorization as output from routine LFTSF/DLFTSF or LFCSF/DLFCSF. (Input)

DET1 — Scalar containing the mantissa of the determinant. (Output)
The value DET1 is normalized so that, 1.0 ≤ |DET1| < 10.0 or DET1 = 0.0.

DET2 — Scalar containing the exponent of the determinant. (Output)
The determinant is returned in the form, det(*A*) = DET1 * 10^{DET2}.

Optional Arguments

N — Order of the matrix. (Input)
Default: N = size (FACT,2).

LDFACT — Leading dimension of FACT exactly as specified in the dimension statement of the calling program. (Input)
Default: LDFACT = size (FACT,1).

FORTRAN 90 Interface

Generic: CALL LFDSF (FACT, IPVT, DET1, DET2 [, …])

Specific: The specific interface names are S_LFDSF and D_LFDSF.

FORTRAN 77 Interface

Single: CALL LFDSF (N, FACT, LDFACT, IPVT, DET1, DET2)

Double: The double precision name is DLFDSF.

Description

Routine `LFDSF` computes the determinant of a real symmetric indefinite coefficient matrix. To compute the determinant, the coefficient matrix must first undergo a $U D U^T$ factorization. This may be done by calling either `LFCSF` or `LFTSF`. Since $\det U = \pm 1$, the formula $\det A = \det U \det D \det U^T = \det D$ is used to compute the determinant. Next $\det D$ is computed as the product of the determinants of its blocks.

`LFDSF` is based on the LINPACK routine `SSIDI`; see Dongarra et al. (1979).

Example

The determinant is computed for a real symmetric 3×3 matrix.

```
      USE LFDSF_INT
      USE LFTSF_INT
      USE UMACH_INT
!                                 Declare variables
      PARAMETER  (LDA=3, N=3)
      INTEGER    IPVT(N), NOUT
      REAL       A(LDA,LDA), FACT(LDA,LDA), DET1, DET2
!
!                                 Set values for A
!                                 A = (  1.0  -2.0   1.0)
!                                     ( -2.0   3.0  -2.0)
!                                     (  1.0  -2.0   3.0)
!
      DATA A/1.0, -2.0, 1.0, -2.0, 3.0, -2.0, 1.0, -2.0, 3.0/
!                                 Factor A
      CALL LFTSF (A, FACT, IPVT)
!                                 Compute the determinant
      CALL LFDSF (FACT, IPVT, DET1, DET2)
!                                 Print the results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) DET1, DET2
99999 FORMAT (' The determinant of A is ', F6.3, ' * 10**', F2.0)
      END
```

Output

```
The determinant of A is -2.000 * 10**0.
```

LSADH

more... more...

Solves a Hermitian positive definite system of linear equations with iterative refinement.

Required Arguments

A — Complex `N` by `N` matrix containing the coefficient matrix of the Hermitian positive definite linear system. (Input)
Only the upper triangle of `A` is referenced.

B — Complex vector of length `N` containing the right-hand side of the linear system. (Input)

X — Complex vector of length `N` containing the solution of the linear system. (Output)

Optional Arguments

N — Number of equations. (Input)
Default: `N` = size (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = size (`A`,1).

FORTRAN 90 Interface

Generic: `CALL LSADH` (`A`, `B`, `X` `[`, `...]`)

Specific: The specific interface names are `S_LSADH` and `D_LSADH`.

FORTRAN 77 Interface

Single: `CALL LSADH` (`N`, `A`, `LDA`, `B`, `X`)

Double: The double precision name is `DLSADH`.

ScaLAPACK Interface

Generic: CALL LSADH (A0, B0, X0 [, ...])

Specific: The specific interface names are S_LSADH and D_LSADH.

See the *ScaLAPACK Usage Notes* below for a description of the arguments for distributed computing.

Description

Routine LSADH solves a system of linear algebraic equations having a complex Hermitian positive definite coefficient matrix. It first uses the routine LFCDH to compute an $R^H R$ Cholesky factorization of the coefficient matrix and to estimate the condition number of the matrix. The matrix R is upper triangular. The solution of the linear system is then found using the iterative refinement routine LFIDH.

LSADH fails if any submatrix of R is not positive definite, if R has a zero diagonal element or if the iterative refinement algorithm fails to converge. These errors occur only if A either is very close to a singular matrix or is a matrix that is not positive definite.

If the estimated condition number is greater than $1/\varepsilon$ (where ε is machine precision), a warning error is issued. This indicates that very small changes in A can cause very large changes in the solution x. Iterative refinement can sometimes find the solution to such a system. LSADH solves the problem that is represented in the computer; however, this problem may differ from the problem whose solution is desired.

The underlying code is based on either LINPACK , LAPACK, or ScaLAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see *Using ScaLAPACK, LAPACK, LINPACK, and EISPACK* in the Introduction section of this manual.

Comments

1. Workspace may be explicitly provided, if desired, by use of L2ADH/DL2ADH. The reference is:

   CALL L2ADH (N, A, LDA, B, X, FACT, WK)

   The additional arguments are as follows:

   FACT — N × N work array containing the $R^H R$ factorization of A on output.

   WK — Complex work vector of length N.

2. Informational errors

Type	Code	Description
3	1	The input matrix is too ill-conditioned. The solution might not be accurate.
3	4	The input matrix is not Hermitian. It has a diagonal entry with a small imaginary part.
4	2	The input matrix is not positive definite.
4	4	The input matrix is not Hermitian. It has a diagonal entry with an imaginary part.

3. *Integer Options* with *Chapter 11* Options Manager

16 This option uses four values to solve memory bank conflict (access inefficiency) problems. In routine L2ADH the leading dimension of FACT is increased by IVAL(3) when N is a multiple of IVAL(4). The values IVAL(3) and IVAL(4) are temporarily replaced by IVAL(1) and IVAL(2), respectively, in LSADH. Additional memory allocation for FACT and option value restoration are done automatically in LSADH. Users directly calling L2ADH can allocate additional space for FACT and set IVAL(3) and IVAL(4) so that memory bank conflicts no longer cause inefficiencies. There is no requirement that users change existing applications that use LSADH or L2ADH. Default values for the option are IVAL(*) = 1, 16, 0, 1.

17 This option has two values that determine if the L_1 condition number is to be computed. Routine LSADH temporarily replaces IVAL(2) by IVAL(1). The routine L2CDH computes the condition number if IVAL(2) = 2. Otherwise L2CDH skips this computation. LSADH restores the option. Default values for the option are IVAL(*) = 1, 2.

ScaLAPACK Usage Notes

The arguments which differ from the standard version of this routine are:

A0 — Complex MXLDA by MXCOL local matrix containing the local portions of the distributed matrix A. A contains the coefficient matrix of the Hermitian positive definite linear system. (Input)
Only the upper triangle of A is referenced.

B0 — Complex local vector of length MXLDA containing the local portions of the distributed vector B. B contains the right-hand side of the linear system. (Input)

X0 — Complex local vector of length MXLDA containing the local portions of the distributed vector X. X contains the solution to the linear system. (Output)

All other arguments are global and are the same as described for the standard version of the routine. In the argument descriptions above, MXLDA and MXCOL can be obtained through a call to SCALAPACK_GETDIM (see *Utilities*) after a call to SCALAPACK_SETUP (see *Utilities*) has been made. See the *ScaLAPACK Example* below.

Examples

Example

A system of five linear equations is solved. The coefficient matrix has complex positive definite form and the right-hand-side vector *b* has five elements.

```
      USE LSADH_INT
      USE WRCRN_INT
!                                 Declare variables
      INTEGER    LDA, N
      PARAMETER  (LDA=5, N=5)
      COMPLEX    A(LDA,LDA), B(N), X(N)
!
!                                 Set values for A and B
!
!        A =   (  2.0+0.0i  -1.0+1.0i   0.0+0.0i   0.0+0.0i   0.0+0.0i )
!              (             4.0+0.0i   1.0+2.0i   0.0+0.0i   0.0+0.0i )
!              (                       10.0+0.0i   0.0+4.0i   0.0+0.0i )
!              (                                   6.0+0.0i   1.0+1.0i )
!              (                                              9.0+0.0i )
!
!        B =   ( 1.0+5.0i  12.0-6.0i  1.0-16.0i  -3.0-3.0i  25.0+16.0i )
!
      DATA A /(2.0,0.0), 4*(0.0,0.0), (-1.0,1.0), (4.0,0.0),&
             4*(0.0,0.0), (1.0,2.0), (10.0,0.0), 4*(0.0,0.0),&
             (0.0,4.0), (6.0,0.0), 4*(0.0,0.0), (1.0,1.0), (9.0,0.0)/
      DATA B /(1.0,5.0), (12.0,-6.0), (1.0,-16.0), (-3.0,-3.0),&
             (25.0,16.0)/
!
      CALL LSADH (A, B, X)
!                                 Print results
      CALL WRCRN ('X', X, 1, N, 1)
!
      END
```

Output

```
                                  X
              1                  2                  3                  4
( 2.000, 1.000)  ( 3.000, 0.000)  (-1.000,-1.000)  ( 0.000,-2.000)
              5
( 3.000, 2.000)
```

ScaLAPACK Example

The same system of five linear equations is solved as a distributed computing example. The coefficient matrix has complex positive definite form and the right-hand-side vector *b* has five elements. `SCALAPACK_MAP` and `SCALAPACK_UNMAP` are IMSL utility routines (see *Utilities*) used to map and unmap arrays to and from the processor grid. They are used here for brevity. `DESCINIT` is a ScaLAPACK tools routine which initializes the descriptors for the local arrays.

```
      USE MPI_SETUP_INT
      USE LSADH_INT
      USE WRCRN_INT
```

```
      USE SCALAPACK_SUPPORT
      IMPLICIT NONE
      INCLUDE 'mpif.h'
!                                Declare variables
      INTEGER    LDA, N, DESCA(9), DESCX(9)
      INTEGER       INFO, MXCOL, MXLDA
      COMPLEX, ALLOCATABLE ::       A(:,:), B(:), X(:)
      COMPLEX, ALLOCATABLE ::       A0(:,:), B0(:), X0(:)
      PARAMETER  (LDA=5, N=5)
!                                Set up for MPI
      MP_NPROCS = MP_SETUP()
      IF(MP_RANK .EQ. 0) THEN
          ALLOCATE (A(LDA,N), B(N), X(N))
!                                Set values for A and B
      A(1,:) = (/(2.0, 0.0),(-1.0, 1.0),( 0.0, 0.0),(0.0, 0.0),(0.0, 0.0)/)
      A(2,:) = (/(0.0, 0.0),( 4.0, 0.0),( 1.0, 2.0),(0.0, 0.0),(0.0, 0.0)/)
      A(3,:) = (/(0.0, 0.0),( 0.0, 0.0),(10.0, 0.0),(0.0, 4.0),(0.0, 0.0)/)
      A(4,:) = (/(0.0, 0.0),( 0.0, 0.0),( 0.0, 0.0),(6.0, 0.0),(1.0, 1.0)/)
      A(5,:) = (/(0.0, 0.0),( 0.0, 0.0),( 0.0, 0.0),(0.0, 0.0),(9.0, 0.0)/)
!
      B = (/(1.0, 5.0),(12.0, -6.0),(1.0, -16.0),(-3.0, -3.0),(25.0, 16.0)/)
      ENDIF
!                                 Set up a 1D processor grid and define
!                                 its context ID, MP_ICTXT
      CALL SCALAPACK_SETUP(N, N, .TRUE., .TRUE.)
!                                 Get the array descriptor entities MXLDA,
!                                 and MXCOL
      CALL SCALAPACK_GETDIM(N, N, MP_MB, MP_NB, MXLDA, MXCOL)
!                                 Set up the array descriptors
      CALL DESCINIT(DESCA, N, N, MP_MB, MP_NB, 0, 0, MP_ICTXT, MXLDA, INFO)
      CALL DESCINIT(DESCX, N, 1, MP_MB, 1, 0, 0, MP_ICTXT, MXLDA, INFO)
!                                 Allocate space for the local arrays
      ALLOCATE (A0(MXLDA,MXCOL), B0(MXLDA), X0(MXLDA))
!                                 Map input arrays to the processor grid
      CALL SCALAPACK_MAP(A, DESCA, A0)
      CALL SCALAPACK_MAP(B, DESCX, B0)
!                                 Solve the system of equations
      CALL LSADH (A0, B0, X0)
!                                 Unmap the results from the distributed
!                                 arrays back to a non-distributed array.
!                                 After the unmap, only Rank=0 has the full
!                                 array.
      CALL SCALAPACK_UNMAP(X0, DESCX, X)
!                                 Print results.
!                                 Only Rank=0 has the solution, X.
      IF(MP_RANK .EQ. 0)CALL WRCRN ('X', X, 1, N, 1)
      IF (MP_RANK .EQ. 0) DEALLOCATE(A, B, X)
      DEALLOCATE(A0, B0, X0)
!                                 Exit ScaLAPACK usage
      CALL SCALAPACK_EXIT(MP_ICTXT)
!                                 Shut down MPI
      MP_NPROCS = MP_SETUP('FINAL')
      END
```

Output

```
                                X
              1                 2                 3                 4
( 2.000, 1.000)  ( 3.000, 0.000)  (-1.000,-1.000)  ( 0.000,-2.000)
              5
( 3.000, 2.000)
```

LSLDH

more...

more...

Solves a complex Hermitian positive definite system of linear equations without iterative refinement.

Required Arguments

A — Complex `N` by `N` matrix containing the coefficient matrix of the Hermitian positive definite linear system. (Input)
Only the upper triangle of `A` is referenced.

B — Complex vector of length `N` containing the right-hand side of the linear system. (Input)

X — Complex vector of length `N` containing the solution to the linear system. (Output)
If `B` is not needed, `B` and `X` can share the same storage locations.

Optional Arguments

N — Number of equations. (Input)
Default: `N` = size (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = size (`A`,1).

FORTRAN 90 Interface

Generic: `CALL LSLDH (A, B, X [, …])`

Specific: The specific interface names are `S_LSLDH` and `D_LSLDH`.

FORTRAN 77 Interface

Single: `CALL LSLDH (N, A, LDA, B, X)`

Double: The double precision name is `DLSLDH`.

ScaLAPACK Interface

Generic: `CALL LSLDH (A0, B0, X0 [, …])`

Specific: The specific interface names are `S_LSLDH` and `D_LSLDH`.

See the *ScaLAPACK Usage Notes* below for a description of the arguments for distributed computing.

Description

Routine `LSLDH` solves a system of linear algebraic equations having a complex Hermitian positive definite coefficient matrix. The underlying code is based on either LINPACK , LAPACK, or ScaLAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see "*Using ScaLAPACK, LAPACK, LINPACK, and EISPACK* in the Introduction section of this manual. `LSLDH` first uses the routine `LFCDH` to compute an $R^H R$ Cholesky factorization of the coefficient matrix and to estimate the condition number of the matrix. The matrix R is upper triangular. The solution of the linear system is then found using the routine `LFSDH`.

`LSLDH` fails if any submatrix of R is not positive definite or if R has a zero diagonal element. These errors occur only if A is very close to a singular matrix or to a matrix which is not positive definite.

If the estimated condition number is greater than $1/\varepsilon$ (where ε is machine precision), a warning error is issued. This indicates that very small changes in A can cause very large changes in the solution x. If the coefficient matrix is ill-conditioned or poorly scaled, it is recommended that `LSADH` be used.

Comments

1. Workspace may be explicitly provided, if desired, by use of `L2LDH`/ `DL2LDH`. The reference is:

   `CALL L2LDH (N, A, LDA, B, X, FACT, WK)`

   The additional arguments are as follows:

   FACT — `N` × `N` work array containing the $R^H R$ factorization of `A` on output. If `A` is not needed, `A` can share the same storage locations as `FACT`.

   WK — Complex work vector of length `N`.

2. Informational errors

Type	Code	Description
3	1	The input matrix is too ill-conditioned. The solution might not be accurate.
3	4	The input matrix is not Hermitian. It has a diagonal entry with a small imaginary part.

Type	Code	Description
4	2	The input matrix is not positive definite.
4	4	The input matrix is not Hermitian. It has a diagonal entry with an imaginary part.

3. *Integer Options* with *Chapter 11* Options Manager

16This option uses four values to solve memory bank conflict (access inefficiency) problems. In routine L2LDH the leading dimension of FACT is increased by IVAL(3) when N is a multiple of IVAL(4). The values IVAL(3) and IVAL(4) are temporarily replaced by IVAL(1) and IVAL(2), respectively, in LSLDH. Additional memory allocation for FACT and option value restoration are done automatically in LSLDH. Users directly calling L2LDH can allocate additional space for FACT and set IVAL(3) and IVAL(4) so that memory bank conflicts no longer cause inefficiencies. There is no requirement that users change existing applications that use LSLDH or L2LDH. Default values for the option are IVAL(*) = 1, 16, 0, 1.

17This option has two values that determine if the L_1 condition number is to be computed. Routine LSLDH temporarily replaces IVAL(2) by IVAL(1). The routine L2CDH computes the condition number if IVAL(2) = 2. Otherwise L2CDH skips this computation. LSLDH restores the option. Default values for the option are IVAL(*) = 1, 2.

ScaLAPACK Usage Notes

The arguments which differ from the standard version of this routine are:

A0 — Complex MXLDA by MXCOL local matrix containing the local portions of the distributed matrix A. A contains the coefficient matrix of the Hermitian positive definite linear system. (Input)
Only the upper triangle of A is referenced.

B0 — Complex local vector of length MXLDA containing the local portions of the distributed vector B. B contains the right-hand side of the linear system. (Input)

X0 — Complex local vector of length MXLDA containing the local portions of the distributed vector X. X contains the solution to the linear system. (Output)
If B is not needed, B and X can share the same storage locations.

All other arguments are global and are the same as described for the standard version of the routine. In the argument descriptions above, MXLDA and MXCOL can be obtained through a call to SCALAPACK_GETDIM (see *Utilities*) after a call to SCALAPACK_SETUP (see *Utilities*) has been made. See the *ScaLAPACK Example* below.

Examples

Example

A system of five linear equations is solved. The coefficient matrix has complex Hermitian positive definite form and the right-hand-side vector *b* has five elements.

```
      USE LSLDH_INT
      USE WRCRN_INT
!                                 Declare variables
      INTEGER    LDA, N
      PARAMETER  (LDA=5, N=5)
      COMPLEX    A(LDA,LDA), B(N), X(N)
!
!                                 Set values for A and B
!
!        A =    (  2.0+0.0i  -1.0+1.0i   0.0+0.0i   0.0+0.0i   0.0+0.0i )
!               (             4.0+0.0i   1.0+2.0i   0.0+0.0i   0.0+0.0i )
!               (                       10.0+0.0i   0.0+4.0i   0.0+0.0i )
!               (                                   6.0+0.0i   1.0+1.0i )
!               (                                              9.0+0.0i )
!
!        B =    ( 1.0+5.0i  12.0-6.0i  1.0-16.0i  -3.0-3.0i  25.0+16.0i )
!
      DATA A /(2.0,0.0), 4*(0.0,0.0), (-1.0,1.0), (4.0,0.0),&
             4*(0.0,0.0), (1.0,2.0), (10.0,0.0), 4*(0.0,0.0),&
             (0.0,4.0), (6.0,0.0), 4*(0.0,0.0), (1.0,1.0), (9.0,0.0)/
      DATA B /(1.0,5.0), (12.0,-6.0), (1.0,-16.0), (-3.0,-3.0),&
             (25.0,16.0)/
!
      CALL LSLDH (A, B, X)
!                                 Print results
      CALL WRCRN ('X', X, 1, N, 1)
!
      END
```

Output

```
                                      X
              1                 2                 3                 4
( 2.000, 1.000)   ( 3.000, 0.000)   (-1.000,-1.000)   ( 0.000,-2.000)
              5
( 3.000, 2.000)
```

ScaLAPACK Example

The same system of five linear equations is solved as a distributed computing example. The coefficient matrix has complex positive definite form and the right-hand-side vector *b* has five elements. `SCALAPACK_MAP` and `SCALAPACK_UNMAP` are IMSL utility routines (see *Utilities*) used to map and unmap arrays to and from the processor grid. They are used here for brevity. `DESCINIT` is a ScaLAPACK tools routine which initializes the descriptors for the local arrays.

```
      USE MPI_SETUP_INT
      USE LSLDH_INT
      USE WRCRN_INT
      USE SCALAPACK_SUPPORT
```

```
      IMPLICIT NONE
      INCLUDE 'mpif.h'
!                                  Declare variables
      INTEGER    LDA, N, DESCA(9), DESCX(9)
      INTEGER       INFO, MXCOL, MXLDA
      COMPLEX, ALLOCATABLE ::        A(:,:), B(:), X(:)
      COMPLEX, ALLOCATABLE ::        A0(:,:), B0(:), X0(:)
      PARAMETER  (LDA=5, N=5)
!                                  Set up for MPI
      MP_NPROCS = MP_SETUP()
      IF(MP_RANK .EQ. 0) THEN
          ALLOCATE (A(LDA,N), B(N), X(N))
!                                  Set values for A and B
      A(1,:) = (/(2.0, 0.0),(-1.0, 1.0),( 0.0, 0.0),(0.0, 0.0),(0.0, 0.0)/)
      A(2,:) = (/(0.0, 0.0),( 4.0, 0.0),( 1.0, 2.0),(0.0, 0.0),(0.0, 0.0)/)
      A(3,:) = (/(0.0, 0.0),( 0.0, 0.0),(10.0, 0.0),(0.0, 4.0),(0.0, 0.0)/)
      A(4,:) = (/(0.0, 0.0),( 0.0, 0.0),( 0.0, 0.0),(6.0, 0.0),(1.0, 1.0)/)
      A(5,:) = (/(0.0, 0.0),( 0.0, 0.0),( 0.0, 0.0),(0.0, 0.0),(9.0, 0.0)/)
!
      B = (/(1.0, 5.0),(12.0, -6.0),(1.0, -16.0),(-3.0, -3.0),(25.0, 16.0)/)
      ENDIF
!                                   Set up a 1D processor grid and define
!                                   its context ID, MP_ICTXT
      CALL SCALAPACK_SETUP(N, N, .TRUE., .TRUE.)
!                                   Get the array descriptor entities MXLDA,
!                                   and MXCOL
      CALL SCALAPACK_GETDIM(N, N, MP_MB, MP_NB, MXLDA, MXCOL)
!                                   Set up the array descriptors
      CALL DESCINIT(DESCA, N, N, MP_MB, MP_NB, 0, 0, MP_ICTXT, MXLDA, INFO)
      CALL DESCINIT(DESCX, N, 1, MP_MB, 1, 0, 0, MP_ICTXT, MXLDA, INFO)
!                                   Allocate space for the local arrays
      ALLOCATE (A0(MXLDA,MXCOL), B0(MXLDA), X0(MXLDA))
!                                  Map input arrays to the processor grid
      CALL SCALAPACK_MAP(A, DESCA, A0)
      CALL SCALAPACK_MAP(B, DESCX, B0)
!                                  Solve the system of equations
      CALL LSLDH (A0, B0, X0)
!                                  Unmap the results from the distributed
!                                  arrays back to a non-distributed array.
!                                  After the unmap, only Rank=0 has the full
!                                  array.
      CALL SCALAPACK_UNMAP(X0, DESCX, X)
!                                  Print results.
!                                  Only Rank=0 has the solution, X.
      IF(MP_RANK .EQ. 0)CALL WRCRN ('X', X, 1, N, 1)
      IF (MP_RANK .EQ. 0) DEALLOCATE(A, B, X)
      DEALLOCATE(A0, B0, X0)
!                                 Exit ScaLAPACK usage
      CALL SCALAPACK_EXIT(MP_ICTXT)

!                                 Shut down MPI
      MP_NPROCS = MP_SETUP('FINAL')
      END
```

Output

```
                                  X
              1                 2                 3                 4
( 2.000, 1.000)  ( 3.000, 0.000)  (-1.000,-1.000)  ( 0.000,-2.000)
              5
( 3.000, 2.000)
```

LFCDH

more...

more...

Computes the $R^H R$ factorization of a complex Hermitian positive definite matrix and estimate its L_1 condition number.

Required Arguments

A — Complex `N` by `N` Hermitian positive definite matrix to be factored. (Input) Only the upper triangle of `A` is referenced.

FACT — Complex `N` by `N` matrix containing the upper triangular matrix *R* of the factorization of `A` in the upper triangle. (Output)
Only the upper triangle of `FACT` will be used. If `A` is not needed, `A` and `FACT` can share the same storage locations.

RCOND — Scalar containing an estimate of the reciprocal of the L_1 condition number of `A`. (Output)

Optional Arguments

N — Order of the matrix. (Input)
Default: `N` = size (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = size (`A`,1).

LDFACT --- Leading dimension of `FACT` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDFACT` = size (`FACT`,1).

FORTRAN 90 Interface

Generic: `CALL LFCDH (A, FACT, RCOND [, …])`

Specific: The specific interface names are `S_LFCDH` and `D_LFCDH`.

FORTRAN 77 Interface

Single: `CALL LFCDH (N, A, LDA, FACT, LDFACT, RCOND)`

Double: The double precision name is `DLFCDH`.

ScaLAPACK Interface

Generic: `CALL LFCDH (A0, FACT0, RCOND [, …])`

Specific: The specific interface names are `S_LFCDH` and `D_LFCDH`.

See the *ScaLAPACK Usage Notes* below for a description of the arguments for distributed computing.

Description

Routine `LFCDH` computes an $R^{\boldsymbol{H}} R$ Cholesky factorization and estimates the condition number of a complex Hermitian positive definite coefficient matrix. The matrix R is upper triangular.

The L_1 condition number of the matrix A is defined to be $\kappa(A) = \|A\|_1 \|A^{-1}\|_1$. Since it is expensive to compute $\|A^{-1}\|_1$, the condition number is only estimated. The estimation algorithm is the same as used by LINPACK and is described by Cline et al. (1979).

If the estimated condition number is greater than $1/\varepsilon$ (where ε is machine precision), a warning error is issued. This indicates that very small changes in A can cause very large changes in the solution x. Iterative refinement can sometimes find the solution to such a system.

`LFCDH` fails if any submatrix of R is not positive definite or if R has a zero diagonal element. These errors occur only if A is very close to a singular matrix or to a matrix which is not positive definite.

The $R^{\boldsymbol{H}} R$ factors are returned in a form that is compatible with routines `LFIDH`, `LFSDH` and `LFDDH`. To solve systems of equations with multiple right-hand-side vectors, use `LFCDH` followed by either `LFIDH` or `LFSDH` called once for each right-hand side. The routine `LFDDH` can be called to compute the determinant of the coefficient matrix after `LFCDH` has performed the factorization.

The underlying code is based on either LINPACK , LAPACK, or ScaLAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see *Using ScaLAPACK, LAPACK, LINPACK, and EISPACK* in the Introduction section of this manual.

Comments

1. Workspace may be explicitly provided, if desired, by use of L2CDH/DL2CDH. The reference is:

   CALL L2CDH (N, A, LDA, FACT, LDFACT, RCOND, WK)

   The additional argument is

   WK — Complex work vector of length N.

2. Informational errors

Type	Code	Description
3	1	The input matrix is algorithmically singular.
3	4	The input matrix is not Hermitian. It has a diagonal entry with a small imaginary part.
4	4	The input matrix is not Hermitian.
4	2	The input matrix is not positive definite. It has a diagonal entry with an imaginary part

ScaLAPACK Usage Notes

The arguments which differ from the standard version of this routine are:

A0 — Complex MXLDA by MXCOL local matrix containing the local portions of the distributed matrix A. A contains the Hermitian positive definite matrix to be factored. (Input)
Only the upper triangle of A is referenced.

FACT0 — Complex MXLDA by MXCOL local matrix containing the local portions of the distributed matrix FACT. FACT contains the upper triangular matrix *R* of the factorization of A in the upper triangle. (Output)
Only the upper triangle of FACT will be used. If A is not needed, A and FACT can share the same storage locations.

All other arguments are global and are the same as described for the standard version of the routine. In the argument descriptions above, MXLDA and MXCOL can be obtained through a call to SCALAPACK_GETDIM (see *Utilities*) after a call to SCALAPACK_SETUP (see *Utilities*) has been made. See the *ScaLAPACK Example* below.

Examples

Example

The inverse of a 5 × 5 Hermitian positive definite matrix is computed. LFCDH is called to factor the matrix and to check for nonpositive definiteness or ill-conditioning. LFIDH is called to determine the columns of the inverse.

```
      USE LFCDH_INT
      USE LFIDH_INT
      USE UMACH_INT
      USE WRCRN_INT
!                                 Declare variables
      INTEGER    LDA, LDFACT, N, NOUT
      PARAMETER  (LDA=5, LDFACT=5, N=5)
      REAL       RCOND
      COMPLEX    A(LDA,LDA), AINV(LDA,LDA), FACT(LDFACT,LDFACT),&
                 RES(N), RJ(N)
!
!                                 Set values for A
!
!         A =    (  2.0+0.0i  -1.0+1.0i   0.0+0.0i   0.0+0.0i   0.0+0.0i )
!                (             4.0+0.0i   1.0+2.0i   0.0+0.0i   0.0+0.0i )
!                (                       10.0+0.0i   0.0+4.0i   0.0+0.0i )
!                (                                   6.0+0.0i   1.0+1.0i )
!                (                                              9.0+0.0i )
!
      DATA A /(2.0,0.0), 4*(0.0,0.0), (-1.0,1.0), (4.0,0.0),&
             4*(0.0,0.0), (1.0,2.0), (10.0,0.0), 4*(0.0,0.0),&
             (0.0,4.0), (6.0,0.0), 4*(0.0,0.0), (1.0,1.0), (9.0,0.0)/
!                                 Factor the matrix A
      CALL LFCDH (A, FACT, RCOND)
!                                 Set up the columns of the identity
!                                 matrix one at a time in RJ
      RJ = (0.0E0, 0.0E0)
      DO 10  J=1, N
         RJ(J) = (1.0E0,0.0E0)
!                                 RJ is the J-th column of the identity
!                                 matrix so the following LFIDH
!                                 reference places the J-th column of
!                                 the inverse of A in the J-th column
!                                 of AINV
         CALL LFIDH (A, FACT, RJ, AINV(:,J), RES)
         RJ(J) = (0.0E0,0.0E0)
   10 CONTINUE
!                                 Print the results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) RCOND, 1.0E0/RCOND
      CALL WRCRN ('AINV', AINV)

!
99999 FORMAT ('  RCOND = ',F5.3,/,'  L1 Condition number = ',F6.3)
      END
```

Output

```
RCOND < 0.075
L1 Condition number < 25.0

                                   AINV
                  1                    2                    3                   4
1 ( 0.7166, 0.0000) ( 0.2166,-0.2166)  (-0.0899,-0.0300)  (-0.0207, 0.0622)
```

```
 2 ( 0.2166, 0.2166) ( 0.4332, 0.0000)  (-0.0599,-0.1198)  (-0.0829, 0.0415)
 3 (-0.0899, 0.0300) (-0.0599, 0.1198)  ( 0.1797, 0.0000)  ( 0.0000,-0.1244)
 4 (-0.0207,-0.0622) (-0.0829,-0.0415)  ( 0.0000, 0.1244)  ( 0.2592, 0.0000)
 5 ( 0.0092, 0.0046) ( 0.0138,-0.0046)  (-0.0138,-0.0138)  (-0.0288, 0.0288)
                    5
 1  ( 0.0092,-0.0046)
 2  ( 0.0138, 0.0046)
 3  (-0.0138, 0.0138)
 4  (-0.0288,-0.0288)
 5  ( 0.1175, 0.0000)
```

ScaLAPACK Example

The inverse of the same 5 × 5 Hermitian positive definite matrix in the preceding example is computed as a distributed computing example. `LFCDH` is called to factor the matrix and to check for nonpositive definiteness or ill-conditioning. `LFIDH` is called to determine the columns of the inverse. `SCALAPACK_MAP` and `SCALAPACK_UNMAP` are IMSL utility routines (see *Utilities*) used to map and unmap arrays to and from the processor grid. They are used here for brevity. `DESCINIT` is a ScaLAPACK tools routine which initializes the descriptors for the local arrays.

```
      USE MPI_SETUP_INT
      USE LFCDH_INT
      USE LFIDH_INT
      USE WRCRN_INT
      USE SCALAPACK_SUPPORT
      IMPLICIT NONE
      INCLUDE 'mpif.h'
!                                  Declare variables
      INTEGER    J, LDA, N, NOUT, DESCA(9), DESCX(9)
      INTEGER       INFO, MXCOL, MXLDA
      REAL          RCOND
      COMPLEX, ALLOCATABLE ::        A(:,:), AINV(:,:), RJ(:), RJ0(:)
      COMPLEX, ALLOCATABLE ::        A0(:,:), FACT0(:,:), RES0(:), X0(:)
      PARAMETER  (LDA=5, N=5)
!                                  Set up for MPI
      MP_NPROCS = MP_SETUP()
      IF(MP_RANK .EQ. 0) THEN
          ALLOCATE (A(LDA,N), AINV(LDA,N))
!                                  Set values for A and B
      A(1,:) = (/(2.0, 0.0),(-1.0, 1.0),( 0.0, 0.0),(0.0, 0.0),(0.0, 0.0)/)
      A(2,:) = (/(0.0, 0.0),( 4.0, 0.0),( 1.0, 2.0),(0.0, 0.0),(0.0, 0.0)/)
      A(3,:) = (/(0.0, 0.0),( 0.0, 0.0),(10.0, 0.0),(0.0, 4.0),(0.0, 0.0)/)
      A(4,:) = (/(0.0, 0.0),( 0.0, 0.0),( 0.0, 0.0),(6.0, 0.0),(1.0, 1.0)/)
      A(5,:) = (/(0.0, 0.0),( 0.0, 0.0),( 0.0, 0.0),(0.0, 0.0),(9.0, 0.0)/)
      ENDIF
!                                   Set up a 1D processor grid and define
!                                   its context ID, MP_ICTXT
      CALL SCALAPACK_SETUP(N, N, .TRUE., .TRUE.)
!                                   Get the array descriptor entities MXLDA,
!                                   and MXCOL
      CALL SCALAPACK_GETDIM(N, N, MP_MB, MP_NB, MXLDA, MXCOL)
!                                   Set up the array descriptors
      CALL DESCINIT(DESCA, N, N, MP_MB, MP_NB, 0, 0, MP_ICTXT, MXLDA, INFO)
      CALL DESCINIT(DESCX, N, 1, MP_MB, 1, 0, 0, MP_ICTXT, MXLDA, INFO)
!                                  Allocate space for the local arrays
      ALLOCATE(A0(MXLDA,MXCOL), X0(MXLDA),FACT0(MXLDA,MXCOL), RJ(N), &
                RJ0(MXLDA), RES0(MXLDA))
!                                  Map input arrays to the processor grid
      CALL SCALAPACK_MAP(A, DESCA, A0)
!                                  Factor the matrix A
```

```
      CALL LFCDH (A0, FACT0, RCOND)
!                                  Set up the columns of the identity
!                                  matrix one at a time in RJ
      RJ = (0.0E0, 0.0E0)
      DO 10  J=1, N
         RJ(J) = (1.0E0,0.0E0)
         CALL SCALAPACK_MAP(RJ, DESCX, RJ0)
!                                  RJ is the J-th column of the identity
!                                  matrix so the following LFIDH
!                                  reference solves for the J-th column of
!                                  the inverse of A
         CALL LFIDH (A0, FACT0, RJ0, X0, RES0)
!                                  Unmap the results from the distributed
!                                  array back to a non-distributed array
         CALL SCALAPACK_UNMAP(X0, DESCX, AINV(:,J))
         RJ(J) = (0.0E0,0.0E0)
   10 CONTINUE
!                                  Print the results.
!                                  After the unmap, only Rank=0 has the full
!                                  array.
      IF(MP_RANK .EQ. 0) THEN
         CALL UMACH (2, NOUT)
         WRITE (NOUT,99999) RCOND, 1.0E0/RCOND
         CALL WRCRN ('AINV', AINV)
      ENDIF
      IF (MP_RANK .EQ. 0) DEALLOCATE(A, AINV)
      DEALLOCATE(A0, FACT0, RJ, RJ0, RES0, X0)
!                                 Exit ScaLAPACK usage
      CALL SCALAPACK_EXIT(MP_ICTXT)
!                                 Shut down MPI
      MP_NPROCS = MP_SETUP('FINAL')
99999 FORMAT ('  RCOND = ',F5.3,/,'  L1 Condition number = ',F6.3)
      END
```

Output

```
RCOND < 0.075
L1 Condition number < 25.0

                                   AINV
                  1                  2                  3                  4
1 ( 0.7166, 0.0000) ( 0.2166,-0.2166)  (-0.0899,-0.0300)  (-0.0207, 0.0622)
2 ( 0.2166, 0.2166) ( 0.4332, 0.0000)  (-0.0599,-0.1198)  (-0.0829, 0.0415)
3 (-0.0899, 0.0300) (-0.0599, 0.1198)  ( 0.1797, 0.0000)  ( 0.0000,-0.1244)
4 (-0.0207,-0.0622) (-0.0829,-0.0415)  ( 0.0000, 0.1244)  ( 0.2592, 0.0000)
5 ( 0.0092, 0.0046) ( 0.0138,-0.0046)  (-0.0138,-0.0138)  (-0.0288, 0.0288)
                   5
1  ( 0.0092,-0.0046)
2  ( 0.0138, 0.0046)
3  (-0.0138, 0.0138)
4  (-0.0288,-0.0288)
5  ( 0.1175, 0.0000)
```

LFTDH

more... more...

Computes the $R^H R$ factorization of a complex Hermitian positive definite matrix.

Required Arguments

A — Complex `N` by `N` Hermitian positive definite matrix to be factored. (Input) Only the upper triangle of `A` is referenced.

FACT — Complex `N` by `N` matrix containing the upper triangular matrix *R* of the factorization of `A` in the upper triangle. (Output)
Only the upper triangle of `FACT` will be used. If `A` is not needed, `A` and `FACT` can share the same storage locations.

Optional Arguments

N — Order of the matrix. (Input)
Default: `N` = size (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = size (`A`,1).

LDFACT — Leading dimension of `FACT` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDFACT` = size (`FACT`,1).

FORTRAN 90 Interface

Generic: `CALL LFTDH (A, FACT [, …])`

Specific: The specific interface names are `S_LFTDH` and `D_LFTDH`.

FORTRAN 77 Interface

Single: `CALL LFTDH (N, A, LDA, FACT, LDFACT)`

Double: The double precision name is DLFTDH.

ScaLAPACK Interface

Generic: `CALL LFTDH (A0, FACT0 [, …])`

Specific: The specific interface names are S_LFTDH and D_LFTDH.

See the *ScaLAPACK Usage Notes* below for a description of the arguments for distributed computing.

Description

Routine LFTDH computes an $R^H R$ Cholesky factorization of a complex Hermitian positive definite coefficient matrix. The matrix *R* is upper triangular.

LFTDH fails if any submatrix of *R* is not positive definite or if *R* has a zero diagonal element. These errors occur only if *A* is very close to a singular matrix or to a matrix which is not positive definite.

The $R^H R$ factors are returned in a form that is compatible with routines LFIDH, LFSDH and LFDDH. To solve systems of equations with multiple right-hand-side vectors, use LFCDH followed by either LFIDH or LFSDH called once for each right-hand side. The IMSL routine LFDDH can be called to compute the determinant of the coefficient matrix after LFCDH has performed the factorization.

The underlying code is based on either LINPACK , LAPACK, or ScaLAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see *Using ScaLAPACK, LAPACK, LINPACK, and EISPACK* in the Introduction section of this manual.

Comments

Informational errors

Type	Code	Description
3	4	The input matrix is not Hermitian. It has a diagonal entry with a small imaginary part.
4	2	The input matrix is not positive definite.
4	4	The input matrix is not Hermitian. It has a diagonal entry with an imaginary part.

ScaLAPACK Usage Notes

The arguments which differ from the standard version of this routine are:

A0 — Complex MXLDA by MXCOL local matrix containing the local portions of the distributed matrix A. A contains the Hermitian positive definite matrix to be factored. (Input)
Only the upper triangle of A is referenced.

FACT0 — Complex MXLDA by MXCOL local matrix containing the local portions of the distributed matrix FACT. FACT contains the upper triangular matrix *R* of the factorization of A in the upper triangle. (Output)
Only the upper triangle of FACT will be used. If A is not needed, A and FACT can share the same storage locations.

All other arguments are global and are the same as described for the standard version of the routine. In the argument descriptions above, MXLDA and MXCOL can be obtained through a call to SCALAPACK_GETDIM (see *Utilities*) after a call to SCALAPACK_SETUP (see *Utilities*) has been made. See the *ScaLAPACK Example* below.

Examples

Example

The inverse of a 5 × 5 matrix is computed. LFTDH is called to factor the matrix and to check for nonpositive definiteness. LFSDH is called to determine the columns of the inverse.

```
      USE LFTDH_INT
      USE LFSDH_INT
      USE WRCRN_INT
!                                 Declare variables
      INTEGER    LDA, LDFACT, N
      PARAMETER  (LDA=5, LDFACT=5, N=5)
      COMPLEX    A(LDA,LDA), AINV(LDA,LDA), FACT(LDFACT,LDFACT), RJ(N)
!
!                                 Set values for A
!
!         A =    (  2.0+0.0i  -1.0+1.0i   0.0+0.0i   0.0+0.0i   0.0+0.0i )
!                (             4.0+0.0i   1.0+2.0i   0.0+0.0i   0.0+0.0i )
!                (                       10.0+0.0i   0.0+4.0i   0.0+0.0i )
!                (                                   6.0+0.0i   1.0+1.0i )
!                (                                              9.0+0.0i )
!
      DATA A /(2.0,0.0), 4*(0.0,0.0), (-1.0,1.0), (4.0,0.0),&
             4*(0.0,0.0), (1.0,2.0), (10.0,0.0), 4*(0.0,0.0),&
             (0.0,4.0), (6.0,0.0), 4*(0.0,0.0), (1.0,1.0), (9.0,0.0)/
!                                 Factor the matrix A
      CALL LFTDH (A, FACT)
!                                 Set up the columns of the identity
!                                 matrix one at a time in RJ
      RJ = (0.0E0,0.0E0)
      DO 10  J=1, N
         RJ(J) = (1.0E0,0.0E0)
!                                 RJ is the J-th column of the identity
```

```
!                                  matrix so the following LFSDH
!                                  reference places the J-th column of
!                                  the inverse of A in the J-th column
!                                  of AINV
         CALL LFSDH (FACT, RJ, AINV(:,J))
         RJ(J) = (0.0E0,0.0E0)
   10 CONTINUE
!                                  Print the results


      CALL WRCRN ('AINV', AINV, ITRING=1)
!
      END
```

Output

```
                                   AINV
                  1                  2                  3                  4
1 ( 0.7166, 0.0000) ( 0.2166,-0.2166)  (-0.0899,-0.0300)  (-0.0207, 0.0622)
2                   ( 0.4332, 0.0000)  (-0.0599,-0.1198)  (-0.0829, 0.0415)
3                                      ( 0.1797, 0.0000)  ( 0.0000,-0.1244)
4                                                         ( 0.2592, 0.0000)
                   5
1  ( 0.0092,-0.0046)
2  ( 0.0138, 0.0046)
3  (-0.0138, 0.0138)
4  (-0.0288,-0.0288)
5  ( 0.1175, 0.0000)
```

ScaLAPACK Example

The inverse of the same 5 × 5 Hermitian positive definite matrix in the preceding example is computed as a distributed computing example. LFTDH is called to factor the matrix and to check for nonpositive definiteness. LFSDH is called to determine the columns of the inverse. SCALAPACK_MAP and SCALAPACK_UNMAP are IMSL utility routines (see *Utilities*) used to map and unmap arrays to and from the processor grid. They are used here for brevity. DESCINIT is a ScaLAPACK tools routine which initializes the descriptors for the local arrays.

```
      USE MPI_SETUP_INT
      USE LFTDH_INT
      USE LFSDH_INT
      USE WRCRN_INT
      USE SCALAPACK_SUPPORT
      IMPLICIT NONE
      INCLUDE 'mpif.h'
!                                  Declare variables
      INTEGER    J, LDA, N, DESCA(9), DESCX(9)
      INTEGER       INFO, MXCOL, MXLDA
      COMPLEX, ALLOCATABLE ::        A(:,:), AINV(:,:), RJ(:), RJ0(:)
      COMPLEX, ALLOCATABLE ::        A0(:,:), FACT0(:,:), X0(:)
      PARAMETER  (LDA=5, N=5)
!                                  Set up for MPI
      MP_NPROCS = MP_SETUP()
      IF(MP_RANK .EQ. 0) THEN
          ALLOCATE (A(LDA,N), AINV(LDA,N))
!                                  Set values for A and B
      A(1,:) = (/(2.0, 0.0),(-1.0, 1.0),( 0.0, 0.0),(0.0, 0.0),(0.0, 0.0)/)
      A(2,:) = (/(0.0, 0.0),( 4.0, 0.0),( 1.0, 2.0),(0.0, 0.0),(0.0, 0.0)/)
      A(3,:) = (/(0.0, 0.0),( 0.0, 0.0),(10.0, 0.0),(0.0, 4.0),(0.0, 0.0)/)
      A(4,:) = (/(0.0, 0.0),( 0.0, 0.0),( 0.0, 0.0),(6.0, 0.0),(1.0, 1.0)/)
      A(5,:) = (/(0.0, 0.0),( 0.0, 0.0),( 0.0, 0.0),(0.0, 0.0),(9.0, 0.0)/)
```

```
      ENDIF
!                                 Set up a 1D processor grid and define
!                                 its context ID, MP_ICTXT
      CALL SCALAPACK_SETUP(N, N, .TRUE., .TRUE.)
!                                 Get the array descriptor entities MXLDA,
!                                 and MXCOL
      CALL SCALAPACK_GETDIM(N, N, MP_MB, MP_NB, MXLDA, MXCOL)
!                                 Set up the array descriptors
      CALL DESCINIT(DESCA, N, N, MP_MB, MP_NB, 0, 0, MP_ICTXT, MXLDA, INFO)
      CALL DESCINIT(DESCX, N, 1, MP_MB, 1, 0, 0, MP_ICTXT, MXLDA, INFO)
!                                 Allocate space for the local arrays
      ALLOCATE(A0(MXLDA,MXCOL), X0(MXLDA),FACT0(MXLDA,MXCOL), RJ(N), &
               RJ0(MXLDA))
!                                Map input arrays to the processor grid
      CALL SCALAPACK_MAP(A, DESCA, A0)
!                                Factor the matrix A
      CALL LFTDH (A0, FACT0)
!                                Set up the columns of the identity
!                                matrix one at a time in RJ
      RJ = (0.0E0, 0.0E0)
      DO 10  J=1, N
         RJ(J) = (1.0E0,0.0E0)
         CALL SCALAPACK_MAP(RJ, DESCX, RJ0)
!                                RJ is the J-th column of the identity
!                                matrix so the following LFIDH
!                                reference solves for the J-th column of
!                                the inverse of A
         CALL LFSDH (FACT0, RJ0, X0)
!                                Unmap the results from the distributed
!                                array back to a non-distributed array
         CALL SCALAPACK_UNMAP(X0, DESCX, AINV(:,J))
         RJ(J) = (0.0E0,0.0E0)
   10 CONTINUE
!
                                 Print the results.
!                                After the unmap, only Rank=0 has the full
!                                array.
      IF(MP_RANK .EQ. 0) CALL WRCRN ('AINV', AINV)
      IF (MP_RANK .EQ. 0) DEALLOCATE(A, AINV)
      DEALLOCATE(A0, FACT0, RJ, RJ0, X0)
!                               Exit ScaLAPACK usage
      CALL SCALAPACK_EXIT(MP_ICTXT)
!                               Shut down MPI
      MP_NPROCS = MP_SETUP('FINAL')
      END
```

Output

```
                                  AINV
                    1                   2                   3                  4
1 ( 0.7166, 0.0000) ( 0.2166,-0.2166)  (-0.0899,-0.0300)  (-0.0207, 0.0622)
2 ( 0.2166, 0.2166) ( 0.4332, 0.0000)  (-0.0599,-0.1198)  (-0.0829, 0.0415)
3 (-0.0899, 0.0300) (-0.0599, 0.1198)  ( 0.1797, 0.0000)  ( 0.0000,-0.1244)
4 (-0.0207,-0.0622) (-0.0829,-0.0415)  ( 0.0000, 0.1244)  ( 0.2592, 0.0000)
5 ( 0.0092, 0.0046) ( 0.0138,-0.0046)  (-0.0138,-0.0138)  (-0.0288, 0.0288)
                     5
1  ( 0.0092,-0.0046)
2  ( 0.0138, 0.0046)
3  (-0.0138, 0.0138)
6  (-0.0288,-0.0288)
7  ( 0.1175, 0.0000)
```

LFSDH

more...

more...

Solves a complex Hermitian positive definite system of linear equations given the $R^H R$ factorization of the coefficient matrix.

Required Arguments

FACT — Complex `N` by `N` matrix containing the factorization of the coefficient matrix `A` as output from routine `LFCDH/DLFCDH` or `LFTDH/DLFTDH`. (Input)

B — Complex vector of length `N` containing the right-hand side of the linear system. (Input)

X — Complex vector of length `N` containing the solution to the linear system. (Output)
If `B` is not needed, `B` and `X` can share the same storage locations.

Optional Arguments

N — Number of equations. (Input)
Default: `N` = size (`FACT`,2).

LDFACT — Leading dimension of `FACT` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDFACT` = size (`FACT`,1).

FORTRAN 90 Interface

Generic: `CALL LFSDH (FACT, B, X [, …])`

Specific: The specific interface names are `S_LFSDH` and `D_LFSDH`.

FORTRAN 77 Interface

Single: `CALL LFSDH (N, FACT, LDFACT, B, X)`

Double: The double precision name is DLFSDH.

ScaLAPACK Interface

Generic: CALL LFSDH (FACT0, B0, X0 [, …])

Specific: The specific interface names are S_LFSDH and D_LFSDH.

See the *ScaLAPACK Usage Notes* below for a description of the arguments for distributed computing.

Description

Routine LFSDH computes the solution for a system of linear algebraic equations having a complex Hermitian positive definite coefficient matrix. To compute the solution, the coefficient matrix must first undergo an $R^H R$ factorization. This may be done by calling either LFCDH or LFTDH. R is an upper triangular matrix.

The solution to $Ax = b$ is found by solving the triangular systems $R^H y = b$ and $Rx = y$.

LFSDH and LFIDH both solve a linear system given its $R^H R$ factorization. LFIDH generally takes more time and produces a more accurate answer than LFSDH. Each iteration of the iterative refinement algorithm used by LFIDH calls LFSDH.

The underlying code is based on either LINPACK , LAPACK, or ScaLAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see *Using ScaLAPACK, LAPACK, LINPACK, and EISPACK* in the Introduction section of this manual.

Comments

Informational error

Type	Code	Description
4	1	The input matrix is singular.

ScaLAPACK Usage Notes

The arguments which differ from the standard version of this routine are:

FACT0 — MXLDA by MXCOL complex local matrix containing the local portions of the distributed matrix FACT as output from routine LFCDH/DLFCDH or LFTDH/DLFTDH. FACT contains the factorization of the matrix A. (Input)

B0 — Complex local vector of length `MXLDA` containing the local portions of the distributed vector `B`. `B` contains the right-hand side of the linear system. (Input)

X0 — Complex local vector of length `MXLDA` containing the local portions of the distributed vector `X`. `X` contains the solution to the linear system. (Output)
If `B` is not needed, `B` and `X` can share the same storage locations.

All other arguments are global and are the same as described for the standard version of the routine. In the argument descriptions above, `MXLDA` and `MXCOL` can be obtained through a call to `SCALAPACK_GETDIM` (see *Utilities*) after a call to `SCALAPACK_SETUP` (*Utilities*) has been made. See the *ScaLAPACK Example* below.

Examples

Example

A set of linear systems is solved successively. `LFTDH` is called to factor the coefficient matrix. `LFSDH` is called to compute the four solutions for the four right-hand sides. In this case, the coefficient matrix is assumed to be well-conditioned and correctly scaled. Otherwise, it would be better to call `LFCDH` to perform the factorization, and `LFIDH` to compute the solutions.

```
      USE LFSDH_INT
      USE LFTDH_INT
      USE WRCRN_INT
!                                 Declare variables
      INTEGER    LDA, LDFACT, N
      PARAMETER  (LDA=5, LDFACT=5, N=5)
      COMPLEX    A(LDA,LDA), B(N,3), FACT(LDFACT,LDFACT), X(N,3)

!                                Set values for A and B
!
!        A =   (  2.0+0.0i  -1.0+1.0i   0.0+0.0i   0.0+0.0i   0.0+0.0i )
!              (             4.0+0.0i   1.0+2.0i   0.0+0.0i   0.0+0.0i )
!              (                       10.0+0.0i   0.0+4.0i   0.0+0.0i )
!              (                                   6.0+0.0i   1.0+1.0i )
!              (                                              9.0+0.0i )
!
!        B =   (  3.0+3.0i    4.0+0.0i    29.0-9.0i )
!              (  5.0-5.0i   15.0-10.0i  -36.0-17.0i )
!              (  5.0+4.0i  -12.0-56.0i  -15.0-24.0i )
!              (  9.0+7.0i  -12.0+10.0i  -23.0-15.0i )
!              (-22.0+1.0i    3.0-1.0i   -23.0-28.0i )

      DATA A /(2.0,0.0), 4*(0.0,0.0), (-1.0,1.0), (4.0,0.0),&
             4*(0.0,0.0), (1.0,2.0), (10.0,0.0), 4*(0.0,0.0),&
             (0.0,4.0), (6.0,0.0), 4*(0.0,0.0), (1.0,1.0), (9.0,0.0)/
      DATA B /(3.0,3.0), (5.0,-5.0), (5.0,4.0), (9.0,7.0), (-22.0,1.0),&
             (4.0,0.0), (15.0,-10.0), (-12.0,-56.0), (-12.0,10.0),&
             (3.0,-1.0), (29.0,-9.0), (-36.0,-17.0), (-15.0,-24.0),&
             (-23.0,-15.0), (-23.0,-28.0)/

!                                 Factor the matrix A
      CALL LFTDH (A, FACT)
!                                 Compute the solutions
      DO 10  I=1, 3
```

```
          CALL LFSDH (FACT, B(:,I), X(:,I))
   10 CONTINUE
!                                 Print solutions
       CALL WRCRN ('X', X)
!
       END
```

Output

```
                           X
                1                  2                  3
1  (  1.00,  0.00)  (  3.00, -1.00)  ( 11.00, -1.00)
2  (  1.00, -2.00)  (  2.00,  0.00)  ( -7.00,  0.00)
3  (  2.00,  0.00)  ( -1.00, -6.00)  ( -2.00, -3.00)
4  (  2.00,  3.00)  (  2.00,  1.00)  ( -2.00, -3.00)
5  ( -3.00,  0.00)  (  0.00,  0.00)  ( -2.00, -3.00)
```

ScaLAPACK Example

The same set of linear systems as in in the preceding example is solved successively as a distributed computing example. LFTDH is called to factor the matrix. LFSDH is called to compute the four solutions for the four right-hand sides. In this case, the coefficient matrix is assumed to be well-conditioned and correctly scaled. Otherwise, it would be better to call LFCDH to perform the factorization, and LFIDH to compute the solutions.

SCALAPACK_MAP and SCALAPACK_UNMAP are IMSL utility routines (see *Utilities*) used to map and unmap arrays to and from the processor grid. They are used here for brevity. DESCINIT is a ScaLAPACK tools routine which initializes the descriptors for the local arrays.

```
       USE MPI_SETUP_INT
       USE LFTDH_INT
       USE LFSDH_INT
       USE WRCRN_INT
       USE SCALAPACK_SUPPORT
       IMPLICIT NONE
       INCLUDE 'mpif.h'
!                                 Declare variables
       INTEGER    J, LDA, N, DESCA(9), DESCX(9)
       INTEGER       INFO, MXCOL, MXLDA
       COMPLEX, ALLOCATABLE ::       A(:,:), B(:,:), B0(:), X(:,:)
       COMPLEX, ALLOCATABLE ::       A0(:,:), FACT0(:,:), X0(:)
       PARAMETER  (LDA=5, N=5)
!                                 Set up for MPI
       MP_NPROCS = MP_SETUP()
       IF(MP_RANK .EQ. 0) THEN
        ALLOCATE (A(LDA,N), B(LDA,3), X(LDA,3))
!                                 Set values for A and B
        A(1,:) = (/(2.0, 0.0),(-1.0, 1.0),( 0.0, 0.0),(0.0, 0.0),(0.0, 0.0)/)
        A(2,:) = (/(0.0, 0.0),( 4.0, 0.0),( 1.0, 2.0),(0.0, 0.0),(0.0, 0.0)/)
        A(3,:) = (/(0.0, 0.0),( 0.0, 0.0),(10.0, 0.0),(0.0, 4.0),(0.0, 0.0)/)
        A(4,:) = (/(0.0, 0.0),( 0.0, 0.0),( 0.0, 0.0),(6.0, 0.0),(1.0, 1.0)/)
        A(5,:) = (/(0.0, 0.0),( 0.0, 0.0),( 0.0, 0.0),(0.0, 0.0),(9.0, 0.0)/)
!
        B(1,:) = (/(3.0,  3.0), (  4.0,  0.0), ( 29.0, -9.0)/)
        B(2,:) = (/(5.0, -5.0), ( 15.0,-10.0), (-36.0,-17.0)/)
        B(3,:) = (/(5.0,  4.0), (-12.0,-56.0), (-15.0,-24.0)/)
        B(4,:) = (/(9.0,  7.0), (-12.0, 10.0), (-23.0,-15.0)/)
        B(5,:) = (/(-22.0,1.0), (  3.0, -1.0), (-23.0,-28.0)/)
       ENDIF
!                                  Set up a 1D processor grid and define
```

```
!                                   its context ID, MP_ICTXT
      CALL SCALAPACK_SETUP(N, N, .TRUE., .TRUE.)
!                                   Get the array descriptor entities MXLDA,
!                                   and MXCOL
      CALL SCALAPACK_GETDIM(N, N, MP_MB, MP_NB, MXLDA, MXCOL)
!                                   Set up the array descriptors
      CALL DESCINIT(DESCA, N, N, MP_MB, MP_NB, 0, 0, MP_ICTXT, MXLDA, INFO)
      CALL DESCINIT(DESCX, N, 1, MP_MB, 1, 0, 0, MP_ICTXT, MXLDA, INFO)
!                                   Allocate space for the local arrays
      ALLOCATE(A0(MXLDA,MXCOL), X0(MXLDA),FACT0(MXLDA,MXCOL), &
               B0(MXLDA))
!                                  Map input arrays to the processor grid
      CALL SCALAPACK_MAP(A, DESCA, A0)
!                                  Factor the matrix A
      CALL LFTDH (A0, FACT0)
!                                  Compute the solutions
      DO 10  J=1, 3
         CALL SCALAPACK_MAP(B(:,J), DESCX, B0)
         CALL LFSDH (FACT0, B0, X0)
!                                  Unmap the results from the distributed
!                                  array back to a non-distributed array
         CALL SCALAPACK_UNMAP(X0, DESCX, X(:,J))
   10 CONTINUE
!                                  Print the results.
!                                  After the unmap, only Rank=0 has the full
!                                  array.
      IF(MP_RANK .EQ. 0) CALL WRCRN ('X', X)
      IF (MP_RANK .EQ. 0) DEALLOCATE(A, B, X)
      DEALLOCATE(A0, B0, FACT0, X0)
!                                 Exit ScaLAPACK usage
      CALL SCALAPACK_EXIT(MP_ICTXT)
!                                 Shut down MPI
      MP_NPROCS = MP_SETUP('FINAL')
      END
```

Output

```
                             X
                 1                 2                 3
 1  (  1.00,  0.00)  (  3.00, -1.00)  ( 11.00, -1.00)
 2  (  1.00, -2.00)  (  2.00,  0.00)  ( -7.00,  0.00)
 3  (  2.00,  0.00)  ( -1.00, -6.00)  ( -2.00, -3.00)
 4  (  2.00,  3.00)  (  2.00,  1.00)  ( -2.00, -3.00)
 5  ( -3.00,  0.00)  (  0.00,  0.00)  ( -2.00, -3.00)
```

LFIDH

more...

more...

Uses iterative refinement to improve the solution of a complex Hermitian positive definite system of linear equations.

Required Arguments

A — Complex N by N matrix containing the coefficient matrix of the linear system. (Input)
Only the upper triangle of A is referenced.

FACT — Complex N by N matrix containing the factorization of the coefficient matrix A as output from routine LFCDH/DLFCDH or LFTDH/DLFTDH. (Input)
Only the upper triangle of FACT is used.

B — Complex vector of length N containing the right-hand side of the linear system. (Input)

X — Complex vector of length N containing the solution. (Output)

RES — Complex vector of length N containing the residual vector at the improved solution. (Output)

Optional Arguments

N — Number of equations. (Input)
Default: N = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

LDFACT — Leading dimension of FACT exactly as specified in the dimension statement of the calling program. (Input)
Default: LDFACT = size (FACT,1).

FORTRAN 90 Interface

Generic: CALL LFIDH (A, FACT, B, X, RES [, …])

Specific: The specific interface names are S_LFIDH and D_LFIDH.

FORTRAN 77 Interface

Single: CALL LFIDH (N, A, LDA, FACT, LDFACT, B, X, RES)

Double: The double precision name is DLFIDH.

ScaLAPACK Interface

Generic: CALL LFIDH (A0, FACT0, B0, X0, RES0 [, …])

Specific: The specific interface names are S_LFIDH and D_LFIDH.

See the *ScaLAPACK Usage Notes* below for a description of the arguments for distributed computing.

Description

Routine LFIDH computes the solution of a system of linear algebraic equations having a complex Hermitian positive definite coefficient matrix. Iterative refinement is performed on the solution vector to improve the accuracy. Usually almost all of the digits in the solution are accurate, even if the matrix is somewhat ill-conditioned.

To compute the solution, the coefficient matrix must first undergo an $R^{H} R$ factorization. This may be done by calling either LFCDH or LFTDH.

Iterative refinement fails only if the matrix is very ill-conditioned.

LFIDH and LFSDH both solve a linear system given its $R^{H} R$ factorization. LFIDH generally takes more time and produces a more accurate answer than LFSDH. Each iteration of the iterative refinement algorithm used by LFIDH calls LFSDH.

Comments

Informational error

Type	Code	Description
3	3	The input matrix is too ill-conditioned for iterative refinement to be effective.

ScaLAPACK Usage Notes

The arguments which differ from the standard version of this routine are:

A0 — MXLDA by MXCOL complex local matrix containing the local portions of the distributed matrix A. A contains the coefficient matrix of the linear system. (Input)
Only the upper triangle of A is referenced.

FACT0 — MXLDA by MXCOL complex local matrix containing the local portions of the distributed matrix FACT as output from routine LFCDH or LFTDH. FACT contains the factorization of the matrix A. (Input)
Only the upper triangle of FACT is referenced.

B0 — Complex local vector of length MXLDA containing the local portions of the distributed vector B. B contains the right-hand side of the linear system. (Input)

X0 — Complex local vector of length MXLDA containing the local portions of the distributed vector X. X contains the solution to the linear system. (Output)

RES0 — Complex local vector of length MXLDA containing the local portions of the distributed vector RES. RES contains the residual vector at the improved solution to the linear system. (Output)

All other arguments are global and are the same as described for the standard version of the routine. In the argument descriptions above, MXLDA and MXCOL can be obtained through a call to SCALAPACK_GETDIM (*Utilities*) after a call to SCALAPACK_SETUP
(Chapter 11, *"Utilities"*) has been made. See the *ScaLAPACK Example* below.

Examples

Example

A set of linear systems is solved successively. The right-hand-side vector is perturbed by adding (1 + *i*)/2 to the second element after each call to LFIDH.

```
      USE LFIDH_INT
      USE LFCDH_INT
      USE UMACH_INT
      USE WRCRN_INT
!                                 Declare variables
      INTEGER    LDA, LDFACT, N
      PARAMETER  (LDA=5, LDFACT=5, N=5)
      REAL       RCOND
      COMPLEX    A(LDA,LDA), B(N), FACT(LDFACT,LDFACT), RES(N,3), X(N,3)
!
!                                 Set values for A and B
!
!        A =    (  2.0+0.0i  -1.0+1.0i   0.0+0.0i   0.0+0.0i   0.0+0.0i )
!               (             4.0+0.0i   1.0+2.0i   0.0+0.0i   0.0+0.0i )
```

```
!               (                        10.0+0.0i   0.0+4.0i   0.0+0.0i )
!               (                                    6.0+0.0i   1.0+1.0i )
!               (                                               9.0+0.0i )
!
!         B =   ( 3.0+3.0i  5.0-5.0i  5.0+4.0i  9.0+7.0i  -22.0+1.0i )
!
      DATA A /(2.0,0.0), 4*(0.0,0.0), (-1.0,1.0), (4.0,0.0),&
             4*(0.0,0.0), (1.0,2.0), (10.0,0.0), 4*(0.0,0.0),&
             (0.0,4.0), (6.0,0.0), 4*(0.0,0.0), (1.0,1.0), (9.0,0.0)/
      DATA B /(3.0,3.0), (5.0,-5.0), (5.0,4.0), (9.0,7.0), (-22.0,1.0)/
!                                Factor the matrix A
      CALL LFCDH (A, FACT, RCOND)
!                                Print the estimated condition number
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) RCOND, 1.0E0/RCOND
!                                Compute the solutions, then perturb B
      DO 10  I=1, 3
         CALL LFIDH (A, FACT, B, X(:,I), RES(:,I))
         B(2) = B(2) + (0.5E0,0.5E0)
   10 CONTINUE
!                                Print solutions and residuals
      CALL WRCRN ('X', X)
      CALL WRCRN ('RES', RES)
!
99999 FORMAT ('  RCOND = ',F5.3,/,'  L1 Condition number = ',F6.3)
      END
```

Output

```
RCOND < 0.07
L1 Condition number < 25.0
                       X
                 1                 2                 3
1  ( 1.000, 0.000)  ( 1.217, 0.000)  ( 1.433, 0.000)
2  ( 1.000,-2.000)  ( 1.217,-1.783)  ( 1.433,-1.567)
3  ( 2.000, 0.000)  ( 1.910, 0.030)  ( 1.820, 0.060)
4  ( 2.000, 3.000)  ( 1.979, 2.938)  ( 1.959, 2.876)
5  (-3.000, 0.000)  (-2.991, 0.005)  (-2.982, 0.009)

                                  RES
                        1                         2                         3
1 ( 1.192E-07, 0.000E+00)  ( 6.592E-08, 1.686E-07)  ( 1.318E-07, 2.010E-14)
2 ( 1.192E-07,-2.384E-07)  (-5.329E-08,-5.329E-08)  ( 1.318E-07,-2.258E-07)
3 ( 2.384E-07, 8.259E-08)  ( 2.390E-07,-3.309E-08)  ( 2.395E-07, 1.015E-07)
4 (-2.384E-07, 2.814E-14)  (-8.240E-08,-8.790E-09)  (-1.648E-07,-1.758E-08)
5 (-2.384E-07,-1.401E-08)  (-2.813E-07, 6.981E-09)  (-3.241E-07,-2.795E-08)
```

ScaLAPACK Example

As in the preceding example, a set of linear systems is solved successively as a distributed computing example. The right-hand-side vector is perturbed by adding (1 + *i*)/2 to the second element after each call to `LFIDH`. `SCALAPACK_MAP` and `SCALAPACK_UNMAP` are IMSL utility routines (see *Utilities*) used to map and unmap arrays to and from the processor grid. They are used here for brevity. `DESCINIT` is a ScaLAPACK tools routine which initializes the descriptors for the local arrays.

```
      USE MPI_SETUP_INT
      USE LFCDH_INT
      USE LFIDH_INT
      USE UMACH_INT
      USE WRCRN_INT
```

```
      USE SCALAPACK_SUPPORT
      IMPLICIT NONE
      INCLUDE 'mpif.h'
!                                Declare variables
      INTEGER    J, LDA, N, NOUT, DESCA(9), DESCX(9)
      INTEGER       INFO, MXCOL, MXLDA
      REAL          RCOND
      COMPLEX, ALLOCATABLE ::        A(:,:), B(:), B0(:), RES(:,:), X(:,:)
      COMPLEX, ALLOCATABLE ::        A0(:,:), FACT0(:,:), X0(:), RES0(:)
      PARAMETER  (LDA=5, N=5)
!                                Set up for MPI
      MP_NPROCS = MP_SETUP()
      IF(MP_RANK .EQ. 0) THEN
       ALLOCATE (A(LDA,N), B(N), RES(N,3), X(N,3))
!                                Set values for A and B
       A(1,:) = (/(2.0, 0.0),(-1.0, 1.0),( 0.0, 0.0),(0.0, 0.0),(0.0, 0.0)/)
       A(2,:) = (/(0.0, 0.0),( 4.0, 0.0),( 1.0, 2.0),(0.0, 0.0),(0.0, 0.0)/)
       A(3,:) = (/(0.0, 0.0),( 0.0, 0.0),(10.0, 0.0),(0.0, 4.0),(0.0, 0.0)/)
       A(4,:) = (/(0.0, 0.0),( 0.0, 0.0),( 0.0, 0.0),(6.0, 0.0),(1.0, 1.0)/)
       A(5,:) = (/(0.0, 0.0),( 0.0, 0.0),( 0.0, 0.0),(0.0, 0.0),(9.0, 0.0)/)
!
       B     = (/(3.0, 3.0),( 5.0,-5.0),( 5.0, 4.0),(9.0, 7.0),(-22.0,1.0)/)
      ENDIF
!                                 Set up a 1D processor grid and define
!                                 its context ID, MP_ICTXT
      CALL SCALAPACK_SETUP(N, N, .TRUE., .TRUE.)
!                                 Get the array descriptor entities MXLDA,
!                                 and MXCOL
      CALL SCALAPACK_GETDIM(N, N, MP_MB, MP_NB, MXLDA, MXCOL)
!                                 Set up the array descriptors
      CALL DESCINIT(DESCA, N, N, MP_MB, MP_NB, 0, 0, MP_ICTXT, MXLDA, INFO)
      CALL DESCINIT(DESCX, N, 1, MP_MB, 1, 0, 0, MP_ICTXT, MXLDA, INFO)
!                                Allocate space for the local arrays
      ALLOCATE(A0(MXLDA,MXCOL), X0(MXLDA),FACT0(MXLDA,MXCOL), &
               B0(MXLDA), RES0(MXLDA))
!                                Map input arrays to the processor grid
      CALL SCALAPACK_MAP(A, DESCA, A0)
!                                Factor the matrix A
      CALL LFCDH (A0, FACT0, RCOND)
!                                Print the estimated condition number
      IF(MP_RANK .EQ. 0) THEN
         CALL UMACH (2, NOUT)
         WRITE (NOUT,99999) RCOND, 1.0E0/RCOND
      ENDIF
!                                Compute the solutions
      DO 10  J=1, 3
         CALL SCALAPACK_MAP(B, DESCX, B0)
         CALL LFIDH (A0, FACT0, B0, X0, RES0)
!                                Unmap the results from the distributed
!                                array back to a non-distributed array
         CALL SCALAPACK_UNMAP(X0, DESCX, X(:,J))
         CALL SCALAPACK_UNMAP(RES0, DESCX, RES(:,J))
         IF(MP_RANK .EQ. 0) B(2) = B(2) + (0.5E0, 0.5E0)
   10 CONTINUE
!                                Print the results.
!                                After the unmap, only Rank=0 has the full
!                                array.
      IF(MP_RANK .EQ. 0) THEN
         CALL WRCRN ('X', X)
         CALL WRCRN ('RES', RES)
      ENDIF
      IF (MP_RANK .EQ. 0) DEALLOCATE(A, B, RES, X)
      DEALLOCATE(A0, B0, FACT0, RES0, X0)

!                               Exit ScaLAPACK usage
      CALL SCALAPACK_EXIT(MP_ICTXT)
```

```
!                                  Shut down MPI
      MP_NPROCS = MP_SETUP('FINAL')
99999 FORMAT ('  RCOND = ',F5.3,/,'  L1 Condition number = ',F6.3)
      END
```

Output

```
RCOND < 0.07
L1 Condition number < 25.0
                        X
                 1                 2                 3
1  ( 1.000, 0.000)  ( 1.217, 0.000)  ( 1.433, 0.000)
2  ( 1.000,-2.000)  ( 1.217,-1.783)  ( 1.433,-1.567)
3  ( 2.000, 0.000)  ( 1.910, 0.030)  ( 1.820, 0.060)
4  ( 2.000, 3.000)  ( 1.979, 2.938)  ( 1.959, 2.876)
5  (-3.000, 0.000)  (-2.991, 0.005)  (-2.982, 0.009)
                                  RES
                        1                         2                         3
1 ( 1.192E-07, 0.000E+00)  ( 6.592E-08, 1.686E-07)  ( 1.318E-07, 2.010E-14)
2 ( 1.192E-07,-2.384E-07)  (-5.329E-08,-5.329E-08)  ( 1.318E-07,-2.258E-07)
3 ( 2.384E-07, 8.259E-08)  ( 2.390E-07,-3.309E-08)  ( 2.395E-07, 1.015E-07)
4 (-2.384E-07, 2.814E-14)  (-8.240E-08,-8.790E-09)  (-1.648E-07,-1.758E-08)
5 (-2.384E-07,-1.401E-08)  (-2.813E-07, 6.981E-09)  (-3.241E-07,-2.795E-08)
```

LFDDH

Computes the determinant of a complex Hermitian positive definite matrix given the $R^H R$ Cholesky factorization of the matrix.

Required Arguments

FACT — Complex N by N matrix containing the $R^H R$ factorization of the coefficient matrix A as output from routine LFCDH/DLFCDH or LFTDH/DLFTDH. (Input)

DET1 — Scalar containing the mantissa of the determinant. (Output)
The value DET1 is normalized so that 1.0 ≤ |DET1| < 10.0 or DET1 = 0.0.

DET2 — Scalar containing the exponent of the determinant. (Output)
The determinant is returned in the form det(*A*) = DET1 * 10^{DET2}.

Optional Arguments

N — Order of the matrix. (Input)
Default: N = size (FACT,2).

LDFACT — Leading dimension of FACT exactly as specified in the dimension statement of the calling program. (Input)
Default: LDFACT = size (FACT,1).

FORTRAN 90 Interface

Generic: CALL LFDDH (FACT, DET1, DET2 [, …])

Specific: The specific interface names are S_LFDDH and D_LFDDH.

FORTRAN 77 Interface

Single: CALL LFDDH (N, FACT, LDFACT, DET1, DET2)

Double: The double precision name is DLFDDH.

Description

Routine `LFDDH` computes the determinant of a complex Hermitian positive definite coefficient matrix. To compute the determinant, the coefficient matrix must first undergo an $R^{\boldsymbol{H}} R$ factorization. This may be done by calling either `LFCDH` or `LFTDH`. The formula det A = det $R^{\boldsymbol{H}}$ det R = (det R)^2 is used to compute the determinant. Since the determinant of a triangular matrix is the product of the diagonal elements,

$$\det R = \prod_{i=1}^{N} R_{ii}$$

(The matrix R is stored in the upper triangle of `FACT`.)

`LFDDH` is based on the LINPACK routine `CPODI`; see Dongarra et al. (1979).

Example

The determinant is computed for a complex Hermitian positive definite 3 × 3 matrix.

```
      USE LFDDH_INT
      USE LFTDH_INT
      USE UMACH_INT
!                                 Declare variables
      INTEGER    LDA, LDFACT, NOUT
      PARAMETER  (LDA=3, LDFACT=3)
      REAL       DET1, DET2
      COMPLEX    A(LDA,LDA), FACT(LDFACT,LDFACT)
!
!                                 Set values for A
!
!         A =    (  6.0+0.0i   1.0-1.0i   4.0+0.0i )
!                (  1.0+1.0i   7.0+0.0i  -5.0+1.0i )
!                (  4.0+0.0i  -5.0-1.0i  11.0+0.0i )
!
      DATA A /(6.0,0.0), (1.0,1.0), (4.0,0.0), (1.0,-1.0), (7.0,0.0),&
             (-5.0,-1.0), (4.0,0.0), (-5.0,1.0), (11.0,0.0)/
!                                 Factor the matrix
      CALL LFTDH (A, FACT)
!                                 Compute the determinant
      CALL LFDDH (FACT, DET1, DET2)
!                                 Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) DET1, DET2
!
99999 FORMAT (' The determinant of A is ',F6.3,' * 10**',F2.0)
      END
```

Output

```
The determinant of A is  1.400 * 10**2.
```

LSAHF

more...

Solves a complex Hermitian system of linear equations with iterative refinement.

Required Arguments

A — Complex `N` by `N` matrix containing the coefficient matrix of the Hermitian linear system. (Input)
Only the upper triangle of `A` is referenced.

B — Complex vector of length `N` containing the right-hand side of the linear system. (Input)

X — Complex vector of length `N` containing the solution to the linear system. (Output)

Optional Arguments

N — Number of equations. (Input)
Default: `N` = size (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = size (`A`,1).

FORTRAN 90 Interface

Generic: `CALL LSAHF (A, B, X [, …])`

Specific: The specific interface names are `S_LSAHF` and `D_LSAHF`.

FORTRAN 77 Interface

Single: `CALL LSAHF (N, A, LDA, B, X)`

Double: The double precision name is `DLSAHF`.

Description

Routine LSAHF solves systems of linear algebraic equations having a complex Hermitian indefinite coefficient matrix. It first uses the routine LFCHF to compute a $U\,DU^{H}$ factorization of the coefficient matrix and to estimate the condition number of the matrix. *D* is a block diagonal matrix with blocks of order 1 or 2 and *U* is a matrix composed of the product of a permutation matrix and a unit upper triangular matrix. The solution of the linear system is then found using the iterative refinement routine LFIHF.

LSAHF fails if a block in *D* is singular or if the iterative refinement algorithm fails to converge. These errors occur only if *A* is singular or very close to a singular matrix.

If the estimated condition number is greater than $1/\varepsilon$ (where ε is machine precision), a warning error is issued. This indicates that very small changes in *A* can cause very large changes in the solution *x*. Iterative refinement can sometimes find the solution to such a system. LSAHF solves the problem that is represented in the computer; however, this problem may differ from the problem whose solution is desired.

Comments

1. Workspace may be explicitly provided, if desired, by use of L2AHF/DL2AHF. The reference is:

   ```
   CALL L2AHF (N, A, LDA, B, X, FACT, IPVT, CWK)
   ```

   The additional arguments are as follows:

   FACT — Complex work vector of length N^2 containing information about the $U\,DU^{H}$ factorization of A on output.

   IPVT — Integer work vector of length N containing the pivoting information for the factorization of A on output.

   CWK — Complex work vector of length N.

2. Informational errors

Type	Code	Description
3	1	The input matrix is algorithmically singular.
3	4	The input matrix is not Hermitian. It has a diagonal entry with a small imaginary part.
4	2	The input matrix singular.
4	4	The input matrix is not Hermitian. It has a diagonal entry with an imaginary part.

3. *Integer Options* with *Chapter 11* Options Manager

   16 This option uses four values to solve memory bank conflict (access inefficiency) problems. In routine L2AHF the leading dimension of FACT is increased by IVAL(3) when N is a multiple of IVAL(4). The values IVAL(3) and IVAL(4) are temporarily replaced by IVAL(1) and

IVAL(2), respectively, in LSAHF. Additional memory allocation for FACT and option value restoration are done automatically in LSAHF. Users directly calling L2AHF can allocate additional space for FACT and set IVAL(3) and IVAL(4) so that memory bank conflicts no longer cause inefficiencies. There is no requirement that users change existing applications that use LSAHF or L2AHF. Default values for the option are IVAL(*) = 1, 16, 0, 1.

17 This option has two values that determine if the L_1 condition number is to be computed. Routine LSAHF temporarily replaces IVAL(2) by IVAL(1). The routine L2CHF computes the condition number if IVAL(2) = 2. Otherwise L2CHF skips this computation. LSAHF restores the option. Default values for the option are IVAL(*) = 1, 2.

Example

A system of three linear equations is solved. The coefficient matrix has complex Hermitian form and the right-hand-side vector b has three elements.

```
      USE LSAHF_INT
      USE WRCRN_INT
!                                 Declare variables
      INTEGER    LDA, N
      PARAMETER  (LDA=3, N=3)
      COMPLEX    A(LDA,LDA), B(N), X(N)
!
!                               Set values for A and B
!
!                               A = ( 3.0+0.0i   1.0-1.0i   4.0+0.0i )
!                                   ( 1.0+1.0i   2.0+0.0i  -5.0+1.0i )
!                                   ( 4.0+0.0i  -5.0-1.0i  -2.0+0.0i )
!
!                               B = ( 7.0+32.0i -39.0-21.0i 51.0+9.0i )
!
      DATA A/(3.0,0.0), (1.0,1.0), (4.0,0.0), (1.0,-1.0), (2.0,0.0),&
            (-5.0,-1.0), (4.0,0.0), (-5.0,1.0), (-2.0,0.0)/
      DATA B/(7.0,32.0), (-39.0,-21.0), (51.0,9.0)/
!
      CALL LSAHF (A, B, X)
!                                 Print results
      CALL WRCRN ('X', X, 1, N, 1)
      END
```

Output

```
                        X
              1                 2                 3
(  2.00,   1.00)  (-10.00, -1.00)  (  3.00,   5.00)
```

LSLHF

more...

Solves a complex Hermitian system of linear equations without iterative refinement.

Required Arguments

A — Complex `N` by `N` matrix containing the coefficient matrix of the Hermitian linear system. (Input)
Only the upper triangle of `A` is referenced.

B — Complex vector of length `N` containing the right-hand side of the linear system. (Input)

X — Complex vector of length `N` containing the solution to the linear system. (Output)

Optional Arguments

N — Number of equations. (Input)
Default: `N` = size (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = size (`A`,1).

FORTRAN 90 Interface

Generic: `CALL LSLHF (A, B, X [, …])`

Specific: The specific interface names are `S_LSLHF` and `D_LSLHF`.

FORTRAN 77 Interface

Single: `CALL LSLHF (N, A, LDA, B, X)`

Double: The double precision name is `DLSLHF`.

Description

Routine LSLHF solves systems of linear algebraic equations having a complex Hermitian indefinite coefficient matrix. It first uses the routine LFCHF to compute a UDU^H factorization of the coefficient matrix. *D* is a block diagonal matrix with blocks of order 1 or 2 and *U* is a matrix composed of the product of a permutation matrix and a unit upper triangular matrix.

The solution of the linear system is then found using the routine LFSHF. LSLHF fails if a block in *D* is singular. This occurs only if *A* is singular or very close to a singular matrix. If the coefficient matrix is ill-conditioned or poorly scaled, it is recommended that LSAHF be used.

Comments

1. Workspace may be explicitly provided, if desired, by use of L2LHF/DL2LHF. The reference is:

   CALL L2LHF (N, A, LDA, B, X, FACT, IPVT, CWK)

   The additional arguments are as follows:

   FACT — Complex work vector of length N^2 containing information about the UDU^H factorization of A on output.

   IPVT — Integer work vector of length N containing the pivoting information for the factorization of A on output.

   CWK — Complex work vector of length N.

2. Informational errors

Type	Code	Description
3	1	The input matrix is algorithmically singular.
3	4	The input matrix is not Hermitian. It has a diagonal entry with a small imaginary part.
4	2	The input matrix singular.
4	4	The input matrix is not Hermitian. It has a diagonal entry with an imaginary part.

3. *Integer Options* with *Chapter 11* Options Manager

   16This option uses four values to solve memory bank conflict (access inefficiency) problems. In routine L2LHF the leading dimension of FACT is increased by IVAL(3) when N is a multiple of IVAL(4). The values IVAL(3) and IVAL(4) are temporarily replaced by IVAL(1) and IVAL(2), respectively, in LSLHF. Additional memory allocation for FACT and option value restoration are done automatically in LSLHF. Users directly calling L2LHF can allocate additional space for FACT and set IVAL(3) and IVAL(4) so that memory bank conflicts no longer cause inefficiencies. There is no requirement that users change existing applications that use LSLHF or L2LHF. Default values for the option are IVAL(*) = 1, 16, 0, 1.

17This option has two values that determine if the L_1 condition number is to be computed. Routine `LSLHF` temporarily replaces `IVAL`(2) by `IVAL`(1). The routine `L2CHF` computes the condition number if `IVAL`(2) = 2. Otherwise `L2CHF` skips this computation. `LSLHF` restores the option. Default values for the option are `IVAL(*)` = 1, 2.

Example

A system of three linear equations is solved. The coefficient matrix has complex Hermitian form and the right-hand-side vector *b* has three elements.

```
      USE LSLHF_INT
      USE WRCRN_INT
!                                 Declare variables
      INTEGER    LDA, N
      PARAMETER  (LDA=3, N=3)
      COMPLEX    A(LDA,LDA), B(N), X(N)
!
!                               Set values for A and B
!
!                               A = ( 3.0+0.0i   1.0-1.0i   4.0+0.0i )
!                                   ( 1.0+1.0i   2.0+0.0i  -5.0+1.0i )
!                                   ( 4.0+0.0i  -5.0-1.0i  -2.0+0.0i )
!
!                               B = ( 7.0+32.0i -39.0-21.0i 51.0+9.0i )
!
      DATA A/(3.0,0.0), (1.0,1.0), (4.0,0.0), (1.0,-1.0), (2.0,0.0),&
            (-5.0,-1.0), (4.0,0.0), (-5.0,1.0), (-2.0,0.0)/
      DATA B/(7.0,32.0), (-39.0,-21.0), (51.0,9.0)/
!
      CALL LSLHF (A, B, X)
!                                 Print results
      CALL WRCRN ('X', X, 1, N, 1)
      END
```

Output

```
                        X
              1                 2                 3
(  2.00,  1.00)  (-10.00, -1.00)  (  3.00,  5.00)
```

LFCHF

more...

Computes the UDU^{H} factorization of a complex Hermitian matrix and estimate its L_1 condition number.

Required Arguments

A — Complex `N` by `N` matrix containing the coefficient matrix of the Hermitian linear system. (Input)
Only the upper triangle of `A` is referenced.

FACT — Complex `N` by `N` matrix containing the information about the factorization of the Hermitian matrix `A`. (Output)
Only the upper triangle of `FACT` is used. If `A` is not needed, `A` and `FACT` can share the same storage locations.

IPVT — Vector of length `N` containing the pivoting information for the factorization. (Output)

RCOND — Scalar containing an estimate of the reciprocal of the L_1 condition number of `A`. (Output)

Optional Arguments

N – Order of the matrix. (Input)
Default: `N` = size (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = size (`A`,1).

LDFACT — Leading dimension of `FACT` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDFACT` = size (`FACT`,1).

FORTRAN 90 Interface

Generic: `CALL LFCHF (A, FACT, IPVT, RCOND [, …])`

Specific: The specific interface names are `S_LFCHF` and `D_LFCHF`.

FORTRAN 77 Interface

Single: `CALL LFCHF (N, A, LDA, FACT, LDFACT, IPVT, RCOND)`

Double: The double precision name is `DLFCHF`.

Description

Routine `LFCHF` performs a $U DU^H$ factorization of a complex Hermitian indefinite coefficient matrix. It also estimates the condition number of the matrix. The $U DU^H$ factorization is called the diagonal pivoting factorization.

The L_1 condition number of the matrix A is defined to be $\kappa(A) = \|A\|_1 \|A^{-1}\|_1$. Since it is expensive to compute $\|A^{-1}\|_1$, the condition number is only estimated. The estimation algorithm is the same as used by LINPACK and is described by Cline et al. (1979).

If the estimated condition number is greater than $1/\varepsilon$ (where ε is machine precision), a warning error is issued. This indicates that very small changes in A can cause very large changes in the solution x. Iterative refinement can sometimes find the solution to such a system.

`LFCHF` fails if A is singular or very close to a singular matrix.

The $U DU^H$ factors are returned in a form that is compatible with routines `LFIHF`, `LFSHF` and `LFDHF`. To solve systems of equations with multiple right-hand-side vectors, use `LFCHF` followed by either `LFIHF` or `LFSHF` called once for each right-hand side. The routine `LFDHF` can be called to compute the determinant of the coefficient matrix after `LFCHF` has performed the factorization.

The underlying code is based on either LINPACK or LAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see *Using ScaLAPACK, LAPACK, LINPACK, and EISPACK* in the Introduction section of this manual.

Comments

1. Workspace may be explicitly provided, if desired, by use of `L2CHF/DL2CHF`. The reference is:

   `CALL L2CHF (N, A, LDA, FACT, LDFACT, IPVT, RCOND, CWK)`

   The additional argument is:

CWK — Complex work vector of length N.

2. Informational errors

Type	Code	Description
3	1	The input matrix is algorithmically singular.
3	4	The input matrix is not Hermitian. It has a diagonal entry with a small imaginary part.
4	2	The input matrix is singular.
4	4	The input matrix is not Hermitian. It has a diagonal entry with an imaginary part.

Example

The inverse of a 3 × 3 complex Hermitian matrix is computed. LFCHF is called to factor the matrix and to check for singularity or ill-conditioning. LFIHF is called to determine the columns of the inverse.

```
      USE LFCHF_INT
      USE UMACH_INT
      USE LFIHF_INT
      USE WRCRN_INT
!                                 Declare variables
      INTEGER    LDA, N
      PARAMETER  (LDA=3, N=3)
      INTEGER    IPVT(N), NOUT
      REAL       RCOND
      COMPLEX    A(LDA,LDA), AINV(LDA,N), FACT(LDA,LDA), RJ(N), RES(N)
!                               Set values for A
!
!                               A = ( 3.0+0.0i   1.0-1.0i   4.0+0.0i )
!                                   ( 1.0+1.0i   2.0+0.0i  -5.0+1.0i )
!                                   ( 4.0+0.0i  -5.0-1.0i  -2.0+0.0i )
!
      DATA A/(3.0,0.0), (1.0,1.0), (4.0,0.0), (1.0,-1.0), (2.0,0.0),&
            (-5.0,-1.0), (4.0,0.0), (-5.0,1.0), (-2.0,0.0)/
!                                 Set output unit number
      CALL UMACH (2, NOUT)
!                                 Factor A and return the reciprocal
!                                 condition number estimate
      CALL LFCHF (A, FACT, IPVT, RCOND)
!                                 Print the estimate of the condition
!                                 number
      WRITE (NOUT,99999) RCOND, 1.0E0/RCOND
!                                 Set up the columns of the identity
!                                 matrix one at a time in RJ
      RJ = (0.0E0,0.0E0)
      DO 10  J=1, N
         RJ(J) = (1.0E0, 0.0E0)
!                                 RJ is the J-th column of the identity
!                                 matrix so the following LFIHF
!                                 reference places the J-th column of
!                                 the inverse of A in the J-th column
!                                 of AINV
         CALL LFIHF (A, FACT, IPVT, RJ, AINV(:,J), RES)
         RJ(J) = (0.0E0, 0.0E0)
   10 CONTINUE
```

```
!                                  Print the inverse
      CALL WRCRN ('AINV', AINV)
!
99999 FORMAT ('  RCOND = ',F5.3,/,'  L1 Condition number = ',F6.3)
      END
```

Output

```
RCOND < 0.25
L1 Condition number <  6.0

                           AINV
                   1                   2                   3
1  ( 0.2000, 0.0000)  ( 0.1200, 0.0400)  ( 0.0800,-0.0400)
2  ( 0.1200,-0.0400)  ( 0.1467, 0.0000)  (-0.1267,-0.0067)
3  ( 0.0800, 0.0400)  (-0.1267, 0.0067)  (-0.0267, 0.0000)
```

LFTHF

more...

Computes the $U\,DU^{H}$ factorization of a complex Hermitian matrix.

Required Arguments

A — Complex `N` by `N` matrix containing the coefficient matrix of the Hermitian linear system. (Input)
Only the upper triangle of `A` is referenced.

FACT — Complex `N` by `N` matrix containing the information about the factorization of the Hermitian matrix `A`. (Output)
Only the upper triangle of `FACT` is used. If `A` is not needed, `A` and `FACT` can share the same storage locations.

IPVT — Vector of length `N` containing the pivoting information for the factorization. (Output)

Optional Arguments

N – Order of the matrix. (Input)
Default: `N` = size (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = size (`A`,1).

LDFACT — Leading dimension of `FACT` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDFACT` = size (`FACT`,1).

FORTRAN 90 Interface

Generic: `CALL LFTHF (A, FACT, IPVT [, …])`

Specific: The specific interface names are `S_LFTHF` and `D_LFTHF`.

FORTRAN 77 Interface

Single:	`CALL LFTHF (N, A, LDA, FACT, LDFACT, IPVT)`
Double:	The double precision name is `DLFTHF`.

Description

Routine `LFTHF` performs a $U\,DU^{H}$ factorization of a complex Hermitian indefinite coefficient matrix. The UDU^{H} factorization is called the diagonal pivoting factorization.

`LFTHF` fails if *A* is singular or very close to a singular matrix.

The $U\,DU^{H}$ factors are returned in a form that is compatible with routines `LFIHF`, `LFSHF` and `LFDHF`. To solve systems of equations with multiple right-hand-side vectors, use `LFTHF` followed by either `LFIHF` or `LFSHF` called once for each right-hand side. The routine `LFDHF` can be called to compute the determinant of the coefficient matrix after `LFTHF` has performed the factorization.

The underlying code is based on either LINPACK or LAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see *Using ScaLAPACK, LAPACK, LINPACK, and EISPACK* in the Introduction section of this manual.

Comments

Informational errors

Type	Code	Description
3	4	The input matrix is not Hermitian. It has a diagonal entry with a small imaginary part.
4	2	The input matrix is singular.
4	4	The input matrix is not Hermitian. It has a diagonal entry with an imaginary part.

Example

The inverse of a 3×3 matrix is computed. `LFTHF` is called to factor the matrix and check for singularity. `LFSHF` is called to determine the columns of the inverse.

```
      USE LFTHF_INT
      USE LFSHF_INT
      USE WRCRN_INT
```

```
!                                  Declare variables
      INTEGER    LDA, N
      PARAMETER  (LDA=3, N=3)
      INTEGER    IPVT(N)
      COMPLEX    A(LDA,LDA), AINV(LDA,N), FACT(LDA,LDA), RJ(N)
!
!                                Set values for A
!
!                                A = ( 3.0+0.0i   1.0-1.0i   4.0+0.0i )
!                                    ( 1.0+1.0i   2.0+0.0i  -5.0+1.0i )
!                                    ( 4.0+0.0i  -5.0-1.0i  -2.0+0.0i )
!
      DATA A/(3.0,0.0), (1.0,1.0), (4.0,0.0), (1.0,-1.0), (2.0,0.0),&
            (-5.0,-1.0), (4.0,0.0), (-5.0,1.0), (-2.0,0.0)/
!                                  Factor A
      CALL LFTHF (A, FACT, IPVT)
!                                  Set up the columns of the identity
!                                  matrix one at a time in RJ
      RJ = (0.0E0,0.0E0)
      DO 10  J=1, N
         RJ(J) = (1.0E0, 0.0E0)
!                                  RJ is the J-th column of the identity
!                                  matrix so the following LFSHF
!                                  reference places the J-th column of
!                                  the inverse of A in the J-th column
!                                  of AINV
         CALL LFSHF (FACT, IPVT, RJ, AINV(:,J))
         RJ(J) = (0.0E0, 0.0E0)
   10 CONTINUE
!                                  Print the inverse
      CALL WRCRN ('AINV', AINV)
      END
```

Output

```
                              AINV
                   1                   2                   3
1  ( 0.2000, 0.0000)  ( 0.1200, 0.0400)  ( 0.0800,-0.0400)
2  ( 0.1200,-0.0400)  ( 0.1467, 0.0000)  (-0.1267,-0.0067)
3  ( 0.0800, 0.0400)  (-0.1267, 0.0067)  (-0.0267, 0.0000)
```

LFSHF

more...

Solves a complex Hermitian system of linear equations given the $U DU^H$ factorization of the coefficient matrix.

Required Arguments

FACT — Complex N by N matrix containing the factorization of the coefficient matrix A as output from routine LFCHF/DLFCHF or LFTHF/DLFTHF. (Input)
Only the upper triangle of FACT is used.

IPVT — Vector of length N containing the pivoting information for the factorization of A as output from routine LFCHF/DLFCHF or LFTHF/DLFTHF. (Input)

B — Complex vector of length N containing the right-hand side of the linear system. (Input)

X — Complex vector of length N containing the solution to the linear system. (Output)
If B is not needed, B and X can share the same storage locations.

Optional Arguments

N — Number of equations. (Input)
Default: N = size (FACT,2).

LDFACT — Leading dimension of FACT exactly as specified in the dimension statement of the calling program. (Input)
Default: LDFACT = size (FACT,1).

FORTRAN 90 Interface

Generic: CALL LFSHF (FACT, IPVT, B, X [, …])

Specific: The specific interface names are S_LFSHF and D_LFSHF.

FORTRAN 77 Interface

Single: CALL LFSHF (N, FACT, LDFACT, IPVT, B, X)

Double: The double precision name is DLFSHF.

Description

Routine LFSHF computes the solution of a system of linear algebraic equations having a complex Hermitian indefinite coefficient matrix.

To compute the solution, the coefficient matrix must first undergo a $UDU^{\boldsymbol{H}}$ factorization. This may be done by calling either LFCHF or LFTHF.

LFSHF and LFIHF both solve a linear system given its $UDU^{\boldsymbol{H}}$ factorization. LFIHF generally takes more time and produces a more accurate answer than LFSHF. Each iteration of the iterative refinement algorithm used by LFIHF calls LFSHF.

The underlying code is based on either LINPACK or LAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see *Using ScaLAPACK, LAPACK, LINPACK, and EISPACK* in the Introduction section of this manual.

Example

A set of linear systems is solved successively. LFTHF is called to factor the coefficient matrix. LFSHF is called to compute the three solutions for the three right-hand sides. In this case the coefficient matrix is assumed to be well-conditioned and correctly scaled. Otherwise, it would be better to call LFCHF to perform the factorization, and LFIHF to compute the solutions.

```
      USE LFSHF_INT
      USE WRCRN_INT
      USE LFTHF_INT
!                                 Declare variables
      INTEGER    LDA, N
      PARAMETER  (LDA=3, N=3)
      INTEGER    IPVT(N), I
      COMPLEX    A(LDA,LDA), B(N,3), X(N,3), FACT(LDA,LDA)
!
!                               Set values for A and B
!
!                               A = ( 3.0+0.0i   1.0-1.0i   4.0+0.0i )
!                                   ( 1.0+1.0i   2.0+0.0i  -5.0+1.0i )
!                                   ( 4.0+0.0i  -5.0-1.0i  -2.0+0.0i )
!
!                               B = (  7.0+32.0i -6.0+11.0i -2.0-17.0i )
!                                   (-39.0-21.0i -5.5-22.5i  4.0+10.0i )
!                                   ( 51.0+ 9.0i 16.0+17.0i -2.0+12.0i )
!
      DATA A/(3.0,0.0), (1.0,1.0), (4.0,0.0), (1.0,-1.0), (2.0,0.0),&
            (-5.0,-1.0), (4.0,0.0), (-5.0,1.0), (-2.0,0.0)/
```

```
      DATA B/(7.0,32.0), (-39.0,-21.0), (51.0,9.0), (-6.0,11.0),&
             (-5.5,-22.5), (16.0,17.0), (-2.0,-17.0), (4.0,10.0),&
             (-2.0,12.0)/
!                                 Factor A
      CALL LFTHF (A, FACT, IPVT)
!                                 Solve for the three right-hand sides
      DO 10  I=1, 3
         CALL LFSHF (FACT, IPVT, B(:,I), X(:,I))
   10 CONTINUE
!                                 Print results
      CALL WRCRN ('X', X)
      END
```

Output

```
                             X
                  1                 2                 3
1  (  2.00,  1.00)  (  1.00,  0.00)  (  0.00, -1.00)
2  (-10.00, -1.00)  ( -3.00, -4.00)  (  0.00, -2.00)
3  (  3.00,  5.00)  ( -0.50,  3.00)  (  0.00, -3.00)
```

LFIHF

more...

Uses iterative refinement to improve the solution of a complex Hermitian system of linear equations.

Required Arguments

A — Complex `N` by `N` matrix containing the coefficient matrix of the Hermitian linear system. (Input)
Only the upper triangle of `A` is referenced.

FACT — Complex `N` by `N` matrix containing the factorization of the coefficient matrix `A` as output from routine `LFCHF/DLFCHF` or `LFTHF/DLFTHF`. (Input)
Only the upper triangle of `FACT` is used.

IPVT — Vector of length `N` containing the pivoting information for the factorization of ***A*** as output from routine `LFCHF/DLFCHF` or `LFTHF/DLFTHF`. (Input)

B — Complex vector of length `N` containing the right-hand side of the linear system. (Input)

X — Complex vector of length `N` containing the solution. (Output)

RES — Complex vector of length `N` containing the residual vector at the improved solution. (Output)

Optional Arguments

N — Number of equations. (Input)
Default: `N` = size (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = size (`A`,1).

LDFACT — Leading dimension of `FACT` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDFACT` = size (`FACT`,1).

FORTRAN 90 Interface

Generic: `CALL LFIHF (A, FACT, IPVT, B, X, RES [, …])`

Specific: The specific interface names are `S_LFIHF` and `D_LFIHF`.

FORTRAN 77 Interface

Single: `CALL LFIHF (N, A, LDA, FACT, LDFACT, IPVT, B, X, RES)`

Double: The double precision name is `DLFIHF`.

Description

Routine `LFIHF` computes the solution of a system of linear algebraic equations having a complex Hermitian indefinite coefficient matrix.

Iterative refinement is performed on the solution vector to improve the accuracy. Usually almost all of the digits in the solution are accurate, even if the matrix is somewhat ill-conditioned.

To compute the solution, the coefficient matrix must first undergo a $U\,DU^{H}$ factorization. This may be done by calling either `LFCHF` or `LFTHF`.

Iterative refinement fails only if the matrix is very ill-conditioned.

`LFIHF` and `LFSHF` both solve a linear system given its $U\,DU^{H}$ factorization. `LFIHF` generally takes more time and produces a more accurate answer than `LFSHF`. Each iteration of the iterative refinement algorithm used by `LFIHF` calls `LFSHF`.

Comments

Informational error

Type	Code	Description
3	3	The input matrix is too ill-conditioned for iterative refinement to be effective.

Example

A set of linear systems is solved successively. The right-hand-side vector is perturbed after solving the system each of the first two times by adding 0.2 + 0.2*i* to the second element.

```
      USE LFIHF_INT
      USE UMACH_INT
      USE LFCHF_INT
      USE WRCRN_INT
!                                  Declare variables
      INTEGER    LDA, N
      PARAMETER  (LDA=3, N=3)
      INTEGER    IPVT(N), NOUT
      REAL       RCOND
      COMPLEX    A(LDA,LDA), B(N), X(N), FACT(LDA,LDA), RES(N)
!
!
!                                Set values for A and B
!
!                                A = ( 3.0+0.0i   1.0-1.0i   4.0+0.0i )
!                                    ( 1.0+1.0i   2.0+0.0i  -5.0+1.0i )
!                                    ( 4.0+0.0i  -5.0-1.0i  -2.0+0.0i )
!
!                                B = ( 7.0+32.0i -39.0-21.0i 51.0+9.0i )
!
      DATA A/(3.0,0.0), (1.0,1.0), (4.0,0.0), (1.0,-1.0), (2.0,0.0),&
            (-5.0,-1.0), (4.0,0.0), (-5.0,1.0), (-2.0,0.0)/
      DATA B/(7.0,32.0), (-39.0,-21.0), (51.0,9.0)/
!                                  Set output unit number
      CALL UMACH (2, NOUT)
!                                  Factor A and compute the estimate
!                                  of the reciprocal condition number
      CALL LFCHF (A, FACT, IPVT, RCOND)
      WRITE (NOUT,99998) RCOND, 1.0E0/RCOND
!                                  Solve, then perturb right-hand side
      DO 10  I=1, 3
         CALL LFIHF (A, FACT, IPVT, B, X, RES)
!                                  Print results
         WRITE (NOUT,99999) I
         CALL WRCRN ('X', X, 1, N, 1)
         CALL WRCRN ('RES', RES, 1, N, 1)
         B(2) = B(2) + (0.2E0, 0.2E0)
   10 CONTINUE
!
99998 FORMAT ('  RCOND = ',F5.3,/,'  L1 Condition number = ',F6.3)
99999 FORMAT (//,'  For problem ', I1)
      END
```

Output

```
RCOND < 0.25
L1 Condition number <  5.0
For problem 1
                        X
              1                 2                 3
(  2.00,  1.00)  (-10.00, -1.00)  (  3.00,  5.00)

                                    RES
                      1                         2                         3
( 2.384E-07,-4.768E-07)  ( 0.000E+00,-3.576E-07)  (-1.421E-14, 1.421E-14)

For problem 2
                        X
              1                 2                 3
( 2.016, 1.032)  (-9.971,-0.971)  ( 2.973, 4.976)

                                   RES
                      1                         2                         3
( 2.098E-07,-1.764E-07)  ( 6.231E-07,-1.518E-07)  ( 1.272E-07, 4.005E-07)
```

```
For problem 3
                        X
              1                 2                 3
( 2.032, 1.064)  (-9.941,-0.941)  ( 2.947, 4.952)

                                   RES
                      1                         2                         3
( 4.196E-07,-3.529E-07)  ( 2.925E-07,-3.632E-07)  ( 2.543E-07, 3.242E-07)
```

LFDHF

Computes the determinant of a complex Hermitian matrix given the UDU^H factorization of the matrix.

Required Arguments

FACT — Complex N by N matrix containing the factorization of the coefficient matrix A as output from routine LFCHF/DLFCHF or LFTHF/DLFTHF. (Input)
Only the upper triangle of FACT is used.

IPVT — Vector of length N containing the pivoting information for the factorization of *A* as output from routine LFCHF/DLFCHF or LFTHF/DLFTHF. (Input)

DET1 — Scalar containing the mantissa of the determinant. (Output)
The value DET1 is normalized so that 1.0 ≤ |DET1| < 10.0 or DET1 = 0.0.

DET2 — Scalar containing the exponent of the determinant. (Output)
The determinant is returned in the form det(*A*) = DET1 * 10^{DET2}.

Optional Arguments

N — Number of equations. (Input)
Default: N = size (FACT,2).

LDFACT — Leading dimension of FACT exactly as specified in the dimension statement of the calling program. (Input)
Default: LDFACT = size (FACT,1).

FORTRAN 90 Interface

Generic: CALL LFDHF (FACT, IPVT, DET1, DET2 [, …])

Specific: The specific interface names are S_LFDHF and D_LFDHF.

FORTRAN 77 Interface

Single: CALL LFDHF (N, FACT, LDFACT, IPVT, DET1, DET2)

Double: The double precision name is DLFDHF.

Description

Routine LFDHF computes the determinant of a complex Hermitian indefinite coefficient matrix. To compute the determinant, the coefficient matrix must first undergo a $U D U^H$ factorization. This may be done by calling either LFCHF or LFTHF since det $U = \pm 1$, the formula det A = det U det D det U^H = det D is used to compute the determinant. det D is computed as the product of the determinants of its blocks.

LFDHF is based on the LINPACK routine CSIDI; see Dongarra et al. (1979).

Example

The determinant is computed for a complex Hermitian 3×3 matrix.

```
      USE LFDHF_INT
      USE LFTHF_INT
      USE UMACH_INT
!                                 Declare variables
      INTEGER    LDA, N
      PARAMETER  (LDA=3, N=3)
      INTEGER    IPVT(N), NOUT
      REAL       DET1, DET2
      COMPLEX    A(LDA,LDA), FACT(LDA,LDA)
!
!                               Set values for A
!
!                               A = ( 3.0+0.0i   1.0-1.0i   4.0+0.0i )
!                                   ( 1.0+1.0i   2.0+0.0i  -5.0+1.0i )
!                                   ( 4.0+0.0i  -5.0-1.0i  -2.0+0.0i )
!
      DATA A/(3.0,0.0), (1.0,1.0), (4.0,0.0), (1.0,-1.0), (2.0,0.0),&
            (-5.0,-1.0), (4.0,0.0), (-5.0,1.0), (-2.0,0.0)/
!                                 Factor A
      CALL LFTHF (A, FACT, IPVT)
!                                 Compute the determinant
      CALL LFDHF (FACT, IPVT, DET1, DET2)
!                                 Print the results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) DET1, DET2
!
99999 FORMAT (' The determinant is', F5.1, ' * 10**', F2.0)
      END
```

Output

```
The determinant is -1.5 * 10**2.
```

LSLTR

Solves a real tridiagonal system of linear equations.

Required Arguments

C — Vector of length N containing the subdiagonal of the tridiagonal matrix in C(2) through C(N). (Input/Output)
On output C is destroyed.

D — Vector of length N containing the diagonal of the tridiagonal matrix. (Input/Output)
On output D is destroyed.

E — Vector of length N containing the superdiagonal of the tridiagonal matrix in E(1) through E(N − 1). (Input/Output)
On output E is destroyed.

B — Vector of length N containing the right-hand side of the linear system on entry and the solution vector on return. (Input/Output)

Optional Arguments

N — Order of the tridiagonal matrix. (Input)
Default: N = size (C,1).

FORTRAN 90 Interface

Generic: CALL LSLTR (C, D, E, B [, …])

Specific: The specific interface names are S_LSLTR and D_LSLTR.

FORTRAN 77 Interface

Single: CALL LSLTR (N, C, D, E, B)

Double: The double precision name is DLSLTR.

Description

Routine LSLTR factors and solves the real tridiagonal linear system $Ax = b$. LSLTR is intended just for tridiagonal systems. The coefficient matrix does not have to be symmetric. The algorithm is Gaussian elimination with partial pivoting for numerical stability. See Dongarra (1979), LINPACK subprograms SGTSL/DGTSL, for details. When computing on vector or parallel computers the cyclic reduction algorithm, LSLCR, should be considered as an alternative method to solve the system.

Comments

Informational error

Type	Code	Description
4	2	An element along the diagonal became exactly zero during execution.

Example

A system of n = 4 linear equations is solved.

```
      USE LSLTR_INT
      USE WRRRL_INT
!                                 Declaration of variables
      INTEGER    N
      PARAMETER  (N=4)
!
      REAL       B(N), C(N), D(N), E(N)
      CHARACTER  CLABEL(1)*6, FMT*8, RLABEL(1)*4
!
      DATA FMT/'(E13.6)'/
      DATA CLABEL/'NUMBER'/
      DATA RLABEL/'NONE'/
!                                 C(*), D(*), E(*), and B(*)
!                                 contain the subdiagonal, diagonal,
!                                 superdiagonal and right hand side.
      DATA C/0.0, 0.0, -4.0, 9.0/, D/6.0, 4.0, -4.0, -9.0/
      DATA E/-3.0, 7.0, -8.0, 0.0/, B/48.0, -81.0, -12.0, -144.0/
!
!
      CALL LSLTR (C, D, E, B)
!                                 Output the solution.
      CALL WRRRL ('Solution:', B, RLABEL, CLABEL, 1, N, 1, FMT=FMT)
      END
```

Output

```
Solution:
        1              2                 3              4
0.400000E+01  -0.800000E+01  -  0.700000E+01   0.900000E+01
```

LSLCR

Computes the LDU factorization of a real tridiagonal matrix A using a cyclic reduction algorithm.

Required Arguments

C — Array of size 2N containing the upper codiagonal of the N by N tridiagonal matrix in the entries C(1), …, C(N − 1). (Input/Output)

A — Array of size 2N containing the diagonal of the N by N tridiagonal matrix in the entries A(1), …, A(N). (Input/Output)

B — Array of size 2N containing the lower codiagonal of the N by N tridiagonal matrix in the entries B(1), …, B(N − 1). (Input/Output)

Y — Array of size 2N containing the right hand side for the system $Ax = y$ in the order Y(1), …, Y(N). (Input/Output)
The vector x overwrites Y in storage.

U — Array of size 2N of flags that indicate any singularities of A. (Output)
A value U(I) = 1. means that a divide by zero would have occurred during the factoring. Otherwise U(I) = 0.

IR — Array of integers that determine the sizes of loops performed in the cyclic reduction algorithm. (Output)

IS — Array of integers that determine the sizes of loops performed in the cyclic reduction algorithm. (Output)
The sizes of IR and IS must be at least $\log_2$ (N) + 3.

Optional Arguments

N — Order of the matrix. (Input)
N must be greater than zero
Default: N = size (C,1).

IJOB — Flag to direct the desired factoring or solving step. (Input)
Default: `IJOB` = 1.

IJOB	**Action**
1	Factor the matrix *A* and solve the system *Ax* = *y*, where *y* is stored in array `Y`.
2	Do the solve step only. Use *y* from array `Y`. (The factoring step has already been done.)
3	Factor the matrix *A* but do not solve a system.
4, 5, 6	Same meaning as with the value `IJOB` = 3. For efficiency, no error checking is done on the validity of any input value.

FORTRAN 90 Interface

Generic: `CALL LSLCR (C, A, B, Y, U, IR, IS [, …])`

Specific: The specific interface names are `S_LSLCR` and `D_LSLCR`.

FORTRAN 77 Interface

Single: `CALL LSLCR (N, C, A, B, IJOB, Y, U, IR, IS)`

Double: The double precision name is `DLSLCR`.

Description

Routine `LSLCR` factors and solves the real tridiagonal linear system *Ax* = *y*. The matrix is decomposed in the form A = *L DU*, where *L* is unit lower triangular, *U* is unit upper triangular, and *D* is diagonal. The algorithm used for the factorization is effectively that described in Kershaw (1982). More details, tests and experiments are reported in Hanson (1990).

`LSLCR` is intended just for tridiagonal systems. The coefficient matrix does not have to be symmetric. The algorithm amounts to Gaussian elimination, with no pivoting for numerical stability, on the matrix whose rows and columns are permuted to a new order. See Hanson (1990) for details. The expectation is that `LSLCR` will outperform either `LSLTR` or `LSLPB` on vector or parallel computers. Its performance may be inferior for small values of *n*, on scalar computers, or high-performance computers with non-optimizing compilers.

Example

A system of n = 1000 linear equations is solved. The coefficient matrix is the symmetric matrix of the second difference operation, and the right-hand-side vector y is the first column of the identity matrix. Note that $a_{n'n}$= 1. The solution vector will be the first column of the inverse matrix of A. Then a new system is solved where y is now the last column of the identity matrix. The solution vector for this system will be the last column of the inverse matrix.

```
      USE LSLCR_INT
      USE UMACH_INT
!                                 Declare variables
      INTEGER    LP, N, N2
      PARAMETER  (LP=12, N=1000, N2=2*N)
!
      INTEGER    I, IJOB, IR(LP), IS(LP), NOUT
      REAL       A(N2), B(N2), C(N2), U(N2), Y1(N2), Y2(N2)
!
!                                 Define matrix entries:
      DO 10  I=1, N - 1
         C(I)    = -1.E0
         A(I)    = 2.E0
         B(I)    = -1.E0
         Y1(I+1) = 0.E0
         Y2(I)   = 0.E0
   10 CONTINUE
      A(N)  = 1.E0
      Y1(1) = 1.E0
      Y2(N) = 1.E0
!
!                                 Obtain decomposition of matrix and
!                                 solve the first system:
      IJOB = 1
      CALL LSLCR (C, A, B, Y1, U, IR, IS, IJOB=IJOB)
!
!                                 Solve the second system with the
!                                 decomposition ready:
      IJOB = 2
      CALL LSLCR (C, A, B, Y2, U, IR, IS, IJOB=IJOB)
      CALL UMACH (2, NOUT)


      WRITE (NOUT,*) ' The value of n is:  ', N
      WRITE (NOUT,*) ' Elements 1, n of inverse matrix columns 1 '//&
                    'and   n:', Y1(1), Y2(N)
      END
```

Output

```
The value of n is:    1000
Elements 1, n of inverse matrix columns 1 and   n:    1.00000   1000.000
```

LSARB

more...

Solves a real system of linear equations in band storage mode with iterative refinement.

Required Arguments

A — (NLCA + NUCA + 1) by N array containing the N by N banded coefficient matrix in band storage mode. (Input)

NLCA — Number of lower codiagonals of A. (Input)

NUCA — Number of upper codiagonals of A. (Input)

B — Vector of length N containing the right-hand side of the linear system. (Input)

X — Vector of length N containing the solution to the linear system. (Output)

Optional Arguments

N — Number of equations. (Input)
Default: N = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

IPATH — Path indicator. (Input)
IPATH = 1 means the system AX = B is solved.
IPATH = 2 means the system $A^T X$ = B is solved.
Default: IPATH =1.

FORTRAN 90 Interface

Generic: CALL LSARB (A, NLCA, NUCA, B, X [, …])

Specific: The specific interface names are S_LSARB and D_LSARB.

FORTRAN 77 Interface

Single: CALL LSARB (N, A, LDA, NLCA, NUCA, B, IPATH, X)

Double: The double precision name is DLSARB.

Description

Routine LSARB solves a system of linear algebraic equations having a real banded coefficient matrix. It first uses the routine LFCRB to compute an *LU* factorization of the coefficient matrix and to estimate the condition number of the matrix. The solution of the linear system is then found using the iterative refinement routine LFIRB.

LSARB fails if *U*, the upper triangular part of the factorization, has a zero diagonal element or if the iterative refinement algorithm fails to converge. These errors occur only if A is singular or very close to a singular matrix.

If the estimated condition number is greater than $1/\varepsilon$ (where ε is machine precision), a warning error is issued. This indicates that very small changes in A can cause very large changes in the solution *x*. Iterative refinement can sometimes find the solution to such a system. LSARB solves the problem that is represented in the computer; however, this problem may differ from the problem whose solution is desired.

Comments

1. Workspace may be explicitly provided, if desired, by use of L2ARB/DL2ARB. The reference is:

   CALL L2ARB (N, A, LDA, NLCA, NUCA, B, IPATH, X, FACT, IPVT, WK)

   The additional arguments are as follows:

   FACT — Work vector of length (2 * NLCA + NUCA + 1) × N containing the *LU* factorization of A on output.

   IPVT — Work vector of length N containing the pivoting information for the *LU* factorization of A on output.

   WK — Work vector of length N.

2. Informational errors

Type	Code	Description
3	1	The input matrix is too ill-conditioned. The solution might not be accurate.
4	2	The input matrix is singular.

3. *Integer Options* with *Chapter 11* Options Manager

16 This option uses four values to solve memory bank conflict (access inefficiency) problems. In routine L2ARB the leading dimension of FACT is increased by IVAL(3) when N is a multiple of IVAL(4). The values IVAL(3) and IVAL(4) are temporarily replaced by IVAL(1) and IVAL(2), respectively, in LSARB. Additional memory allocation for FACT and option value restoration are done automatically in LSARB. Users directly calling L2ARB can allocate additional space for FACT and set IVAL(3) and IVAL(4) so that memory bank conflicts no longer cause inefficiencies. There is no requirement that users change existing applications that use LSARB or L2ARB. Default values for the option are IVAL(*) = 1, 16, 0, 1.

17 This option has two values that determine if the L_1 condition number is to be computed. Routine LSARB temporarily replaces IVAL(2) by IVAL(1). The routine L2CRB computes the condition number if IVAL(2) = 2. Otherwise L2CRB skips this computation. LSARB restores the option. Default values for the option are IVAL(*) = 1, 2.

Example

A system of four linear equations is solved. The coefficient matrix has real banded form with 1 upper and 1 lower codiagonal. The right-hand-side vector *b* has four elements.

```
      USE LSARB_INT
      USE WRRRN_INT
!                                 Declare variables
      INTEGER    LDA, N, NLCA, NUCA
      PARAMETER  (LDA=3, N=4, NLCA=1, NUCA=1)
      REAL       A(LDA,N), B(N), X(N)
!                                 Set values for A in band form, and B
!
!                                 A = (  0.0  -1.0  -2.0   2.0)
!                                     (  2.0   1.0  -1.0   1.0)
!                                     ( -3.0   0.0   2.0   0.0)
!
!                                 B = (  3.0   1.0  11.0  -2.0)
!
      DATA A/0.0, 2.0, -3.0, -1.0, 1.0, 0.0, -2.0, -1.0, 2.0,&
            2.0, 1.0, 0.0/
      DATA B/3.0, 1.0, 11.0, -2.0/
!
      CALL LSARB (A, NLCA, NUCA, B, X)
!                                 Print results
      CALL WRRRN ('X', X, 1, N, 1)
!
      END
```

Output

```
                 X
     1        2        3        4
 2.000    1.000   -3.000    4.000
```

LSLRB

more...

more...

Solves a real system of linear equations in band storage mode without iterative refinement.

Required Arguments

A — (NLCA + NUCA + 1) by N array containing the N by N banded coefficient matrix in band storage mode. (Input)

NLCA — Number of lower codiagonals of A. (Input)

NUCA — Number of upper codiagonals of A. (Input)

B — Vector of length N containing the right-hand side of the linear system. (Input)

X — Vector of length N containing the solution to the linear system. (Output)

Optional Arguments

N — Number of equations. (Input)
Default: N = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

IPATH — Path indicator. (Input)
IPATH = 1 means the system $AX = B$ is solved.
IPATH = 2 means the system $A^T X = B$ is solved.
Default: IPATH = 1.

FORTRAN 90 Interface

Generic: CALL LSLRB (A, NLCA, NUCA, B, X [, …])

Specific: The specific interface names are S_LSLRB and D_LSLRB.

FORTRAN 77 Interface

Single: CALL LSLRB (N, A, LDA, NLCA, NUCA, B, IPATH, X)

Double: The double precision name is DLSLRB.

ScaLAPACK Interface

Generic: CALL LSLRB (A0, NLCA, NUCA, B0, X0 [, …])

Specific: The specific interface names are S_LSLRB and D_LSLRB.

See the *ScaLAPACK Usage Notes* below for a description of the arguments for distributed computing.

Description

Routine LSLRB solves a system of linear algebraic equations having a real banded coefficient matrix. It first uses the routine LFCRB to compute an *LU* factorization of the coefficient matrix and to estimate the condition number of the matrix. The solution of the linear system is then found using LFSRB. LSLRB fails if *U*, the upper triangular part of the factorization, has a zero diagonal element. This occurs only if *A* is singular or very close to a singular matrix. If the estimated condition number is greater than $1/\varepsilon$ (where ε is machine precision), a warning error is issued. This indicates that very small changes in *A* can cause very large changes in the solution *x*. If the coefficient matrix is ill-conditioned or poorly scaled, it is recommended that LSARB be used.

The underlying code is based on either LINPACK , LAPACK, or ScaLAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see *Using ScaLAPACK, LAPACK, LINPACK, and EISPACK* in the Introduction section of this manual.

Comments

1. Workspace may be explicitly provided, if desired, by use of L2LRB/DL2LRB. The reference is:

   CALL L2LRB (N, A, LDA, NLCA, NUCA, B, IPATH, X, FACT, IPVT, WK)

   The additional arguments are as follows:

   FACT — (2 × NLCA + NUCA + 1) × N containing the *LU* factorization of A on output. If A is not needed, A can share the first (NLCA + NUCA + 1) * N storage locations with FACT.

   IPVT — Work vector of length N containing the pivoting information for the *LU* factorization of A on output.

   WK — Work vector of length N.

2. Informational errors

Type	Code	Description
3	1	The input matrix is too ill-conditioned. The solution might not be accurate.
4	2	The input matrix is singular.

3. *Integer Options* with *Chapter 11* Options Manager

16 This option uses four values to solve memory bank conflict (access inefficiency) problems. In routine L2LRB the leading dimension of FACT is increased by IVAL(3) when N is a multiple of IVAL(4). The values IVAL(3) and IVAL(4) are temporarily replaced by IVAL(1) and IVAL(2), respectively, in LSLRB. Additional memory allocation for FACT and option value restoration are done automatically in LSLRB. Users directly calling L2LRB can allocate additional space for FACT and set IVAL(3) and IVAL(4) so that memory bank conflicts no longer cause inefficiencies. There is no requirement that users change existing applications that use LSLRB or L2LRB. Default values for the option are IVAL(*) = 1, 16, 0, 1.

17 This option has two values that determine if the L_1 condition number is to be computed. Routine LSLRB temporarily replaces IVAL(2) by IVAL(1). The routine L2CRB computes the condition number if IVAL(2) = 2. Otherwise L2CRB skips this computation. LSLRB restores the option. Default values for the option are IVAL(*) = 1, 2.

ScaLAPACK Usage Notes

The arguments which differ from the standard version of this routine are:

A0 — (2*NLCA + 2*NUCA+1) by MXCOL local matrix containing the local portions of the distributed matrix A. A contains the N by N banded coefficient matrix in band storage mode. (Input)

B0 — Local vector of length MXCOL containing the local portions of the distributed vector B. B contains the right-hand side of the linear system. (Input)

X0 — Local vector of length MXCOL containing the local portions of the distributed vector X. X contains the solution to the linear system. (Output)

All other arguments are global and are the same as described for the standard version of the routine. In the argument descriptions above, MXCOL can be obtained through a call to SCALAPACK_GETDIM (see *Utilities*) after a call to SCALAPACK_SETUP (see *Utilities*) has been made. See the *ScaLAPACK Example* below.

Examples

Example

A system of four linear equations is solved. The coefficient matrix has real banded form with 1 upper and 1 lower codiagonal. The right-hand-side vector *b* has four elements.

```
      USE LSLRB_INT
      USE WRRRN_INT
!                                 Declare variables
      INTEGER    LDA, N, NLCA, NUCA
      PARAMETER  (LDA=3, N=4, NLCA=1, NUCA=1)
      REAL       A(LDA,N), B(N), X(N)
!                                 Set values for A in band form, and B
!
!                                 A = (  0.0  -1.0  -2.0   2.0)
!                                     (  2.0   1.0  -1.0   1.0)
!                                     ( -3.0   0.0   2.0   0.0)
!
!                                 B = (  3.0   1.0  11.0  -2.0)
!
      DATA A/0.0, 2.0, -3.0, -1.0, 1.0, 0.0, -2.0, -1.0, 2.0,&
            2.0, 1.0, 0.0/
      DATA B/3.0, 1.0, 11.0, -2.0/
!
      CALL LSLRB (A, NLCA, NUCA, B, X)
!                                 Print results
      CALL WRRRN ('X', X, 1, N, 1)
!
      END
```

Output

```
                X
    1       2        3        4
2.000   1.000   -3.000    4.000
```

ScaLAPACK Example

The same system of four linear equations is solved as a distributed computing example. The coefficient matrix has real banded form with 1 upper and 1 lower codiagonal. The right-hand-side vector *b* has four elements. `SCALAPACK_MAP` and `SCALAPACK_UNMAP` are IMSL utility routines (see *Utilities*) used to map and unmap arrays to and from the processor grid. They are used here for brevity. `DESCINIT` is a ScaLAPACK tools routine which initializes the descriptors for the local arrays.

```
      USE MPI_SETUP_INT
      USE LSLRB_INT
      USE WRRRN_INT
      USE SCALAPACK_SUPPORT
      IMPLICIT NONE
      INCLUDE 'mpif.h'
!                                 Declare variables
      INTEGER    LDA, M, N, NLCA, NUCA, NRA, DESCA(9), DESCX(9)
      INTEGER       INFO, MXCOL, MXLDA
      REAL, ALLOCATABLE ::        A(:,:), B(:), X(:)
      REAL, ALLOCATABLE ::        A0(:,:), B0(:), X0(:)
```

```
      PARAMETER  (LDA=3, N=6, NLCA=1, NUCA=1)
!                                   Set up for MPI
      MP_NPROCS = MP_SETUP()
      IF(MP_RANK .EQ. 0) THEN
          ALLOCATE (A(LDA,N), B(N), X(N))
!                                   Set values for A and B
          A(1,:) = (/  0.0,   0.0,  -3.0,   0.0, -1.0, -3.0/)
          A(2,:) = (/ 10.0,  10.0,  15.0,  10.0,  1.0,  6.0/)
          A(3,:) = (/  0.0,   0.0,   0.0,  -5.0,  0.0,  0.0/)!

          B      = (/ 10.0,   7.0,  45.0,  33.0, -34.0, 31.0/)
      ENDIF
      NRA = NLCA + NUCA + 1
      M = 2*NLCA + 2*NUCA + 1
!                                    Set up a 1D processor grid and define
!                                    its context ID, MP_ICTXT
      CALL SCALAPACK_SETUP(M, N, .FALSE., .TRUE.)
!                                    Get the array descriptor entities MXLDA,
!                                    and MXCOL
      CALL SCALAPACK_GETDIM(M, N, MP_MB, MP_NB, MXLDA, MXCOL)
!                                    Reset MXLDA to M
      MXLDA = M
!                                    Set up the array descriptors
      CALL DESCINIT(DESCA,NRA,N,MP_MB, MP_NB, 0, 0, MP_ICTXT, MXLDA, INFO)
      CALL DESCINIT(DESCX, 1, N, 1, MP_NB, 0, 0, MP_ICTXT, 1, INFO)
!                                    Allocate space for the local arrays
      ALLOCATE (A0(MXLDA,MXCOL), B0(MXCOL), X0(MXCOL))
!                                   Map input arrays to the processor grid
      CALL SCALAPACK_MAP(A, DESCA, A0)
      CALL SCALAPACK_MAP(B, DESCX, B0, 1, .FALSE.)
!                                   Solve the system of equations
      CALL LSLRB (A0, NLCA, NUCA, B0, X0)
!                                   Unmap the results from the distributed
!                                   arrays back to a non-distributed array.
!                                   After the unmap, only Rank=0 has the full
!                                   array.
      CALL SCALAPACK_UNMAP(X0, DESCX, X, 1, .FALSE.)
!                                 Print results.
!                                 Only Rank=0 has the solution, X.
      IF(MP_RANK .EQ. 0)CALL WRRRN ('X', X, 1, N, 1)
      IF (MP_RANK .EQ. 0) DEALLOCATE(A, B, X)
      DEALLOCATE(A0, B0, X0)
!                                 Exit ScaLAPACK usage
      CALL SCALAPACK_EXIT(MP_ICTXT)
!                                 Shut down MPI
      MP_NPROCS = MP_SETUP('FINAL')
      END
```

Output

```
                X
    1       2       3       4        5       6
1.000   1.600   3.000   2.900   -4.000   5.167
```

LFCRB

more...

Computes the *LU* factorization *of a* real matrix in band storage mode and estimate its L_1 condition number.

Required Arguments

A — (NLCA + NUCA + 1) by N array containing the N by N matrix in band storage mode to be factored. (Input)

NLCA — Number of lower codiagonals of A. (Input)

NUCA — Number of upper codiagonals of A. (Input)

FACT — (2 * NLCA + NUCA + 1) by N array containing the *LU* factorization of the matrix A. (Output)
If A is not needed, A can share the first (NLCA + NUCA + 1) * N locations with FACT.

IPVT — Vector of length N containing the pivoting information for the *LU* factorization. (Output)

RCOND — Scalar containing an estimate of the reciprocal of the L_1 condition number of A. (Output)

Optional Arguments

N — Order of the matrix. (Input)
Default: N = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

LDFACT — Leading dimension of FACT exactly as specified in the dimension statement of the calling program. (Input)
Default: LDFACT = size (FACT,1).

FORTRAN 90 Interface

Generic: `CALL LFCRB (A, NLCA, NUCA, FACT, IPVT, RCOND [, …])`

Specific: The specific interface names are `S_LFCRB` and `D_LFCRB`.

FORTRAN 77 Interface

Single: `CALL LFCRB (N, A, LDA, NLCA, NUCA, FACT, LDFACT, IPVT, RCOND)`

Double: The double precision name is `DLFCRB`.

Description

Routine `LFCRB` performs an *LU* factorization of a real banded coefficient matrix. It also estimates the condition number of the matrix. The *LU* factorization is done using scaled partial pivoting. Scaled partial pivoting differs from partial pivoting in that the pivoting strategy is the same as if each row were scaled to have the same ∞-norm.

The L_1 condition number of the matrix *A* is defined to be

$$\kappa(A) = \|A\|_1 \|A^{-1}\|_1$$

Since it is expensive to compute

$$\|A^{-1}\|_1$$

the condition number is only estimated. The estimation algorithm is the same as used by LINPACK and is described by Cline et al. (1979).

If the estimated condition number is greater than 1/**ε** (where **ε** is machine precision), a warning error is issued. This indicates that very small changes in *A* can cause very large changes in the solution *x*. Iterative refinement can sometimes find the solution to such a system.

`LSCRB` fails if *U*, the upper triangular part of the factorization, has a zero diagonal element. This can occur only if *A* is singular or very close to a singular matrix. The *LU* factors are returned in a form that is compatible with routines `LFIRB`, `LFSRB` and `LFDRB`. To solve systems of equations with multiple right-hand-side vectors, use `LFCRB` followed by either `LFIRB` or `LFSRB` called once for each right-hand side. The routine `LFDRB` can be called to compute the determinant of the coefficient matrix after `LFCRB` has performed the factorization.

Let *F* be the matrix `FACT`, let m_l = `NLCA` and let m_u = `NUCA`. The first $m_l + m_u + 1$ rows of F contain the triangular matrix *U* in band storage form. The lower m_l rows of F contain the multipliers needed to reconstruct L^{-1} .

The underlying code is based on either LINPACK or LAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see *Using ScaLAPACK, LAPACK, LINPACK, and EISPACK* in the Introduction section of this manual.

Comments

1. Workspace may be explicitly provided, if desired, by use of L2CRB/DL2CRB. The reference is:

   CALL L2CRB (N, A, LDA, NLCA, NUCA, FACT, LDFACT, IPVT, RCOND, WK)

   The additional argument is:

   WK — Work vector of length N.

2. Informational errors

Type	Code	Description
3	1	The input matrix is algorithmically singular.
4	2	The input matrix is singular.

Example

The inverse of a 4 × 4 band matrix with one upper and one lower codiagonal is computed. LFCRB is called to factor the matrix and to check for singularity or ill-conditioning. LFIRB is called to determine the columns of the inverse.

```
      USE LFCRB_INT
      USE UMACH_INT
      USE LFIRB_INT
      USE WRRRN_INT
!                                 Declare variables
      INTEGER    LDA, LDFACT, N, NLCA, NUCA, NOUT
      PARAMETER  (LDA=3, LDFACT=4, N=4, NLCA=1, NUCA=1)
      INTEGER    IPVT(N)
      REAL       A(LDA,N), AINV(N,N), FACT(LDFACT,N), RCOND, RJ(N), RES(N)
!                                 Set values for A in band form
!                                 A = (  0.0  -1.0  -2.0   2.0)
!                                     (  2.0   1.0  -1.0   1.0)
!                                     ( -3.0   0.0   2.0   0.0)
!
      DATA A/0.0, 2.0, -3.0, -1.0, 1.0, 0.0, -2.0, -1.0, 2.0,&
            2.0, 1.0, 0.0/
!
      CALL LFCRB (A, NLCA, NUCA, FACT, IPVT, RCOND)
!                                 Print the reciprocal condition number
!                                 and the L1 condition number
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) RCOND, 1.0E0/RCOND
!                                 Set up the columns of the identity
!                                 matrix one at a time in RJ
      RJ = 0.0E0
      DO 10  J=1, N
         RJ(J) = 1.0E0
```

```
!                                  RJ is the J-th column of the identity
!                                  matrix so the following LFIRB
!                                  reference places the J-th column of
!                                  the inverse of A in the J-th column
!                                  of AINV
         CALL LFIRB (A, NLCA, NUCA, FACT, IPVT, RJ, AINV(:,J), RES)
         RJ(J) = 0.0E0
   10 CONTINUE
!                                  Print results
      CALL WRRRN ('AINV', AINV)


!
99999 FORMAT ('  RCOND = ',F5.3,/,'  L1 Condition number = ',F6.3)
      END
```

Output

```
RCOND < .07
L1 Condition number = 25.0

               AINV
        1       2       3       4
1  -1.000  -1.000   0.400  -0.800
2  -3.000  -2.000   0.800  -1.600
3   0.000   0.000  -0.200   0.400
4   0.000   0.000   0.400   0.200
```

LFTRB

more...

Computes the *LU* factorization of a real matrix in band storage mode.

Required Arguments

A — (`NLCA` + `NUCA` + 1) by `N` array containing the `N` by `N` matrix in band storage mode to be factored. (Input)

NLCA — Number of lower codiagonals of `A`. (Input)

NUCA — Number of upper codiagonals of `A`. (Input)

FACT — (2 * `NLCA` + `NUCA` + 1) by `N` array containing the *LU* factorization of the matrix `A`. (Output)
If `A` is not needed, `A` can share the first (`NLCA` + `NUCA` + 1) * `N` locations with `FACT`.

IPVT — Vector of length `N` containing the pivoting information for the *LU* factorization. (Output)

Optional Arguments

N — Order of the matrix. (Input)
Default: `N` = size (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = size (`A`,1).

LDFACT — Leading dimension of `FACT` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDFACT` = size (`FACT`,1).

FORTRAN 90 Interface

Generic: `CALL LFTRB (A, NLCA, NUCA, FACT [, …])`

Specific: The specific interface names are S_LFTRB and D_LFTRB.

FORTRAN 77 Interface

Single: CALL LFTRB (N, A, LDA, NLCA, NUCA, FACT, LDFACT, IPVT)

Double: The double precision name is DLFTRB.

Description

Routine LFTRB performs an *LU* factorization of a real banded coefficient matrix using Gaussian elimination with partial pivoting. *A* failure occurs if *U*, the upper triangular factor, has a zero diagonal element. This can happen if *A* is close to a singular matrix. The *LU* factors are returned in a form that is compatible with routines LFIRB, LFSRB and LFDRB. To solve systems of equations with multiple right-hand-side vectors, use LFTRB followed by either LFIRB or LFSRB called once for each right-hand side. The routine LFDRB can be called to compute the determinant of the coefficient matrix after LFTRB has performed the factorization

Let m_l = NLCA, and let m_u = NUCA. The first $m_l + m_u + 1$ rows of FACT contain the triangular matrix *U* in band storage form. The next m_l rows of FACT contain the multipliers needed to produce *L*.

The routine LFTRB is based on the the blocked *LU* factorization algorithm for banded linear systems given in Du Croz, et al. (1990). Level-3 BLAS invocations were replaced by in-line loops. The blocking factor *nb* has the default value 1 in LFTRB. It can be reset to any positive value not exceeding 32.

Comments

1. Workspace may be explicitly provided, if desired, by use of L2TRB/DL2TRB. The reference is:

   CALL L2TRB (N, A, LDA, NLCA, NUCA, FACT, LDFACT, IPVT, WK)

   The additional argument is:

   WK — Work vector of length N used for scaling.

2 Informational error

Type	Code	Description
4	2	The input matrix is singular.

3. *Utilities* with *Chapter 11* Options Manager

21 The performance of the *LU* factorization may improve on high-performance computers if the blocking factor, NB, is increased. The current version of the routine allows NB to be reset to a value no larger than 32. Default value is NB = 1.

Example

A linear system with multiple right-hand sides is solved. LFTRB is called to factor the coefficient matrix. LFSRB is called to compute the two solutions for the two right-hand sides. In this case the coefficient matrix is assumed to be appropriately scaled. Otherwise, it may be better to call routine LFCRB to perform the factorization, and LFIRB to compute the solutions.

```
      USE LFTRB_INT
      USE LFSRB_INT
      USE WRRRN_INT
!                                 Declare variables
      INTEGER    LDA, LDFACT, N, NLCA, NUCA
      PARAMETER  (LDA=3, LDFACT=4, N=4, NLCA=1, NUCA=1)
      INTEGER    IPVT(N)
      REAL       A(LDA,N), B(N,2), FACT(LDFACT,N), X(N,2)
!                                 Set values for A in band form, and B
!
!                                 A = (  0.0  -1.0  -2.0   2.0)
!                                     (  2.0   1.0  -1.0   1.0)
!                                     ( -3.0   0.0   2.0   0.0)
!
!                                 B = ( 12.0 -17.0)
!                                     (-19.0  23.0)
!                                     (  6.0   5.0)
!                                     (  8.0   5.0)
!
      DATA A/0.0, 2.0, -3.0, -1.0, 1.0, 0.0, -2.0, -1.0, 2.0,&
            2.0, 1.0, 0.0/
      DATA B/12.0, -19.0, 6.0, 8.0, -17.0, 23.0, 5.0, 5.0/
!                                 Compute factorization
      CALL LFTRB (A, NLCA, NUCA, FACT, IPVT)
!                                 Solve for the two right-hand sides
      DO 10  J=1, 2
         CALL LFSRB (FACT, NLCA, NUCA, IPVT, B(:,J), X(:,J))
   10 CONTINUE
!                                 Print results
      CALL WRRRN ('X', X)
!
      END
```

Output

```
         X
         1       2
1    3.000  -8.000
2   -6.000   1.000
3    2.000   1.000
4    4.000   3.000
```

LFSRB

more...

Solves a real system of linear equations given the *LU* factorization of the coefficient matrix in band storage mode.

Required Arguments

FACT — (2 * NLCA + NUCA + 1) by N array containing the *LU* factorization of the coefficient matrix A as output from routine LFCRB/DLFCRB or LFTRB/DLFTRB. (Input)

NLCA — Number of lower codiagonals of A. (Input)

NUCA — Number of upper codiagonals of A. (Input)

IPVT — Vector of length N containing the pivoting information for the *LU* factorization of A as output from routine LFCRB/DLFCRB or LFTRB/DLFTRB. (Input)

B — Vector of length N containing the right-hand side of the linear system. (Input)

X — Vector of length N containing the solution to the linear system. (Output)
If B is not needed, B and X can share the same storage locations.

Optional Arguments

N — Number of equations. (Input)
Default: N = size (FACT,2).

LDFACT — Leading dimension of FACT exactly as specified in the dimension statement of the calling program. (Input)
Default: LDFACT = size (FACT,1).

IPATH — Path indicator. (Input)
IPATH = 1 means the system $AX = B$ is solved.
IPATH = 2 means the system $A^T X = B$ is solved.
Default: IPATH = 1.

FORTRAN 90 Interface

Generic: CALL LFSRB (FACT, NLCA, NUCA, IPVT, B, X [, …])

Specific: The specific interface names are S_LFSRB and D_LFSRB.

FORTRAN 77 Interface

Single: CALL LFSRB (N, FACT, LDFACT, NLCA, NUCA, IPVT, B, IPATH, X)

Double: The double precision name is DLFSRB.

Description

Routine LFSRB computes the solution of a system of linear algebraic equations having a real banded coefficient matrix. To compute the solution, the coefficient matrix must first undergo an *LU* factorization. This may be done by calling either LFCRB or LFTRB. The solution to $Ax = b$ is found by solving the banded triangular systems $Ly = b$ and $Ux = y$. The forward elimination step consists of solving the system $Ly = b$ by applying the same permutations and elimination operations to b that were applied to the columns of A in the factorization routine. The backward substitution step consists of solving the banded triangular system $Ux = y$ for x.

LFSRB and LFIRB both solve a linear system given its *LU* factorization. LFIRB generally takes more time and produces a more accurate answer than LFSRB. Each iteration of the iterative refinement algorithm used by LFIRB calls LFSRB.

The underlying code is based on either LINPACK or LAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see *Using ScaLAPACK, LAPACK, LINPACK, and EISPACK* in the Introduction section of this manual.

Example

The inverse is computed for a real banded 4 × 4 matrix with one upper and one lower codiagonal. The input matrix is assumed to be well-conditioned, hence LFTRB is used rather than LFCRB.

```
      USE LFSRB_INT
      USE LFTRB_INT
      USE WRRRN_INT
!                                 Declare variables
      INTEGER    LDA, LDFACT, N, NLCA, NUCA
      PARAMETER  (LDA=3, LDFACT=4, N=4, NLCA=1, NUCA=1)
      INTEGER    IPVT(N)
      REAL       A(LDA,N), AINV(N,N), FACT(LDFACT,N), RJ(N)
!                                 Set values for A in band form
!                                 A = (  0.0  -1.0  -2.0   2.0)
!                                     (  2.0   1.0  -1.0   1.0)
```

```
!                                        ( -3.0   0.0   2.0   0.0)
!
      DATA A/0.0, 2.0, -3.0, -1.0, 1.0, 0.0, -2.0, -1.0, 2.0,&
            2.0, 1.0, 0.0/
!
      CALL LFTRB (A, NLCA, NUCA, FACT, IPVT)
!                                   Set up the columns of the identity
!                                   matrix one at a time in RJ
      RJ = 0.0E0
      DO 10  J=1, N
         RJ(J) = 1.0E0
!                                   RJ is the J-th column of the identity
!                                   matrix so the following LFSRB
!                                   reference places the J-th column of
!                                   the inverse of A in the J-th column
!                                   of AINV
         CALL LFSRB (FACT, NLCA, NUCA, IPVT, RJ, AINV(:,J))
         RJ(J) = 0.0E0
   10 CONTINUE
!                                   Print results
      CALL WRRRN ('AINV', AINV)
!
      END
```

Output

```
                AINV
          1        2        3        4
1  -1.000   -1.000    0.400   -0.800
2  -3.000   -2.000    0.800   -1.600
3   0.000    0.000   -0.200    0.400
4   0.000    0.000    0.400    0.200
```

LFIRB

more...

Uses iterative refinement to improve the solution of a real system of linear equations in band storage mode.

Required Arguments

A — (NUCA + NLCA + 1) by N array containing the N by N banded coefficient matrix in band storage mode. (Input)

NLCA — Number of lower codiagonals of A. (Input)

NUCA — Number of upper codiagonals of A. (Input)

FACT — (2 * NLCA + NUCA + 1) by N array containing the *LU* factorization of the matrix A as output from routines LFCRB/DLFCRB or LFTRB/DLFTRB. (Input)

IPVT — Vector of length N containing the pivoting information for the *LU* factorization of A as output from routine LFCRB/DLFCRB or LFTRB/DLFTRB. (Input)

B — Vector of length N containing the right-hand side of the linear system. (Input)

X — Vector of length N containing the solution to the linear system. (Output)

RES — Vector of length N containing the residual vector at the improved solution . (Output)

Optional Arguments

N — Number of equations. (Input)
Default: N = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

LDFACT — Leading dimension of FACT exactly as specified in the dimension statement of the calling program. (Input)
Default: LDFACT = size (FACT,1).

IPATH — Path indicator. (Input)
IPATH = 1 means the system $AX = B$ is solved.
IPATH = 2 means the system $A^T X = B$ is solved.
Default: IPATH =1.

FORTRAN 90 Interface

Generic: CALL LFIRB (A, NLCA, NUCA, FACT, IPVT, B, X, RES [, …])

Specific: The specific interface names are S_LFIRB and D_LFIRB.

FORTRAN 77 Interface

Single: CALL LFIRB (N, A, LDA, NLCA, NUCA, FACT, LDFACT, IPVT, B, IPATH, X, RES)

Double: The double precision name is DLFIRB.

Description

Routine LFIRB computes the solution of a system of linear algebraic equations having a real banded coefficient matrix. Iterative refinement is performed on the solution vector to improve the accuracy. Usually almost all of the digits in the solution are accurate, even if the matrix is somewhat ill-conditioned.

To compute the solution, the coefficient matrix must first undergo an *LU* factorization. This may be done by calling either LFCRB or LFTRB.

Iterative refinement fails only if the matrix is very ill-conditioned.

LFIRB and LFSRB both solve a linear system given its *LU* factorization. LFIRB generally takes more time and produces a more accurate answer than LFSRB. Each iteration of the iterative refinement algorithm used by LFIRB calls LFSRB.

Comments

Informational error

Type	Code	Description
3	2	The input matrix is too ill-conditioned for iterative refinement to be effective

Example

A set of linear systems is solved successively. The right-hand-side vector is perturbed after solving the system each of the first two times by adding 0.5 to the second element.

```
      USE LFIRB_INT
      USE LFCRB_INT
      USE UMACH_INT
      USE WRRRN_INT
!                                 Declare variables
      INTEGER    LDA, LDFACT, N, NLCA, NUCA, NOUT
      PARAMETER  (LDA=3, LDFACT=4, N=4, NLCA=1, NUCA=1)
      INTEGER    IPVT(N)
      REAL       A(LDA,N), B(N), FACT(LDFACT,N), RCOND, RES(N), X(N)
!                                 Set values for A in band form, and B
!
!                                 A = (  0.0  -1.0  -2.0   2.0)
!                                     (  2.0   1.0  -1.0   1.0)
!                                     ( -3.0   0.0   2.0   0.0)
!
!                                 B = (  3.0   5.0   7.0  -9.0)
!
      DATA A/0.0, 2.0, -3.0, -1.0, 1.0, 0.0, -2.0, -1.0, 2.0,&
            2.0, 1.0, 0.0/
      DATA B/3.0, 5.0, 7.0, -9.0/
!
      CALL LFCRB (A, NLCA, NUCA, FACT, IPVT, RCOND)
!                                 Print the reciprocal condition number
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) RCOND, 1.0E0/RCOND
!                                 Solve the three systems
      DO 10  J=1, 3
         CALL LFIRB (A, NLCA, NUCA, FACT, IPVT, B, X, RES)
!                                 Print results
         CALL WRRRN ('X', X, 1, N, 1)
!                                 Perturb B by adding 0.5 to B(2)
         B(2) = B(2) + 0.5E0
   10 CONTINUE
!
99999 FORMAT ('  RCOND = ',F5.3,/,'  L1 Condition number = ',F6.3)
      END
```

Output

```
RCOND < .07
L1 Condition number = 25.0
                X
    1       2       3       4
2.000   1.000  -5.000   1.000

                X
    1       2       3       4
1.500   0.000  -5.000   1.000

                X
    1       2       3       4
1.000  -1.000  -5.000   1.000
```

LFDRB

Computes the determinant of a real matrix in band storage mode given the *LU* factorization of the matrix.

Required Arguments

FACT — (2 * NLCA + NUCA + 1) by N array containing the *LU* factorization of the matrix A as output from routine LFTRB/DLFTRB or LFCRB/DLFCRB. (Input)

NLCA — Number of lower codiagonals of A. (Input)

NUCA — Number of upper codiagonals of A. (Input)

IPVT — Vector of length N containing the pivoting information for the *LU* factorization as output from routine LFTRB/DLFTRB or LFCRB/DLFCRB. (Input)

DET1 — Scalar containing the mantissa of the determinant. (Output)
The value DET1 is normalized so that 1.0 ≤ |DET1| < 10.0 or DET1 = 0.0.

DET2 — Scalar containing the exponent of the determinant. (Output)
The determinant is returned in the form det(*A*) = DET1 * 10^{DET2}.

Optional Arguments

N — Order of the matrix. (Input)
Default: N = size (FACT,2).

LDFACT — Leading dimension of FACT exactly as specified in the dimension statement of the calling program. (Input)
Default: LDFACT = size (FACT,1).

FORTRAN 90 Interface

Generic: CALL LFDRB (FACT, NLCA, NUCA, IPVT, DET1, DET2 [, …])

Specific: The specific interface names are S_LFDRB and D_LFDRB.

FORTRAN 77 Interface

Single: CALL LFDRB (N, FACT, LDFACT, NLCA, NUCA, IPVT, DET1, DET2)

Double: The double precision name is DLFDRB.

Description

Routine LFDRB computes the determinant of a real banded coefficient matrix. To compute the determinant, the coefficient matrix must first undergo an *LU* factorization. This may be done by calling either LFCRB or LFTRB. The formula det *A* = det *L* det *U* is used to compute the determinant. Since the determinant of a triangular matrix is the product of the diagonal elements,

$$\det U = \prod_{i=1}^{N} U_{ii}$$

(The matrix *U* is stored in the upper NUCA + NLCA + 1 rows of FACT as a banded matrix.) Since *L* is the product of triangular matrices with unit diagonals and of permutation matrices, det $L = (-1)^k$, where *k* is the number of pivoting interchanges.

LFDRB is based on the LINPACK routine CGBDI; see Dongarra et al. (1979).

Example

The determinant is computed for a real banded 4 × 4 matrix with one upper and one lower codiagonal.

```
      USE LFDRB_INT
      USE LFTRB_INT
      USE UMACH_INT
!                                 Declare variables
      INTEGER    LDA, LDFACT, N, NLCA, NUCA, NOUT
      PARAMETER  (LDA=3, LDFACT=4, N=4, NLCA=1, NUCA=1)
      INTEGER    IPVT(N)
      REAL       A(LDA,N), DET1, DET2, FACT(LDFACT,N)
!                                 Set values for A in band form
!                                 A = (  0.0  -1.0  -2.0   2.0)
!                                     (  2.0   1.0  -1.0   1.0)
!                                     ( -3.0   0.0   2.0   0.0)
!
      DATA A/0.0, 2.0, -3.0, -1.0, 1.0, 0.0, -2.0, -1.0, 2.0,&
            2.0, 1.0, 0.0/
!
      CALL LFTRB (A, NLCA, NUCA, FACT, IPVT)
!                                 Compute the determinant
      CALL LFDRB (FACT, NLCA, NUCA, IPVT, DET1, DET2)
!                                 Print the results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) DET1, DET2
99999 FORMAT (' The determinant of A is ', F6.3, ' * 10**', F2.0)
      END
```

Output

```
The determinant of A is  5.000 * 10**0.
```

LSAQS

Solves a real symmetric positive definite system of linear equations in band symmetric storage mode with iterative refinement.

Required Arguments

A — NCODA + 1 by N array containing the N by N positive definite band coefficient matrix in band symmetric storage mode. (Input)

NCODA — Number of upper codiagonals of A. (Input)

B — Vector of length N containing the right-hand side of the linear system. (Input)

X — Vector of length N containing the solution to the linear system. (Output)

Optional Arguments

N — Number of equations. (Input)
Default: N = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

FORTRAN 90 Interface

Generic: CALL LSAQS (A, NCODA, B, X [, …])

Specific: The specific interface names are S_LSAQS and D_LSAQS.

FORTRAN 77 Interface

Single: CALL LSAQS (N, A, LDA, NCODA, B, X)

Double: The double precision name is DLSAQS.

Description

Routine LSAQS solves a system of linear algebraic equations having a real symmetric positive definite band coefficient matrix. It first uses the routine LFCQS to compute an $R^T R$ Cholesky factorization of the coefficient matrix and to estimate the condition number of the matrix. R is an upper triangular band matrix. The solution of the linear system is then found using the iterative refinement routine LFIQS.

LSAQS fails if any submatrix of R is not positive definite, if R has a zero diagonal element or if the iterative refinement algorithm fails to converge. These errors occur only if A is very close to a singular matrix or to a matrix which is not positive definite.

If the estimated condition number is greater than $1/\varepsilon$ (where ε is machine precision), a warning error is issued. This indicates that very small changes in A can cause very large changes in the solution x. Iterative refinement can sometimes find the solution to such a system. LSAQS solves the problem that is represented in the computer; however, this problem may differ from the problem whose solution is desired.

Comments

1. Workspace may be explicitly provided, if desired, by use of L2AQS/DL2AQS. The reference is:

   CALL L2AQS (N, A, LDA, NCODA, B, X, FACT, WK)

   The additional arguments are as follows:

   FACT — Work vector of length NCODA + 1 by N containing the $R^T R$ factorization of A in band symmetric storage form on output.

   WK — Work vector of length N.

2. Informational errors

Type	Code	Description
3	1	The input matrix is too ill-conditioned. The solution might not be accurate.
4	2	The input matrix is not positive definite.

3. *Integer Options* with *Chapter 11* Options Manager

   16 This option uses four values to solve memory bank conflict (access inefficiency) problems. In routine L2AQS the leading dimension of FACT is increased by IVAL(3) when N is a multiple of IVAL(4). The values IVAL(3) and IVAL(4) are temporarily replaced by IVAL(1) and IVAL(2), respectively, in LSAQS. Additional memory allocation for FACT and option value restoration are done automatically in LSAQS.

Users directly calling L2AQS can allocate additional space for FACT and set IVAL(3) and IVAL(4) so that memory bank conflicts no longer cause inefficiencies. There is no requirement that users change existing applications that use LSAQS or L2AQS. Default values for the option are IVAL(*) = 1, 16, 0, 1.

17 This option has two values that determine if the L_1 condition number is to be computed. Routine LSAQS temporarily replaces IVAL(2) by IVAL(1). The routine L2CQS computes the condition number if IVAL(2) = 2. Otherwise L2CQS skips this computation. LSAQS restores the option. Default values for the option are IVAL(*) = 1,2.

Example

A system of four linear equations is solved. The coefficient matrix has real positive definite band form, and the right-hand-side vector b has four elements.

```
      USE LSAQS_INT
      USE WRRRN_INT
!                                 Declare variables
      INTEGER    LDA, N, NCODA
      PARAMETER  (LDA=3, N=4, NCODA=2)
      REAL       A(LDA,N), B(N), X(N)
!
!                     Set values for A in band symmetric form, and B
!
!                                 A = (  0.0   0.0  -1.0   1.0 )
!                                     (  0.0   0.0   2.0  -1.0 )
!                                     (  2.0   4.0   7.0   3.0 )
!
!                                 B = (  6.0 -11.0 -11.0  19.0 )
!
      DATA A/2*0.0, 2.0, 2*0.0, 4.0, -1.0, 2.0, 7.0, 1.0, -1.0, 3.0/
      DATA B/6.0, -11.0, -11.0, 19.0/
!                                 Solve A*X = B
      CALL LSAQS (A, NCODA, B, X)
!                                 Print results
      CALL WRRRN ('X', X, 1, N, 1)
!
      END
```

Output

```
                   X
     1        2        3        4
   4.000   -6.000    2.000    9.000
```

LSLQS

Solves a real symmetric positive definite system of linear equations in band symmetric storage mode without iterative refinement.

Required Arguments

A — `NCODA` + 1 by `N` array containing the `N` by `N` positive definite band symmetric coefficient matrix in band symmetric storage mode. (Input)

NCODA — Number of upper codiagonals of `A`. (Input)

B — Vector of length `N` containing the right-hand side of the linear system. (Input)

X — Vector of length `N` containing the solution to the linear system. (Output)

Optional Arguments

N — Number of equations. (Input)
Default: `N` = size (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = size (`A`,1).

FORTRAN 90 Interface

Generic: `CALL LSLQS (A, NCODA, B, X [, …])`

Specific: The specific interface names are `S_LSLQS` and `D_LSLQS`.

FORTRAN 77 Interface

Single: `CALL LSLQS (N, A, LDA, NCODA, B, X)`

Double: The double precision name is `DLSLQS`.

Description

Routine LSLQS solves a system of linear algebraic equations having a real symmetric positive definite band coefficient matrix. It first uses the routine LFCQS to compute an R^TR Cholesky factorization of the coefficient matrix and to estimate the condition number of the matrix. *R* is an upper triangular band matrix. The solution of the linear system is then found using the routine LFSQS.

LSLQS fails if any submatrix of *R* is not positive definite or if *R* has a zero diagonal element. These errors occur only if *A* is very close to a singular matrix or to a matrix which is not positive definite.

If the estimated condition number is greater than $1/\varepsilon$ (where ε is machine precision), a warning error is issued. This indicates that very small changes in *A* can cause very large changes in the solution *x*. If the coefficient matrix is ill-conditioned or poorly scaled, it is recommended that LSAQS be used.

Comments

1. Workspace may be explicitly provided, if desired, by use of L2LQS/DL2LQS. The reference is:

   CALL L2LQS (N, A, LDA, NCODA, B, X, FACT, WK)

   The additional arguments are as follows:

   FACT — NCODA + 1 by N work array containing the R^TR factorization of A in band symmetric form on output. If A is not needed, A and FACT can share the same storage locations.

   WK — Work vector of length N.

2. Informational errors

Type	Code	Description
3	1	The input matrix is too ill-conditioned. The solution might not be accurate.
4	2	The input matrix is not positive definite.

3. *Integer Options* with *Chapter 11* Options Manager

   16 This option uses four values to solve memory bank conflict (access inefficiency) problems. In routine L2LQS the leading dimension of FACT is increased by IVAL(3) when N is a multiple of IVAL(4). The values IVAL(3) and IVAL(4) are temporarily replaced by IVAL(1) and IVAL(2), respectively, in LSLQS. Additional memory allocation for FACT and option value restoration are done automatically in LSLQS. Users directly calling L2LQS can allocate additional space for FACT and set IVAL(3) and IVAL(4) so that memory bank conflicts no longer cause inefficiencies. There is no requirement that users change existing applications that use LSLQS or L2LQS. Default values for the option are IVAL(*) = 1,16,0,1.

17 This option has two values that determine if the L_1 condition number is to be computed. Routine LSLQS temporarily replaces IVAL(2) by IVAL(1). The routine L2CQS computes the condition number if IVAL(2) = 2. Otherwise L2CQS skips this computation. LSLQS restores the option. Default values for the option are IVAL(*) = 1,2.

Example

A system of four linear equations is solved. The coefficient matrix has real positive definite band form and the right-hand-side vector *b* has four elements.

```
      USE LSLQS_INT
      USE WRRRN_INT
!                                 Declare variables
      INTEGER    LDA, N, NCODA
      PARAMETER  (LDA=3, N=4, NCODA=2)
      REAL       A(LDA,N), B(N), X(N)
!
!                       Set values for A in band symmetric form, and B
!
!                                 A = (  0.0   0.0  -1.0   1.0 )
!                                     (  0.0   0.0   2.0  -1.0 )
!                                     (  2.0   4.0   7.0   3.0 )
!
!                                 B = (  6.0 -11.0 -11.0  19.0 )
!
      DATA A/2*0.0, 2.0, 2*0.0, 4.0, -1.0, 2.0, 7.0, 1.0, -1.0, 3.0/
      DATA B/6.0, -11.0, -11.0, 19.0/
!                                 Solve A*X = B
      CALL LSLQS (A, NCODA, B, X)


!                                 Print results
      CALL WRRRN ('X', X, 1, N, 1)
      END
```

Output

```
                X
       1        2        3        4
   4.000   -6.000    2.000    9.000
```

LSLPB

Computes the $R^T DR$ Cholesky factorization of a real symmetric positive definite matrix *A* in codiagonal band symmetric storage mode. Solve a system $Ax = b$.

Required Arguments

A — Array containing the N by N positive definite band coefficient matrix and right hand side in codiagonal band symmetric storage mode. (Input/Output)
The number of array columns must be at least NCODA + 2. The number of column is not an input to this subprogram.

On output, A contains the solution and factors. See Comments section for details.

NCODA — Number of upper codiagonals of matrix A. (Input)
Must satisfy NCODA ≥ 0 and NCODA < N.

U — Array of flags that indicate any singularities of A, namely loss of positive-definiteness of a leading minor. (Output)
A value U(I) = 0. means that the leading minor of dimension I is not positive-definite. Otherwise, U(I) = 1.

Optional Arguments

N — Order of the matrix. (Input)
Must satisfy N > 0.
Default: N = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Must satisfy LDA ≥ N + NCODA.
Default: LDA = size (A,1).

IJOB — Flag to direct the desired factorization or solving step. (Input)
Default: IJOB = 1.

IJOBMeaning

1 factor the matrix A and solve the system Ax = b, where b is stored in column NCODA + 2 of array A. The vector x overwrites b in storage.

2 solve step only. Use *b* as column NCODA + 2 of A. (The factorization step has already been done.) The vector *x* overwrites *b* in storage.

3 factor the matrix A but do not solve a system.

4,5,6 same meaning as with the value IJOB – 3. For efficiency, no error checking is done on values LDA, N, NCODA, and U(*).

FORTRAN 90 Interface

Generic: CALL LSLPB (A, NCODA, U [, …])

Specific: The specific interface names are S_LSLPB and D_LSLPB.

FORTRAN 77 Interface

Single: CALL LSLPB (N, A, LDA, NCODA, IJOB, U)

Double: The double precision name is DLSLPB.

Description

Routine LSLPB factors and solves the symmetric positive definite banded linear system $Ax = b$. The matrix is factored so that $A = R^T DR$, where R is unit upper triangular and D is diagonal. The reciprocals of the diagonal entries of D are computed and saved to make the solving step more efficient. Errors will occur if D has a non-positive diagonal element. Such events occur only if A is very close to a singular matrix or is not positive definite.

LSLPB is efficient for problems with a small band width. The particular cases NCODA = 0, 1, 2 are done with special loops within the code. These cases will give good performance. See Hanson (1989) for details. When solving tridiagonal systems, NCODA = 1, the cyclic reduction code LSLCR should be considered as an alternative. The expectation is that LSLCR will outperform LSLPB on vector or parallel computers. It may be inferior on scalar computers or even parallel computers with non-optimizing compilers.

Comments

1. Workspace may be explicitly provided, if desired, by use of L2LPB/DL2LPB. The reference is:

   CALL L2LPB (N, A, LDA, NCODA, IJOB, U, WK)

   The additional argument is:

   WK — Work vector of length NCODA.

2. If IJOB=1, 3, 4, or 6, A contains the factors R and D on output. These are stored in codiagonal band symmetric storage mode. Column 1 of A contains the reciprocal of diagonal matrix D. Columns 2 through NCODA+1 contain the upper diagonal values for upper unit diagonal matrix R. If IJOB=1,2, 4, or 5, the last column of A contains the solution on output, replacing b.

3. Informational error

Type	Code	Description
4	2	The input matrix is not positive definite.

Example

A system of four linear equations is solved. The coefficient matrix has real positive definite codiagonal band form and the right-hand-side vector *b* has four elements.

```
      USE LSLPB_INT
      USE WRRRN_INT
!                                  Declare variables
      INTEGER LDA, N, NCODA
      PARAMETER (N=4, NCODA=2, LDA=N+NCODA)
!
      INTEGER IJOB
      REAL A(LDA,NCODA+2), U(N)
      REAL R(N,N), RT(N,N), D(N,N), WK(N,N), AA(N,N)!!
!
!                                  Set values for A and right side in
!                                  codiagonal band symmetric form:
!
!                             A    =    (  *     *      *       * )
!                                       (  *     *      *       * )
!                                       (2.0     *      *      6.0)
!                                       (4.0    0.0     *    -11.0)
!                                       (7.0    2.0   -1.0   -11.0)
!                                       (3.0   -1.0    1.0    19.0)
!
      DATA ((A(I+NCODA,J),I=1,N),J=1,NCODA+2)/2.0, 4.0, 7.0, 3.0, 0.0,&
      0.0, 2.0, -1.0, 0.0, 0.0, -1.0, 1.0, 6.0, -11.0, -11.0,&
      19.0/
      DATA R/16*0.0/, D/16*0.0/, RT/16*0.0/
!                                  Factor and solve A*x = b.
      CALL LSLPB(A, NCODA, U)
!                                  Print results
      CALL WRRRN ('X', A((NCODA+1):,(NCODA+2):), NRA=1, NCA=N, LDA=1)

      END
```

Output

```
                 X
       1        2        3        4
   4.000   -6.000    2.000    9.000
```

LFCQS

Computes the $R^T R$ Cholesky factorization of a real symmetric positive definite matrix in band symmetric storage mode and estimate its L_1condition number.

Required Arguments

A — NCODA + 1 by N array containing the N by N positive definite band coefficient matrix in band symmetric storage mode to be factored. (Input)

NCODA — Number of upper codiagonals of A. (Input)

FACT — NCODA + 1 by N array containing the $R^T R$ factorization of the matrix A in band symmetric form. (Output)
If A is not needed, A and FACT can share the same storage locations.

RCOND — Scalar containing an estimate of the reciprocal of the L_1condition number of A. (Output)

Optional Arguments

N — Order of the matrix. (Input)
Default: N = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

LDFACT — Leading dimension of FACT exactly as specified in the dimension statement of the calling program. (Input)
Default: LDFACT = size (FACT,1).

FORTRAN 90 Interface

Generic: CALL LFCQS (A, NCODA, FACT, RCOND [, …])

Specific: The specific interface names are S_LFCQS and D_LFCQS.

FORTRAN 77 Interface

Single: CALL LFCQS (N, A, LDA, NCODA, FACT, LDFACT, RCOND)

Double: The double precision name is DLFCQS.

Description

Routine LFCQS computes an R^TR Cholesky factorization and estimates the condition number of a real symmetric positive definite band coefficient matrix. R is an upper triangular band matrix.

The L_1condition number of the matrix A is defined to be $\kappa(A) = \|A\|_1 \|A^{-1}\|_1$. Since it is expensive to compute $\|A^{-1}\|_1$, the condition number is only estimated. The estimation algorithm is the same as used by LINPACK and is described by Cline et al. (1979).

If the estimated condition number is greater than $1/\varepsilon$ (where ε is machine precision), a warning error is issued. This indicates that very small changes in A can cause very large changes in the solution x. Iterative refinement can sometimes find the solution to such a system.

LFCQS fails if any submatrix of R is not positive definite or if R has a zero diagonal element. These errors occur only if A is very close to a singular matrix or to a matrix which is not positive definite.

The R^TR factors are returned in a form that is compatible with routines LFIQS, LFSQS and LFDQS. To solve systems of equations with multiple right-hand-side vectors, use LFCQS followed by either LFIQS or LFSQS called once for each right-hand side. The routine LFDQS can be called to compute the determinant of the coefficient matrix after LFCQS has performed the factorization.

LFCQS is based on the LINPACK routine SPBCO; see Dongarra et al. (1979).

Comments

1. Workspace may be explicitly provided, if desired, by use of L2CQS/DL2CQS. The reference is:

   ```
   CALL L2CQS (N, A, LDA, NCODA, FACT, LDFACT, RCOND, WK)
   ```

   The additional argument is:

   WK — Work vector of length N.

2. Informational errors

Type	Code	Description
3	3	The input matrix is algorithmically singular.
4	2	The input matrix is not positive definite.

Example

The inverse of a 4 × 4 symmetric positive definite band matrix with one codiagonal is computed. LFCQS is called to factor the matrix and to check for nonpositive definiteness or ill-conditioning. LFIQS is called to determine the columns of the inverse.

```
      USE LFCQS_INT
      USE LFIQS_INT
      USE UMACH_INT
      USE WRRRN_INT
!                                 Declare variables
      INTEGER    LDA, LDFACT, N, NCODA, NOUT
      PARAMETER  (LDA=2, LDFACT=2, N=4, NCODA=1)
      REAL       A(LDA,N), AINV(N,N), RCOND, FACT(LDFACT,N),&
                RES(N), RJ(N)
!
!                              Set values for A in band symmetric form
!
!                                 A = (  0.0   1.0   1.0   1.0 )
!                                     (  2.0   2.5   2.5   2.0 )
!
      DATA A/0.0, 2.0, 1.0, 2.5, 1.0, 2.5, 1.0, 2.0/
!                                 Factor the matrix A
      CALL LFCQS (A, NCODA, FACT, RCOND)
!                                 Set up the columns of the identity
!                                 matrix one at a time in RJ
      RJ = 0.0E0
      DO 10  J=1, N
         RJ(J) = 1.0E0
!                                 RJ is the J-th column of the identity
!                                 matrix so the following LFIQS
!                                 reference places the J-th column of
!                                 the inverse of A in the J-th column
!                                 of AINV
         CALL LFIQS (A, NCODA, FACT, RJ, AINV(:,J), RES)
         RJ(J) = 0.0E0
   10 CONTINUE
!                                 Print the results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) RCOND, 1.0E0/RCOND
      CALL WRRRN ('AINV', AINV)
99999 FORMAT ('  RCOND = ',F5.3,/,'  L1 Condition number = ',F6.3)
      END
```

Output

```
RCOND = 0.160
L1 Condition number =  6.239
                 AINV
          1         2         3         4
    1   0.6667   -0.3333    0.1667   -0.0833
    2  -0.3333    0.6667   -0.3333    0.1667
    3   0.1667   -0.3333    0.6667   -0.3333
    4  -0.0833    0.1667   -0.3333    0.6667
```

LFTQS

Computes the $R^T R$ Cholesky factorization of a real symmetric positive definite matrix in band symmetric storage mode.

Required Arguments

A — NCODA + 1 by N array containing the N by N positive definite band coefficient matrix in band symmetric storage mode to be factored. (Input)

NCODA — Number of upper codiagonals of A. (Input)

FACT — NCODA + 1 by N array containing the $R^T R$ factorization of the matrix A. (Output)
If A s not needed, A and FACT can share the same storage locations.

Optional Arguments

N — Order of the matrix. (Input)
Default: N = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

LDFACT — Leading dimension of FACT exactly as specified in the dimension statement of the calling program. (Input)
Default: LDFACT = size (FACT,1).

FORTRAN 90 Interface

Generic: CALL LFTQS (A, NCODA, FACT [, …])

Specific: The specific interface names are S_LFTQS and D_LFTQS.

FORTRAN 77 Interface

Single: CALL LFTQS (N, A, LDA, NCODA, FACT, LDFACT)

Double: The double precision name is DLFTQS.

Description

Routine LFTQS computes an $R^T R$ Cholesky factorization of a real symmetric positive definite band coefficient matrix. R is an upper triangular band matrix.

LFTQS fails if any submatrix of R is not positive definite or if R has a zero diagonal element. These errors occur only if A is very close to a singular matrix or to a matrix which is not positive definite.

The $R^T R$ factors are returned in a form that is compatible with routines LFIQS, LFSQS and LFDQS. To solve systems of equations with multiple right hand-side vectors, use LFTQS followed by either LFIQS or LFSQS called once for each right-hand side. The routine LFDQS can be called to compute the determinant of the coefficient matrix after LFTQS has performed the factorization.

LFTQS is based on the LINPACK routine CPBFA; see Dongarra et al. (1979).

Comments

Informational error

Type	Code	Description
4	2	The input matrix is not positive definite.

Example

The inverse of a 3 × 3 matrix is computed. LFTQS is called to factor the matrix and to check for nonpositive definiteness. LFSQS is called to determine the columns of the inverse.

```
      USE LFTQS_INT
      USE WRRRN_INT
      USE LFSQS_INT
!                                 Declare variables
      INTEGER    LDA, LDFACT, N, NCODA
      PARAMETER  (LDA=2, LDFACT=2, N=4, NCODA=1)
      REAL       A(LDA,N), AINV(N,N), FACT(LDFACT,N), RJ(N)
!
!                              Set values for A in band symmetric form
!
!                                 A = (  0.0   1.0   1.0   1.0 )
!                                     (  2.0   2.5   2.5   2.0 )
!
      DATA A/0.0, 2.0, 1.0, 2.5, 1.0, 2.5, 1.0, 2.0/
!                                 Factor the matrix A
      CALL LFTQS (A, NCODA, FACT)
!                                 Set up the columns of the identity
!                                 matrix one at a time in RJ
      RJ = 0.0E0
      DO 10  J=1, N
         RJ(J) = 1.0E0
!                                 RJ is the J-th column of the identity
```

```
!                                  matrix so the following LFSQS
!                                  reference places the J-th column of
!                                  the inverse of A in the J-th column
!                                  of AINV
         CALL LFSQS (FACT, NCODA, RJ, AINV(:,J))
         RJ(J) = 0.0E0
   10 CONTINUE
!                                  Print the results
      CALL WRRRN ('AINV', AINV, ITRING=1)
      END
```

Output

```
                 AINV
          1         2         3         4
1    0.6667   -0.3333    0.1667   -0.0833
2              0.6667   -0.3333    0.1667
3                        0.6667   -0.3333
4                                  0.6667
```

LFSQS

Solves a real symmetric positive definite system of linear equations given the factorization of the coefficient matrix in band symmetric storage mode.

Required Arguments

FACT — NCODA + 1 by N array containing the $R^T R$ factorization of the positive definite band matrix A in band symmetric storage mode as output from subroutine LFCQS/DLFCQS or LFTQS/DLFTQS. (Input)

NCODA — Number of upper codiagonals of A. (Input)

B — Vector of length N containing the right-hand side of the linear system. (Input)

X — Vector of length N containing the solution to the linear system. (Output)
If B is not needed, B and X an share the same storage locations.

Optional Arguments

N — Number of equations. (Input)
Default: N = size (FACT,2).

LDFACT — Leading dimension of FACT exactly as specified in the dimension statement of the calling program. (Input)
Default: LDFACT = size (FACT,1).

FORTRAN 90 Interface

Generic: CALL LFSQS (FACT, NCODA, B, X [, …])

Specific: The specific interface names are S_LFSQS and D_LFSQS.

FORTRAN 77 Interface

Single: CALL LFSQS (N, FACT, LDFACT, NCODA, B, X)

Double: The double precision name is DLFSQS.

Description

Routine LFSQS computes the solution for a system of linear algebraic equations having a real symmetric positive definite band coefficient matrix. To compute the solution, the coefficient matrix must first undergo an $R^T R$ factorization. This may be done by calling either LFCQS or LFTQS. R is an upper triangular band matrix.

The solution to $Ax = b$ is found by solving the triangular systems $R^T y = b$ and $Rx = y$.

LFSQS and LFIQS both solve a linear system given its $R^T R$ factorization. LFIQS generally takes more time and produces a more accurate answer than LFSQS. Each iteration of the iterative refinement algorithm used by LFIQS calls LFSQS.

LFSQS is based on the LINPACK routine SPBSL; see Dongarra et al. (1979).

Comments

Informational error

Type	Code	Description
4	1	The factored matrix is singular.

Example

A set of linear systems is solved successively. LFTQS is called to factor the coefficient matrix. LFSQS is called to compute the four solutions for the four right-hand sides. In this case the coefficient matrix is assumed to be well-conditioned and correctly scaled. Otherwise, it would be better to call LFCQS to perform the factorization, and LFIQS to compute the solutions.

```
      USE LFSQS_INT
      USE LFTQS_INT
      USE WRRRN_INT
!                                 Declare variables
      INTEGER    LDA, LDFACT, N, NCODA
      PARAMETER  (LDA=3, LDFACT=3, N=4, NCODA=2)
      REAL       A(LDA,N), B(N,4), FACT(LDFACT,N), X(N,4)
!
!
!                   Set values for A in band symmetric form, and B
!
!                                 A = (  0.0   0.0  -1.0   1.0 )
!                                     (  0.0   0.0   2.0  -1.0 )
!                                     (  2.0   4.0   7.0   3.0 )
!
!                                 B = (  4.0  -3.0   9.0  -1.0 )
!                                     (  6.0  10.0  29.0   3.0 )
!                                     ( 15.0  12.0  11.0   6.0 )
!                                     ( -7.0   1.0  14.0   2.0 )
!
```

```
      DATA A/2*0.0, 2.0, 2*0.0, 4.0, -1.0, 2.0, 7.0, 1.0, -1.0, 3.0/
      DATA B/4.0, 6.0, 15.0, -7.0, -3.0, 10.0, 12.0, 1.0, 9.0, 29.0,&
            11.0, 14.0, -1.0, 3.0, 6.0, 2.0/
!                                 Factor the matrix A
      CALL LFTQS (A, NCODA, FACT)
!                                 Compute the solutions
      DO 10  I=1, 4
         CALL LFSQS (FACT, NCODA, B(:,I), X(:,I))
   10 CONTINUE
!                                 Print solutions
      CALL WRRRN ('X', X)
!
      END
```

Output

```
                X
        1        2        3        4
1   3.000   -1.000    5.000    0.000
2   1.000    2.000    6.000    0.000
3   2.000    1.000    1.000    1.000
4  -2.000    0.000    3.000    1.000
```

LFIQS

Uses iterative refinement to improve the solution of a real symmetric positive definite system of linear equations in band symmetric storage mode.

Required Arguments

A — NCODA + 1 by N array containing the N by N positive definite band coefficient matrix in band symmetric storage mode. (Input)

NCODA — Number of upper codiagonals of A. (Input)

FACT — NCODA + 1 by N array containing the $R^T R$ factorization of the matrix A from routine LFCQS/DLFCQS or LFTQS/DLFTQS. (Input)

B — Vector of length N containing the right-hand side of the linear system. (Input)

X — Vector of length N containing the solution to the system. (Output)

RES — Vector of length N containing the residual vector at the improved solution. (Output)

Optional Arguments

N — Number of equations. (Input)
Default: N = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

LDFACT — Leading dimension of FACT exactly as specified in the dimension statement of the calling program. (Input)
Default: LDFACT = size (FACT,1).

FORTRAN 90 Interface

Generic: CALL LFIQS (A, NCODA, FACT, B, X, RES [, …])

Specific: The specific interface names are S_LFIQS and D_LFIQS.

FORTRAN 77 Interface

Single: CALL LFIQS (N, A, LDA, NCODA, FACT, LDFACT, B, X, RES)

Double: The double precision name is DLFIQS.

Description

Routine LFIQS computes the solution of a system of linear algebraic equations having a real symmetric positive-definite band coefficient matrix. Iterative refinement is performed on the solution vector to improve the accuracy. Usually almost all of the digits in the solution are accurate, even if the matrix is somewhat ill-conditioned.

To compute the solution, the coefficient matrix must first undergo an $R^T R$ factorization. This may be done by calling either IMSL routine LFCQS or LFTQS.

Iterative refinement fails only if the matrix is very ill-conditioned.

LFIQS and LFSQS both solve a linear system given its $R^T R$ factorization. LFIQS generally takes more time and produces a more accurate answer than LFSQS. Each iteration of the iterative refinement algorithm used by LFIQS calls LFSQS.

Comments

Informational error

Type	Code	Description
3	4	The input matrix is too ill-conditioned for iterative refinement to be effective.

Example

A set of linear systems is solved successively. The right-hand-side vector is perturbed after solving the system each of the first two times by adding 0.5 to the second element.

```
      USE LFIQS_INT
      USE UMACH_INT
      USE LFCQS_INT
      USE WRRRN_INT
!                                 Declare variables
      INTEGER    LDA, LDFACT, N, NCODA, NOUT
      PARAMETER  (LDA=2, LDFACT=2, N=4, NCODA=1)
      REAL       A(LDA,N), B(N), RCOND, FACT(LDFACT,N), RES(N,3),&
                X(N,3)
!
!                       Set values for A in band symmetric form, and B
!
!                                 A = (  0.0   1.0   1.0   1.0 )
```

```
!                                    (  2.0   2.5   2.5   2.0 )
!
!                               B = (  3.0   5.0   7.0   4.0 )
!
      DATA A/0.0, 2.0, 1.0, 2.5, 1.0, 2.5, 1.0, 2.0/
      DATA B/3.0, 5.0, 7.0, 4.0/
!                               Factor the matrix A
      CALL LFCQS (A, NCODA, FACT, RCOND)
!                               Print the estimated condition number
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) RCOND, 1.0E0/RCOND
!                               Compute the solutions
      DO 10  I=1, 3
         CALL LFIQS (A, NCODA, FACT, B, X(:,I), RES(:,I))
         B(2) = B(2) + 0.5E0
   10 CONTINUE
!                               Print solutions and residuals
      CALL WRRRN ('X', X)
      CALL WRRRN ('RES', RES)
99999 FORMAT ('  RCOND = ',F5.3,/,'  L1 Condition number = ',F6.3)
      END
```

Output

```
RCOND = 0.160
L1 Condition number =  6.239
             X
        1       2       3
1   1.167   1.000   0.833
2   0.667   1.000   1.333
3   2.167   2.000   1.833
4   0.917   1.000   1.083
                 RES
            1           2           3
1   7.947E-08   0.000E+00   9.934E-08
2   7.947E-08   0.000E+00   3.974E-08
3   7.947E-08   0.000E+00   1.589E-07
4  -3.974E-08   0.000E+00  -7.947E-08
```

LFDQS

Computes the determinant of a real symmetric positive definite matrix given the $R^T R$ Cholesky factorization of the matrix in band symmetric storage mode.

Required Arguments

FACT — NCODA + 1 by N array containing the $R^T R$ factorization of the positive definite band matrix, A, in band symmetric storage mode as output from subroutine LFCQS/DLFCQS or LFTQS/DLFTQS. (Input)

NCODA — Number of upper codiagonals of A. (Input)

DET1 — Scalar containing the mantissa of the determinant. (Output)
The value DET1 is normalized so that 1.0 ≤ |DET1| < 10.0 or DET1 = 0.0.

DET2 — Scalar containing the exponent of the determinant. (Output)
The determinant is returned in the form det(A) = DET1 * 10^{DET2}.

Optional Arguments

N — Number of equations. (Input)
Default: N = size (FACT,2).

LDFACT — Leading dimension of FACT exactly as specified in the dimension statement of the calling program. (Input)
Default: LDFACT = size (FACT,1).

FORTRAN 90 Interface

Generic: CALL LFDQS (FACT, NCODA, DET1, DET2 [, …])

Specific: The specific interface names are S_LFDQS and D_LFDQS.

FORTRAN 77 Interface

Single: CALL LFDQS (N, FACT, LDFACT, NCODA, DET1, DET2)

Double: The double precision name is DLFDQS.

Description

Routine LFDQS computes the determinant of a real symmetric positive-definite band coefficient matrix. To compute the determinant, the coefficient matrix must first undergo an $R^T R$ factorization. This may be done by calling either IMSL routine LFCQS or LFTQS. The formula

$\det A = \det R^T \det R = (\det R)^2$ is used to compute the determinant. Since the determinant of a triangular matrix is the product of the diagonal elements,

$$\det R = \prod_{i=1}^{N} R_{ii}$$

LFDQS is based on the LINPACK routine SPBDI; see Dongarra et al. (1979).

Example

The determinant is computed for a real positive definite 4 × 4 matrix with 2 codiagonals.

```
      USE LFDQS_INT
      USE LFTQS_INT
      USE UMACH_INT
!                                 Declare variables
      INTEGER    LDA, LDFACT, N, NCODA, NOUT
      PARAMETER  (LDA=3, N=4, LDFACT=3, NCODA=2)
      REAL       A(LDA,N), DET1, DET2, FACT(LDFACT,N)
!
!                     Set values for A in band symmetric form
!
!                                 A = (  0.0   0.0   1.0  -2.0 )
!                                     (  0.0   2.0   1.0   3.0 )
!                                     (  7.0   6.0   6.0   8.0 )
!
      DATA A/2*0.0, 7.0, 0.0, 2.0, 6.0, 1.0, 1.0, 6.0, -2.0, 3.0, 8.0/
!                                 Factor the matrix
      CALL LFTQS (A, NCODA, FACT)
!                                 Compute the determinant
      CALL LFDQS (FACT, NCODA, DET1, DET2)
!                                 Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) DET1, DET2
!
99999 FORMAT (' The determinant of A is ',F6.3,' * 10**',F2.0)
      END
```

Output

```
The determinant of A is 1.186 * 10**3.
```

LSLTQ

Solves a complex tridiagonal system of linear equations.

Required Arguments

C — Complex vector of length N containing the subdiagonal of the tridiagonal matrix in C(2) through C(N). (Input/Output)
On output C is destroyed.

D — Complex vector of length N containing the diagonal of the tridiagonal matrix. (Input/Output)
On output D is destroyed.

E — Complex vector of length N containing the superdiagonal of the tridiagonal matrix in E(1) through E(N − 1). (Input/Output)
On output E is destroyed.

B — Complex vector of length N containing the right-hand side of the linear system on entry and the solution vector on return. (Input/Output)

Optional Arguments

N — Order of the tridiagonal matrix. (Input)
Default: N = size (C,1).

FORTRAN 90 Interface

Generic: `CALL LSLTQ (C, D, E, B [, …])`

Specific: The specific interface names are `S_LSLTQ` and `D_LSLTQ`.

FORTRAN 77 Interface

Single: `CALL LSLTQ (N, C, D, E, B)`

Double: The double precision name is `DLSLTQ`.

Description

Routine `LSLTQ` factors and solves the complex tridiagonal linear system $Ax = b$. `LSLTQ` is intended just for tridiagonal systems. The coefficient matrix does not have to be symmetric. The algorithm is Gaussian elimination with pivoting for numerical stability. See Dongarra et al. (1979), LINPACK subprograms `CGTSL`/`ZGTSL`, for details. When computing on vector or parallel computers the cyclic reduction algorithm, `LSLCQ`, should be considered as an alternative method to solve the system.

Comments

Informational error

Type	Code	Description
4	2	An element along the diagonal became exactly zero during execution.

Example

A system of $n = 4$ linear equations is solved.

```
      USE LSLTQ_INT
      USE WRCRL_INT
!                                  Declaration of variables
      INTEGER    N
      PARAMETER  (N=4)
!
      COMPLEX    B(N), C(N), D(N), E(N)
      CHARACTER  CLABEL(1)*6, FMT*8, RLABEL(1)*4
!
      DATA FMT/'(E13.6)'/
      DATA CLABEL/'NUMBER'/
      DATA RLABEL/'NONE'/
!                                 C(*), D(*), E(*) and B(*)
!                                 contain the subdiagonal,
!                                 diagonal, superdiagonal and
!                                 right hand side.
      DATA C/(0.0,0.0), (-9.0,3.0), (2.0,7.0), (7.0,-4.0)/
      DATA D/(3.0,-5.0), (4.0,-9.0), (-5.0,-7.0), (-2.0,-3.0)/
      DATA E/(-9.0,8.0), (1.0,8.0), (8.0,3.0), (0.0,0.0)/
      DATA B/(-16.0,-93.0), (128.0,179.0), (-60.0,-12.0), (9.0,-108.0)/
!
!
      CALL LSLTQ (C, D, E, B)
!                                  Output the solution.
      CALL WRCRL ('Solution:', B, RLABEL, CLABEL, 1, N, 1, FMT=FMT)
      END
```

Output

```
Solution:
                           1                               2
(-0.400000E+01,-0.700000E+01)   (-0.700000E+01, 0.400000E+01)
```

```
                              3                                 4
( 0.700000E+01,-0.700000E+01)  ( 0.900000E+01, 0.200000E+01)
```

LSLCQ

Computes the *LDU* factorization of a complex tridiagonal matrix *A* using a cyclic reduction algorithm.

Required Arguments

C — Complex array of size 2N containing the upper codiagonal of the N by N tridiagonal matrix in the entries C(1), …, C(N − 1). (Input/Output)

A — Complex array of size 2N containing the diagonal of the N by N tridiagonal matrix in the entries A(1), …, A(N). (Input/Output)

B — Complex array of size 2N containing the lower codiagonal of the N by N tridiagonal matrix in the entries B(1), …, B(N − 1). (Input/Output)

Y — Complex array of size 2N containing the right-hand side of the system $Ax = y$ in the order Y(1), …, Y(N). (Input/Output)
The vector *x* overwrites *Y* in storage.

U — Real array of size 2N of flags that indicate any singularities of A. (Output)
A value U(I) = 1. means that a divide by zero would have occurred during the factoring. Otherwise U(I) = 0.

IR — Array of integers that determine the sizes of loops performed in the cyclic reduction algorithm. (Output)

IS — Array of integers that determine the sizes of loops performed in the cyclic reduction algorithm. (Output)
The sizes of these arrays must be at least $\log_2$ (N) + 3.

Optional Arguments

N — Order of the matrix. (Input)
N must be greater than zero.
Default: N = size (C,1).

IJOB — Flag to direct the desired factoring or solving step. (Input)
Default: IJOB =1.

IJOB	Action
1	Factor the matrix *A* and solve the system *Ax* = *y*, where *y* is stored in array *Y*.
2	Do the solve step only. Use *y* from array *Y*. (The factoring step has already been done.)
3	Factor the matrix *A* but do not solve a system.
4	Same meaning as with the value IJOB = 3. For efficiency, no error checking is done on the validity of any input value.

FORTRAN 90 Interface

Generic: CALL LSLCQ (C, A, B, Y, U, IR, IS [, …])

Specific: The specific interface names are S_LSLCQ and D_LSLCQ.

FORTRAN 77 Interface

Single: CALL LSLCQ (N, C, A, B, IJOB, Y, U, IR, IS)

Double: The double precision name is DLSLCQ.

Description

Routine LSLCQ factors and solves the complex tridiagonal linear system *Ax* = *y*. The matrix is decomposed in the form *A* = *LDU*, where *L* is unit lower triangular, *U* is unit upper triangular, and *D* is diagonal. The algorithm used for the factorization is effectively that described in Kershaw (1982). More details, tests and experiments are reported in Hanson (1990).

LSLCQ is intended just for tridiagonal systems. The coefficient matrix does not have to be Hermitian. The algorithm amounts to Gaussian elimination, with no pivoting for numerical stability, on the matrix whose rows and columns are permuted to a new order. See Hanson (1990) for details. The expectation is that LSLCQ will outperform either LSLTQ or LSLQB on vector or parallel computers. Its performance may be inferior for small values of *n*, on scalar computers, or high-performance computers with non-optimizing compilers.

Example

A real skew-symmetric tridiagonal matrix, *A*, of dimension $n = 1000$ is given by $c_k = -k$, $a_k = 0$, and $b_k = k$, $k = 1, \ldots, n-1$, $a_n = 0$. This matrix will have eigenvalues that are purely imaginary. The eigenvalue closest to the imaginary unit is required. This number is obtained by using inverse iteration to approximate a complex eigenvector *y*. The eigenvalue is approximated by $\lambda = y^H Ay / y^H y$. (This example is contrived in the sense that the given tridiagonal skew-symmetric matrix eigenvalue problem is essentially equivalent to the tridiagonal symmetic eigenvalue problem where the $c_k = k$ and the other data are unchanged.)

```
      USE LSLCQ_INT
      USE UMACH_INT
!                                  Declare variables
      INTEGER    LP, N, N2
      PARAMETER  (LP=12, N=1000, N2=2*N)
!
      INTEGER    I, IJOB, IR(LP), IS(LP), K, NOUT
      REAL       AIMAG, U(N2)
      COMPLEX    A(N2), B(N2), C(N2), CMPLX, CONJG, S, T, Y(N2)
      INTRINSIC  AIMAG, CMPLX, CONJG
!                                  Define entries of skew-symmetric
!                                  matrix, A:
      DO 10  I=1, N - 1
         C(I) = -I
!                                  This amounts to subtracting the
!                                  positive imaginary unit from the
!                                  diagonal.  (The eigenvalue closest
!                                  to this value is desired.)
         A(I) = CMPLX(0.E0,-1.0E0)
         B(I) = I
!                                  This initializes the approximate
!                                  eigenvector.
         Y(I) = 1.E0
   10 CONTINUE
      A(N) = CMPLX(0.E0,-1.0E0)
      Y(N) = 1.E0
!                                  First step of inverse iteration
!                                  follows. Obtain decomposition of
!                                  matrix and solve the first system:
      IJOB = 1
      CALL LSLCQ (C, A, B, Y, U, IR, IS, N=N, IJOB=IJOB)
!
!                                  Next steps of inverse iteration
!                                  follow. Solve the system again with
!                                  the decomposition ready:
      IJOB = 2
      DO 20  K=1, 3
         CALL LSLCQ (C, A, B, Y, U, IR, IS, N=N, IJOB=IJOB)
   20 CONTINUE
!
!                                  Compute the Raleigh quotient to
!                                  estimate the eigenvalue closest to
!                                  the positive imaginary unit. After
!                                  the approximate eigenvector, y, is
!                                  computed, the estimate of the
!                                  eigenvalue is ctrans(y)*A*y/t,
!                                  where t = ctrans(y)*y.
      S = -CONJG(Y(1))*Y(2)
      T = CONJG(Y(1))*Y(1)
      DO 30  I=2, N - 1
         S = S + CONJG(Y(I))*((I-1)*Y(I-1)-I*Y(I+1))
```

```
          T = T + CONJG(Y(I))*Y(I)
   30 CONTINUE
      S = S + CONJG(Y(N))*(N-1)*Y(N-1)
      T = T + CONJG(Y(N))*Y(N)
      S = S/T
      CALL UMACH (2, NOUT)
      WRITE (NOUT,*) ' The value of n is:  ', N
      WRITE (NOUT,*) ' Value of approximate imaginary eigenvalue:',&
                   AIMAG(S)
      STOP
      END
```

Output

```
The value of n is:    1000
Value of approximate imaginary eigenvalue:    1.03811
```

LSACB

Solves a complex system of linear equations in band storage mode with iterative refinement.

Required Arguments

A — Complex NLCA + NUCA + 1 by N array containing the N by N banded coefficient matrix in band storage mode. (Input)

NLCA — Number of lower codiagonals of A. (Input)

NUCA — Number of upper codiagonals of A. (Input)

B — Complex vector of length N containing the right-hand side of the linear system. (Input)

X — Complex vector of length N containing the solution to the linear system. (Output)

Optional Arguments

N — Number of equations. (Input)
Default: N = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

IPATH — Path indicator. (Input)
IPATH = 1 means the system $AX = B$ is solved.
IPATH = 2 means the system $A^H X = B$ is solved.
Default: IPATH = 1.

FORTRAN 90 Interface

Generic: CALL LSACB (A, NLCA, NUCA, B, X [, …])

Specific: The specific interface names are S_LSACB and D_LSACB.

FORTRAN 77 Interface

Single: CALL LSACB (N, A, LDA, NLCA, NUCA, B, IPATH, X)

Double: The double precision name is DLSACB.

Description

Routine LSACB solves a system of linear algebraic equations having a complex banded coefficient matrix. It first uses the routine LFCCB to compute an *LU* factorization of the coefficient matrix and to estimate the condition number of the matrix. The solution of the linear system is then found using the iterative refinement routine LFICB.

LSACB fails if *U*, the upper triangular part of the factorization, has a zero diagonal element or if the iterative refinement algorithm fails to converge. These errors occur only if A is singular or very close to a singular matrix.

If the estimated condition number is greater than $1/\varepsilon$ (where ε is machine precision), a warning error is issued. This indicates that very small changes in A can cause very large changes in the solution *x*. Iterative refinement can sometimes find the solution to such a system. LSACB solves the problem that is represented in the computer; however, this problem may differ from the problem whose solution is desired.

Comments

1. Workspace may be explicitly provided, if desired, by use of L2ACB/DL2ACB. The reference is:

   CALL L2ACB (N, A, LDA, NLCA, NUCA, B, IPATH, X, FACT, IPVT, WK)

   The additional arguments are as follows:

   FACT — Complex work vector of length (2 * NLCA + NUCA + 1) * N containing the *LU* factorization of A on output.

   IPVT — Integer work vector of length N containing the pivoting information for the *LU* factorization of A on output.

   WK — Complex work vector of length N.

2. Informational errors

Type	Code	Description
3	3	The input matrix is too ill-conditioned. The solution might not be accurate.
4	2	The input matrix is singular.

3. *Integer Options* with *Chapter 11* Options Manager

   16 This option uses four values to solve memory bank conflict (access inefficiency) problems. In routine L2ACB the leading dimension of FACT is increased by IVAL(3) when N is a multiple of IVAL(4). The values IVAL(3) and IVAL(4) are temporarily replaced by IVAL(1) and IVAL(2), respectively, in LSACB. Additional memory allocation for FACT and option value restoration are done automatically in LSACB. Users directly calling L2ACB can allocate additional space for FACT and set IVAL(3) and IVAL(4) so that memory bank conflicts no longer cause inefficiencies. There is no requirement that users change existing applications that use LSACB or L2ACB. Default values for the option are IVAL(*) = 1,16,0,1.

17 This option has two values that determine if the L_1 condition number is to be computed. Routine LSACB temporarily replaces IVAL(2) by IVAL(1). The routine L2CCB computes the condition number if IVAL(2) = 2. Otherwise L2CCB skips this computation. LSACB restores the option. Default values for the option are IVAL(*) = 1,2.

Example

A system of four linear equations is solved. The coefficient matrix has complex banded form with one upper and one lower codiagonal. The right-hand-side vector *b* has four elements.

```
      USE LSACB_INT
      USE WRCRN_INT
!                                 Declare variables
      INTEGER    LDA, N, NLCA, NUCA
      PARAMETER  (LDA=3, N=4, NLCA=1, NUCA=1)
      COMPLEX    A(LDA,N), B(N), X(N)
!
!                Set values for A in band form, and B
!
!                A = (  0.0+0.0i  4.0+0.0i -2.0+2.0i -4.0-1.0i )
!                    ( -2.0-3.0i -0.5+3.0i  3.0-3.0i  1.0-1.0i )
!                    (  6.0+1.0i  1.0+1.0i  0.0+2.0i  0.0+0.0i )
!
!                B = ( -10.0-5.0i  9.5+5.5i  12.0-12.0i  0.0+8.0i )
!
      DATA A/(0.0,0.0), (-2.0,-3.0), (6.0,1.0), (4.0,0.0), (-0.5,3.0),&
            (1.0,1.0), (-2.0,2.0), (3.0,-3.0), (0.0,2.0), (-4.0,-1.0),&
            (1.0,-1.0), (0.0,0.0)/
      DATA B/(-10.0,-5.0), (9.5,5.5), (12.0,-12.0), (0.0,8.0)/
!                                 Solve A*X = B
      CALL LSACB (A, NLCA, NUCA, B, X)
!                                 Print results
      CALL WRCRN ('X', X, 1, N, 1)
!
      END
```

Output

```
                                  X
             1                 2                 3                 4
( 3.000, 0.000)   (-1.000, 1.000)   ( 3.000, 0.000)   (-1.000, 1.000)
```

LSLCB

Solves a complex system of linear equations in band storage mode without iterative refinement.

Required Arguments

A — Complex NLCA + NUCA + 1 by N array containing the N by N banded coefficient matrix in band storage mode. (Input)

NLCA — Number of lower codiagonals of A. (Input)

NUCA — Number of upper codiagonals of A. (Input)

B — Complex vector of length N containing the right-hand side of the linear system. (Input)

X — Complex vector of length N containing the solution to the linear system. (Output)
If B is not needed, then B and X may share the same storage locations)

Optional Arguments

N — Number of equations. (Input)
Default: N = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

IPATH — Path indicator. (Input)
IPATH = 1 means the system $AX = B$ is solved.
IPATH = 2 means the system $A^H X = B$ is solved.
Default: IPATH = 1.

FORTRAN 90 Interface

Generic: CALL LSLCB (A, NLCA, NUCA, B, X [, …])

Specific: The specific interface names are S_LSLCB and D_LSLCB.

FORTRAN 77 Interface

Single: CALL LSLCB (N, A, LDA, NLCA, NUCA, B, IPATH, X)

Double: The double precision name is DLSLCB.

Description

Routine LSLCB solves a system of linear algebraic equations having a complex banded coefficient matrix. It first uses the routine LFCCB to compute an *LU* factorization of the coefficient matrix and to estimate the condition number of the matrix. The solution of the linear system is then found using LFSCB.

LSLCB fails if *U*, the upper triangular part of the factorization, has a zero diagonal element. This occurs only if *A* is singular or very close to a singular matrix.

If the estimated condition number is greater than $1/\varepsilon$ (where ε is machine precision), a warning error is issued. This indicates that very small changes in A can cause very large changes in the solution *x*. If the coefficient matrix is ill-conditioned or poorly scaled, it is recommended that LSACB be used.

Comments

1. Workspace may be explicitly provided, if desired, by use of L2LCB/DL2LCB The reference is:

   CALL L2LCB (N, A, LDA, NLCA, NUCA, B, IPATH, X, FACT, IPVT, WK)

   The additional arguments are as follows:

   FACT — (2 * NLCA + NUCA + 1) × N complex work array containing the *LU* factorization of A on output. If A is not needed, A can share the first (NLCA + NUCA + 1) * N locations with FACT.

   IPVT — Integer work vector of length N containing the pivoting information for the *LU* factorization of A on output.

   WK — Complex work vector of length N.

2. Informational errors

Type	Code	Description
3	3	The input matrix is too ill-conditioned. The solution might not be accurate.
4	2	The input matrix is singular.

3. *Integer Options* with *Chapter 11* Options Manager

   16 This option uses four values to solve memory bank conflict (access inefficiency) problems. In routine L2LCB the leading dimension of FACT is increased by IVAL(3) when N is a multiple of IVAL(4). The values IVAL(3) and IVAL(4) are temporarily replaced by IVAL(1) and IVAL(2), respectively, in LSLCB. Additional memory allocation for FACT and option value restoration are done automatically in LSLCB. Users directly calling L2LCB can allocate additional space for FACT and set IVAL(3) and IVAL(4) so that memory bank conflicts no longer cause inefficiencies. There is no requirement that users change existing applications that use LSLCB or L2LCB. Default values for the option are IVAL(*) = 1,16,0,1.

17 This option has two values that determine if the L_1 condition number is to be computed. Routine LSLCB temporarily replaces IVAL(2) by IVAL(1). The routine L2CCB computes the condition number if IVAL(2) = 2. Otherwise L2CCB skips this computation. LSLCB restores the option. Default values for the option are IVAL(*) = 1,2.

Example

A system of four linear equations is solved. The coefficient matrix has complex banded form with one upper and one lower codiagonal. The right-hand-side vector *b* has four elements.

```
      USE LSLCB_INT
      USE WRCRN_INT
!                                 Declare variables
      INTEGER    LDA, N, NLCA, NUCA
      PARAMETER  (LDA=3, N=4, NLCA=1, NUCA=1)
      COMPLEX    A(LDA,N), B(N), X(N)
!
!                Set values for A in band form, and B
!
!                A = (  0.0+0.0i  4.0+0.0i -2.0+2.0i -4.0-1.0i )
!                    ( -2.0-3.0i -0.5+3.0i  3.0-3.0i  1.0-1.0i )
!                    (  6.0+1.0i  1.0+1.0i  0.0+2.0i  0.0+0.0i )
!
!                B = ( -10.0-5.0i  9.5+5.5i  12.0-12.0i  0.0+8.0i )
!
      DATA A/(0.0,0.0), (-2.0,-3.0), (6.0,1.0), (4.0,0.0), (-0.5,3.0),&
            (1.0,1.0), (-2.0,2.0), (3.0,-3.0), (0.0,2.0), (-4.0,-1.0),&
            (1.0,-1.0), (0.0,0.0)/
      DATA B/(-10.0,-5.0), (9.5,5.5), (12.0,-12.0), (0.0,8.0)/
!                                 Solve A*X = B
      CALL LSLCB (A, NLCA, NUCA, B, X)
!                                 Print results
      CALL WRCRN ('X', X, 1, N, 1)
!
      END
```

Output

```
                                   X
             1                  2                  3                  4
 ( 3.000, 0.000)  (-1.000, 1.000)  ( 3.000, 0.000)  (-1.000, 1.000)
```

LFCCB

Computes the *LU* factorization *of a* complex matrix in band storage mode and estimate its L_1 condition number.

Required Arguments

A — Complex NLCA + NUCA + 1 by N array containing the N by N matrix in band storage mode to be factored. (Input)

NLCA — Number of lower codiagonals of A. (Input)

NUCA — Number of upper codiagonals of A. (Input)

FACT — Complex 2 * NLCA + NUCA + 1 by N array containing the *LU* factorization of the matrix A. (Output)
If A is not needed, A can share the first (NLCA + NUCA + 1) * N locations with FACT .

IPVT — Vector of length N containing the pivoting information for the *LU* factorization. (Output)

RCOND — Scalar containing an estimate of the reciprocal of the L_1 condition number of A. (Output)

Optional Arguments

N — Order of the matrix. (Input)
Default: N = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

LDFACT — Leading dimension of FACT exactly as specified in the dimension statement of the calling program. (Input)
Default: LDFACT = size (FACT,1).

FORTRAN 90 Interface

Generic: CALL LFCCB (A, NLCA, NUCA, FACT, IPVT, RCOND [, …])

Specific: The specific interface names are S_LFCCB and D_LFCCB.

FORTRAN 77 Interface

Single: `CALL LFCCB (N, A, LDA, NLCA, NUCA, FACT, LDFACT, IPVT, RCOND)`

Double: The double precision name is `DLFCCB`.

Description

Routine `LFCCB` performs an *LU* factorization of a complex banded coefficient matrix. It also estimates the condition number of the matrix. The *LU* factorization is done using scaled partial pivoting. Scaled partial pivoting differs from partial pivoting in that the pivoting strategy is the same as if each row were scaled to have the same ∞-norm.

The L_1 condition number of the matrix *A* is defined to be $\kappa(A) = \|A\|_1 \|A^{-1}\|_1$ Since it is expensive to compute $\|A^{-1}\|_1$, the condition number is only estimated. The estimation algorithm is the same as used by LINPACK and is described by Cline et al. (1979).

If the estimated condition number is greater than $1/\varepsilon$ (where ε is machine precision), a warning error is issued. This indicates that very small changes in *A* can cause very large changes in the solution *x*. Iterative refinement can sometimes find the solution to such a system.

`LFCCB` fails if *U*, the upper triangular part of the factorization, has a zero diagonal element. This can occur only if *A* is singular or very close to a singular matrix.

The *LU* factors are returned in a form that is compatible with IMSL routines `LFICB`, `LFSCB` and `LFDCB`. To solve systems of equations with multiple right-hand-side vectors, use `LFCCB` followed by either `LFICB` or `LFSCB` called once for each right-hand side. The routine `LFDCB` can be called to compute the determinant of the coefficient matrix after `LFCCB` has performed the factorization.

Let *F* be the matrix `FACT`, let m_l = `NLCA` and let m_u = `NUCA`. The first $m_l + m_u + 1$ rows of *F* contain the triangular matrix *U* in band storage form. The lower m_l rows of *F* contain the multipliers needed to reconstruct *L*.

`LFCCB` is based on the LINPACK routine `CGBCO`; see Dongarra et al. (1979). `CGBCO` uses unscaled partial pivoting.

Comments

1. Workspace may be explicitly provided, if desired, by use of `L2CCB/DL2CCB`. The reference is:

   `CALL L2CCB (N, A, LDA, NLCA, NUCA, FACT, LDFACT, IPVT, RCOND, WK)`

   The additional argument is

   WK — Complex work vector of length `N`.

2. Informational errors

Type	Code	Description
3	1	The input matrix is algorithmically singular.
4	2	The input matrix is singular.

Example

The inverse of a 4 × 4 band matrix with one upper and one lower codiagonal is computed. LFCCB is called to factor the matrix and to check for singularity or ill-conditioning. LFICB is called to determine the columns of the inverse.

```
      USE LFCCB_INT
      USE UMACH_INT
      USE LFICB_INT
      USE WRCRN_INT
!                                 Declare variables
      INTEGER    LDA, LDFACT, N, NLCA, NUCA, NOUT
      PARAMETER  (LDA=3, LDFACT=4, N=4, NLCA=1, NUCA=1)
      INTEGER    IPVT(N)
      REAL       RCOND
      COMPLEX    A(LDA,N), AINV(N,N), FACT(LDFACT,N), RJ(N), RES(N)
!
!                Set values for A in band form
!
!                A = (  0.0+0.0i  4.0+0.0i -2.0+2.0i -4.0-1.0i )
!                    (  0.0-3.0i -0.5+3.0i  3.0-3.0i  1.0-1.0i )
!                    (  6.0+1.0i  4.0+1.0i  0.0+2.0i  0.0+0.0i )
!
      DATA A/(0.0,0.0), (0.0,-3.0), (6.0,1.0), (4.0,0.0), (-0.5,3.0),&
            (4.0,1.0), (-2.0,2.0), (3.0,-3.0), (0.0,2.0), (-4.0,-1.0),&
            (1.0,-1.0), (0.0,0.0)/
!
      CALL LFCCB (A, NLCA, NUCA, FACT, IPVT, RCOND)
!                                 Print the reciprocal condition number
!                                 and the L1 condition number
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) RCOND, 1.0E0/RCOND
!                                 Set up the columns of the identity
!                                 matrix one at a time in RJ
      RJ = (0.0E0,0.0E0)
      DO 10  J=1, N
         RJ(J) = (1.0E0,0.0E0)
!                                 RJ is the J-th column of the identity
!                                 matrix so the following LFICB
!                                 reference places the J-th column of
!                                 the inverse of A in the J-th column
!                                 of AINV
         CALL LFICB (A, NLCA, NUCA, FACT, IPVT, RJ, AINV(:,J), RES)
         RJ(J) = (0.0E0,0.0E0)
   10 CONTINUE
!                                 Print results
      CALL WRCRN ('AINV', AINV)

!
99999 FORMAT ('  RCOND = ',F5.3,/,'  L1 condition number = ',F6.3)
      END
```

Output

```
RCOND = 0.022
L1 condition number = 45.933
                                 AINV
                    1                  2                  3                  4
    1  ( 0.562, 0.170)  ( 0.125, 0.260)  (-0.385,-0.135)  (-0.239,-1.165)
    2  ( 0.122, 0.421)  (-0.195, 0.094)  ( 0.101,-0.289)  ( 0.874,-0.179)
    3  ( 0.034, 0.904)  (-0.437, 0.090)  (-0.153,-0.527)  ( 1.087,-1.172)
    4  ( 0.938, 0.870)  (-0.347, 0.527)  (-0.679,-0.374)  ( 0.415,-1.759)
```

LFTCB

Computes the *LU* factorization *of a* complex matrix in band storage mode.

Required Arguments

A — Complex NLCA + NUCA + 1 by N array containing the N by N matrix in band storage mode to be factored. (Input)

NLCA — Number of lower codiagonals of A. (Input)

NUCA — Number of upper codiagonals of A. (Input)

FACT — Complex 2 * NLCA + NUCA + 1 by N array containing the *LU* factorization of the matrix A. (Output)
If A is not needed, A can share the first (NLCA + NUCA + 1) * N locations with FACT.

IPVT — Integer vector of length N containing the pivoting information for the *LU* factorization. (Output)

Optional Arguments

N — Order of the matrix. (Input)
Default: N = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

LDFACT — Leading dimension of FACT exactly as specified in the dimension statement of the calling program. (Input)
Default: LDFACT = size (FACT,1).

FORTRAN 90 Interface

Generic: CALL LFTCB (A, NLCA, NUCA, FACT, IPVT [, …])

Specific: The specific interface names are S_LFTCB and D_LFTCB.

FORTRAN 77 Interface

Single: CALL LFTCB (N, A, LDA, NLCA, NUCA, FACT, LDFACT, IPVT)

Double: The double precision name is DLFTCB.

Description

Routine LFTCB performs an *LU* factorization of a complex banded coefficient matrix. The *LU* factorization is done using scaled partial pivoting. Scaled partial pivoting differs from partial pivoting in that the pivoting strategy is the same as if each row were scaled to have the same ∞-norm.

LFTCB fails if *U*, the upper triangular part of the factorization, has a zero diagonal element. This can occur only if *A* is singular or very close to a singular matrix.

The *LU* factors are returned in a form that is compatible with routines LFICB, LFSCB and LFDCB. To solve systems of equations with multiple right-hand-side vectors, use LFTCB followed by either LFICB or LFSCB called once for each right-hand side. The routine LFDCB can be called to compute the determinant of the coefficient matrix after LFTCB has performed the factorization.

Let *F* be the matrix FACT, let m_l = NLCA and let m_u = NUCA. The first $m_l + m_u + 1$ rows of *F* contain the triangular matrix *U* in band storage form. The lower m_l rows of *F* contain the multipliers needed to reconstruct L^{-1}. LFTCB is based on the LINPACK routine CGBFA; see Dongarra et al. (1979). CGBFA uses unscaled partial pivoting.

Comments

1. Workspace may be explicitly provided, if desired, by use of L2TCB/DL2TCB The reference is:

   CALL L2TCB (N, A, LDA, NLCA, NUCA, FACT, LDFACT, IPVT, WK)

   The additional argument is:

   WK — Complex work vector of length N used for scaling.

2. Informational error

Type	Code	Description
4	2	The input matrix is singular.

Example

A linear system with multiple right-hand sides is solved. LFTCB is called to factor the coefficient matrix. LFSCB is called to compute the two solutions for the two right-hand sides. In this case the coefficient matrix is assumed to be well-conditioned and correctly scaled. Otherwise, it would be better to call LFCCB to perform the factorization, and LFICB to compute the solutions.

```
      USE LFTCB_INT
```

```
      USE LFSCB_INT
      USE WRCRN_INT
!                                 Declare variables
      INTEGER    LDA, LDFACT, N, NLCA, NUCA
      PARAMETER  (LDA=3, LDFACT=4, N=4, NLCA=1, NUCA=1)
      INTEGER    IPVT(N)
      COMPLEX    A(LDA,N), B(N,2), FACT(LDFACT,N), X(N,2)
!
!                Set values for A in band form, and B
!
!                A = (  0.0+0.0i  4.0+0.0i -2.0+2.0i -4.0-1.0i )
!                    (  0.0-3.0i -0.5+3.0i  3.0-3.0i  1.0-1.0i )
!                    (  6.0+1.0i  4.0+1.0i  0.0+2.0i  0.0+0.0i )
!
!                B = (  -4.0-5.0i  16.0-4.0i )
!                    (   9.5+5.5i  -9.5+19.5i )
!                    (   9.0-9.0i  12.0+12.0i )
!                    (   0.0+8.0i  -8.0-2.0i  )
!
      DATA A/(0.0,0.0), (0.0,-3.0), (6.0,1.0), (4.0,0.0), (-0.5,3.0),&
            (4.0,1.0), (-2.0,2.0), (3.0,-3.0), (0.0,2.0), (-4.0,-1.0),&
            (1.0,-1.0), (0.0,0.0)/
      DATA B/(-4.0,-5.0), (9.5,5.5), (9.0,-9.0), (0.0,8.0),&
            (16.0,-4.0), (-9.5,19.5), (12.0,12.0), (-8.0,-2.0)/
!
      CALL LFTCB (A, NLCA, NUCA, FACT, IPVT)
!                                 Solve for the two right-hand sides
      DO 10  J=1, 2
         CALL LFSCB (FACT, NLCA, NUCA, IPVT, B(:,J), X(:,J))
   10 CONTINUE
!                                 Print results
      CALL WRCRN ('X', X)
!
      END
```

Output

```
                 X
              1                 2
1  ( 3.000, 0.000)  ( 0.000, 4.000)
2  (-1.000, 1.000)  ( 1.000,-1.000)
3  ( 3.000, 0.000)  ( 0.000, 4.000)
4  (-1.000, 1.000)  ( 1.000,-1.000)
```

LFSCB

Solves a complex system of linear equations given the *LU* factorization of the coefficient matrix in band storage mode.

Required Arguments

FACT — Complex 2 * NLCA + NUCA + 1 by N array containing the *LU* factorization of the coefficient matrix A as output from subroutine LFCCB/DLFCCB or LFTCB/DLFTCB. (Input)

NLCA — Number of lower codiagonals of A. (Input)

NUCA — Number of upper codiagonals of A. (Input)

IPVT — Vector of length N containing the pivoting information for the *LU* factorization of A as output from subroutine LFCCB/DLFCCB or LFTCB/DLFTCB. (Input)

B — Complex vector of length N containing the right-hand side of the linear system. (Input)

X — Complex vector of length N containing the solution to the linear system. (Output)
If B is not needed, B and X can share the same storage locations.

Optional Arguments

N — Number of equations. (Input)
Default: N = size (FACT,2).

LDFACT — Leading dimension of FACT exactly as specified in the dimension statement of the calling program. (Input)
Default: LDFACT = size (FACT,1).

IPATH — Path indicator. (Input)
IPATH = 1 means the system AX = B is solved.
IPATH = 2 means the system $A^H X$ = B is solved.
Default: IPATH = 1.

FORTRAN 90 Interface

Generic: CALL LFSCB (FACT, NLCA, NUCA, IPVT, B, X [, …])

Specific: The specific interface names are S_LFSCB and D_LFSCB.

FORTRAN 77 Interface

Single: `CALL LFSCB (N, FACT, LDFACT, NLCA, NUCA, IPVT, B, IPATH, X)`

Double: The double precision name is `DLFSCB`.

Description

Routine `LFSCB` computes the solution of a system of linear algebraic equations having a complex banded coefficient matrix. To compute the solution, the coefficient matrix must first undergo an *LU* factorization. This may be done by calling either `LFCCB` or `LFTCB`. The solution to $Ax = b$ is found by solving the banded triangular systems $Ly = b$ and $Ux = y$. The forward elimination step consists of solving the system $Ly = b$ by applying the same permutations and elimination operations to b that were applied to the columns of A in the factorization routine. The backward substitution step consists of solving the banded triangular system $Ux = y$ for x.

`LFSCB` and `LFICB` both solve a linear system given its *LU* factorization. `LFICB` generally takes more time and produces a more accurate answer than `LFSCB`. Each iteration of the iterative refinement algorithm used by `LFICB` calls `LFSCB`.

`LFSCB` is based on the LINPACK routine `CGBSL`; see Dongarra et al. (1979).

Example

The inverse is computed for a real banded 4 × 4 matrix with one upper and one lower codiagonal. The input matrix is assumed to be well-conditioned; hence `LFTCB` is used rather than `LFCCB`.

```
      USE LFSCB_INT
      USE LFTCB_INT
      USE WRCRN_INT
!                                  Declare variables
      INTEGER    LDA, LDFACT, N, NLCA, NUCA
      PARAMETER  (LDA=3, LDFACT=4, N=4, NLCA=1, NUCA=1)
      INTEGER    IPVT(N)
      COMPLEX    A(LDA,N), AINV(N,N), FACT(LDFACT,N), RJ(N)
!
!                Set values for A in band form
!
!                A = (  0.0+0.0i  4.0+0.0i -2.0+2.0i -4.0-1.0i )
!                    ( -2.0-3.0i -0.5+3.0i  3.0-3.0i  1.0-1.0i )
!                    (  6.0+1.0i  1.0+1.0i  0.0+2.0i  0.0+0.0i )
!
      DATA A/(0.0,0.0), (-2.0,-3.0), (6.0,1.0), (4.0,0.0), (-0.5,3.0),&
            (1.0,1.0), (-2.0,2.0), (3.0,-3.0), (0.0,2.0), (-4.0,-1.0),&
            (1.0,-1.0), (0.0,0.0)/
!
      CALL LFTCB (A, NLCA, NUCA, FACT, IPVT)
!                                  Set up the columns of the identity
!                                  matrix one at a time in RJ
      RJ = (0.0E0,0.0E0)
      DO 10  J=1, N
         RJ(J) = (1.0E0,0.0E0)
!                                  RJ is the J-th column of the identity
```

```
!                                 matrix so the following LFSCB
!                                 reference places the J-th column of
!                                 the inverse of A in the J-th column
!                                 of AINV
         CALL LFSCB (FACT, NLCA, NUCA, IPVT, RJ, AINV(:,J))
         RJ(J) = (0.0E0,0.0E0)
   10 CONTINUE
!                                 Print results
      CALL WRCRN ('AINV', AINV)
!
      END
```

Output

```
                 1                 2                 3                 4
1  ( 0.165,-0.341)  ( 0.376,-0.094)  (-0.282, 0.471)  (-1.600, 0.000)
2  ( 0.588,-0.047)  ( 0.259, 0.235)  (-0.494, 0.024)  (-0.800,-1.200)
3  ( 0.318, 0.271)  ( 0.012, 0.247)  (-0.759,-0.235)  (-0.550,-2.250)
4  ( 0.588,-0.047)  ( 0.259, 0.235)  (-0.994, 0.524)  (-2.300,-1.200)
```

LFICB

Uses iterative refinement to improve the solution of a complex system of linear equations in band storage mode.

Required Arguments

A — Complex NLCA + NUCA + 1 by N array containing the N by N coefficient matrix in band storage mode. (Input)

NLCA — Number of lower codiagonals of A. (Input)

NUCA — Number of upper codiagonals of A. (Input)

FACT — Complex 2 * NLCA + NUCA + 1 by N array containing the *LU* factorization of the matrix A as output from routine LFCCB/DLFCCB or LFTCB/DLFTCB. (Input)

IPVT — Vector of length N containing the pivoting information for the *LU* factorization of A as output from routine LFCCB/DLFCCB or LFTCB/DLFTCB. (Input)

B — Complex vector of length N containing the right-hand side of the linear system. (Input)

X — Complex vector of length N containing the solution. (Output)

RES — Complex vector of length N containing the residual vector at the improved solution. (Output)

Optional Arguments

N — Number of equations. (Input)
Default: N = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

LDFACT — Leading dimension of FACT exactly as specified in the dimension statement of the calling program. (Input)
Default: LDFACT = size (FACT,1).

IPATH — Path indicator. (Input)
IPATH = 1 means the system AX = B is solved.
IPATH = 2 means the system $A^H X$ = B is solved.
Default: IPATH = 1.

FORTRAN 90 Interface

Generic: CALL LFICB (A, NLCA, NUCA, FACT, IPVT, B, X, RES [, …])

Specific: The specific interface names are S_LFICB and D_LFICB.

FORTRAN 77 Interface

Single: CALL LFICB (N, A, LDA, NLCA, NUCA, FACT, LDFACT, IPVT, B, IPATH, X, RES)

Double: The double precision name is DLFICB.

Description

Routine LFICB computes the solution of a system of linear algebraic equations having a complex banded coefficient matrix. Iterative refinement is performed on the solution vector to improve the accuracy. Usually almost all of the digits in the solution are accurate, even if the matrix is somewhat ill-conditioned.

To compute the solution, the coefficient matrix must first undergo an *LU* factorization. This may be done by calling either LFCCB or LFTCB.

Iterative refinement fails only if the matrix is very ill-conditioned.

LFICB and LFSCB both solve a linear system given its *LU* factorization. LFICB generally takes more time and produces a more accurate answer than LFSCB. Each iteration of the iterative refinement algorithm used by LFICB calls LFSCB.

Comments

Informational error

Type	Code	Description
3	3	The input matrix is too ill-conditioned for iterative refinement be effective.

Example

A set of linear systems is solved successively. The right-hand-side vector is perturbed after solving the system each of the first two times by adding (1 + *i*)/2 to the second element.

```
      USE LFICB_INT
      USE LFCCB_INT
      USE WRCRN_INT
      USE UMACH_INT
!                                 Declare variables
```

```
      INTEGER    LDA, LDFACT, N, NLCA, NUCA, NOUT
      PARAMETER  (LDA=3, LDFACT=4, N=4, NLCA=1, NUCA=1)
      INTEGER    IPVT(N)
      REAL       RCOND
      COMPLEX    A(LDA,N), B(N), FACT(LDFACT,N), RES(N), X(N)
!
!                Set values for A in band form, and B
!
!                A = (  0.0+0.0i  4.0+0.0i -2.0+2.0i -4.0-1.0i )
!                    ( -2.0-3.0i -0.5+3.0i  3.0-3.0i  1.0-1.0i )
!                    (  6.0+1.0i  1.0+1.0i  0.0+2.0i  0.0+0.0i )
!
!                B = ( -10.0-5.0i  9.5+5.5i  12.0-12.0i  0.0+8.0i )
!
      DATA A/(0.0,0.0), (-2.0,-3.0), (6.0,1.0), (4.0,0.0), (-0.5,3.0),&
            (1.0,1.0), (-2.0,2.0), (3.0,-3.0), (0.0,2.0), (-4.0,-1.0),&
            (1.0,-1.0), (0.0,0.0)/
      DATA B/(-10.0,-5.0), (9.5,5.5), (12.0,-12.0), (0.0,8.0)/
!
      CALL LFCCB (A, NLCA, NUCA, FACT, IPVT, RCOND)
!                                 Print the reciprocal condition number
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99998) RCOND, 1.0E0/RCOND
!                                 Solve the three systems
      DO 10  J=1, 3
         CALL LFICB (A, NLCA, NUCA, FACT, IPVT, B, X, RES)
!                                 Print results
         WRITE (NOUT, 99999) J
         CALL WRCRN ('X', X, 1, N, 1)
         CALL WRCRN ('RES', RES, 1, N, 1)
!                                 Perturb B by adding 0.5+0.5i to B(2)
         B(2) = B(2) + (0.5E0,0.5E0)
   10 CONTINUE
!
99998 FORMAT ('  RCOND = ',F5.3,/,'  L1 Condition number = ',F6.3)
99999 FORMAT (//,'  For system ',I1)
      END
```

Output

```
RCOND = 0.014
L1 Condition number = 72.414

For system 1
                                  X
            1                 2                 3                 4
( 3.000, 0.000)  (-1.000, 1.000)  ( 3.000, 0.000)  (-1.000, 1.000)

                                    RES
                      1                         2                         3
( 0.000E+00, 0.000E+00)  ( 0.000E+00, 0.000E+00)  ( 0.000E+00, 5.684E-14)
                      4
( 3.494E-22,-6.698E-22)

For system 2
                                  X
              1                 2                 3                 4
( 3.235, 0.141)  (-0.988, 1.247)  ( 2.882, 0.129)  (-0.988, 1.247)

                                    RES
                      1                         2                         3
(-1.402E-08, 6.486E-09)  (-7.012E-10, 4.488E-08)  (-1.122E-07, 7.188E-09)
                      4
(-7.012E-10, 4.488E-08)
```

```
For system 3
                                  X
              1                 2                 3                 4
( 3.471, 0.282)  (-0.976, 1.494)  ( 2.765, 0.259)  (-0.976, 1.494)

                                    RES
                      1                         2                         3
(-2.805E-08, 1.297E-08)  (-1.402E-09,-2.945E-08)  ( 1.402E-08, 1.438E-08)
                      4
(-1.402E-09,-2.945E-08)
```

LFDCB

Computes the determinant of a complex matrix given the *LU* factorization of the matrix in band storage mode.

Required Arguments

FACT — Complex (2 * NLCA + NUCA + 1) by N array containing the *LU* factorization of the matrix A as output from routine LFTCB/DLFTCB or LFCCB/DLFCCB. (Input)

NLCA — Number of lower codiagonals in matrix A. (Input)

NUCA — Number of upper codiagonals in matrix A. (Input)

IPVT — Vector of length N containing the pivoting information for the *LU* factorization as output from routine LFTCB/DLFTCB or LFCCB/DLFCCB. (Input)

DET1 — Complex scalar containing the mantissa of the determinant. (Output)
The value DET1 is normalized so that 1.0 ≤ |DET1 | < 10.0 or DET1 = 0.0.

DET2 — Scalar containing the exponent of the determinant. (Output)
The determinant is returned in the form det (*A*) = DET1 * 10^{DET2}.

Optional Arguments

N — Order of the matrix. (Input)
Default: N = size (FACT,2).

LDFACT — Leading dimension of FACT exactly as specified in the dimension statement of the calling program. (Input)
Default: LDFACT = size (FACT,1).

FORTRAN 90 Interface

Generic: CALL LFDCB (FACT, NLCA, NUCA, IPVT, DET1, DET2 [, …])

Specific: The specific interface names are S_LFDCB and D_LFDCB.

FORTRAN 77 Interface

Single: CALL LFDCB (N, FACT, LDFACT, NLCA, NUCA, IPVT, DET1, DET2)

Double: The double precision name is DLFDCB.

Description

Routine LFDCB computes the determinant of a complex banded coefficient matrix. To compute the determinant, the coefficient matrix must first undergo an *LU* factorization. This may be done by calling either LFCCB or LFTCB. The formula det *A* = det *L* det *U* is used to compute the determinant. Since the determinant of a triangular matrix is the product of the diagonal elements,

$$\det U = \prod_{i=1}^{N} U_{ii}$$

(The matrix *U* is stored in the upper NUCA + NLCA + 1 rows of FACT as a banded matrix.) Since *L* is the product of triangular matrices with unit diagonals and of permutation matrices, det $L = (-1)^k$, where *k* is the number of pivoting interchanges.

LFDCB is based on the LINPACK routine CGBDI; see Dongarra et al. (1979).

Example

The determinant is computed for a complex banded 4 × 4 matrix with one upper and one lower codiagonal.

```
      USE LFDCB_INT
      USE LFTCB_INT
      USE UMACH_INT
!                                 Declare variables
      INTEGER    LDA, LDFACT, N, NLCA, NUCA, NOUT
      PARAMETER  (LDA=3, LDFACT=4, N=4, NLCA=1, NUCA=1)
      INTEGER    IPVT(N)
      REAL       DET2
      COMPLEX    A(LDA,N), DET1, FACT(LDFACT,N)
!
!                Set values for A in band form
!
!                A = (  0.0+0.0i  4.0+0.0i -2.0+2.0i -4.0-1.0i )
!                    ( -2.0-3.0i -0.5+3.0i  3.0-3.0i  1.0-1.0i )
!                    (  6.0+1.0i  1.0+1.0i  0.0+2.0i  0.0+0.0i )
!
      DATA A/(0.0,0.0), (-2.0,-3.0), (6.0,1.0), (4.0,0.0), (-0.5,3.0),&
            (1.0,1.0), (-2.0,2.0), (3.0,-3.0), (0.0,2.0), (-4.0,-1.0),&
            (1.0,-1.0), (0.0,0.0)/
!
      CALL LFTCB (A, NLCA, NUCA, FACT, IPVT)
!                                 Compute the determinant
      CALL LFDCB (FACT, NLCA, NUCA, IPVT, DET1, DET2)
!                                 Print the results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) DET1, DET2
!
99999 FORMAT (' The determinant of A is (', F6.3, ',', F6.3, ') * 10**',&
             F2.0)
      END
```

Output

```
The determinant of A is ( 2.500,-1.500) * 10**1.
```

LSAQH

Solves a complex Hermitian positive definite system of linear equations in band Hermitian storage mode with iterative refinement.

Required Arguments

A — Complex NCODA + 1 by N array containing the N by N positive definite band Hermitian coefficient matrix in band Hermitian storage mode. (Input)

NCODA — Number of upper or lower codiagonals of A. (Input)

B — Complex vector of length N containing the right-hand side of the linear system. (Input)

X — Complex vector of length N containing the solution to the linear system. (Output)

Optional Arguments

N — Number of equations. (Input)
Default: N = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

FORTRAN 90 Interface

Generic: CALL LSAQH (A, NCODA, B, X [, …])

Specific: The specific interface names are S_LSAQH and D_LSAQH.

FORTRAN 77 Interface

Single: CALL LSAQH (N, A, LDA, NCODA, B, X)

Double: The double precision name is DLSAQH.

Description

Routine LSAQH solves a system of linear algebraic equations having a complex Hermitian positive definite band coefficient matrix. It first uses the IMSL routine LFCQH to compute an $R^H R$ Cholesky factorization of the coefficient matrix and to estimate the condition number of the matrix. R is an upper triangular band matrix. The solution of the linear system is then found using the iterative refinement IMSL routine LFIQH.

LSAQH fails if any submatrix of R is not positive definite, if R has a zero diagonal element, or if the iterative refinement agorithm fails to converge. These errors occur only if the matrix A either is very close to a singular matrix or is a matrix that is not positive definite.

If the estimated condition number is greater than $1/\varepsilon$ (where ε is machine precision), a warning error is issued. This indicates that very small changes in A can cause very large changes in the solution x. Iterative refinement can sometimes find the solution to such a system. LSAQH solves the problem that is represented in the computer; however, this problem may differ from the problem whose solution is desired.

Comments

1. Workspace may be explicitly provided, if desired, by use of L2AQH/DL2AQH The reference is:

   CALL L2AQH (N, A, LDA, NCODA, B, X, FACT, WK)

   The additional arguments are as follows:

   FACT — Complex work vector of length (NCODA + 1) * N containing the $R^H R$ factorization of A in band Hermitian storage form on output.

   WK — Complex work vector of length N.

2. Informational errors

Type	Code	Description
3	3	The input matrix is too ill-conditioned. The solution might not be accurate.
3	4	The input matrix is not Hermitian. It has a diagonal entry with a small imaginary part.
4	2	The input matrix is not positive definite.
4	4	The input matrix is not Hermitian. It has a diagonal entry with an imaginary part.

3. *Integer Options* with *Chapter 11* Options Manager

   16 This option uses four values to solve memory bank conflict (access inefficiency) problems. In routine L2AQH the leading dimension of FACT is increased by IVAL(3) when N is a multiple of IVAL(4). The values IVAL(3) and IVAL(4) are temporarily replaced by IVAL(1) and IVAL(2), respectively, in LSAQH. Additional memory allocation for FACT and option value restoration are done automatically in LSAQH. Users directly calling L2AQH can allocate additional space for FACT and set IVAL(3) and IVAL(4) so that memory bank conflicts no longer cause inefficiencies. There is no requirement that users change existing applications that use LSAQH or L2AQH. Default values for the option are IVAL(*) = 1, 16, 0, 1.

17 This option has two values that determine if the L_1 condition number is to be computed. Routine LSAQH temporarily replaces IVAL(2) by IVAL(1). The routine L2CQH computes the condition number if IVAL(2) = 2. Otherwise L2CQH skips this computation. LSAQH restores the option. Default values for the option are IVAL(*) = 1, 2.

Example

A system of five linear equations is solved. The coefficient matrix has complex Hermitian positive definite band form with one codiagonal and the right-hand-side vector *b* has five elements.

```
      USE LSAQH_INT
      USE WRCRN_INT
!                                 Declare variables
      INTEGER    LDA, N, NCODA
      PARAMETER  (LDA=2, N=5, NCODA=1)
      COMPLEX    A(LDA,N), B(N), X(N)
!
!             Set values for A in band Hermitian form, and B
!
!             A = ( 0.0+0.0i -1.0+1.0i  1.0+2.0i  0.0+4.0i  1.0+1.0i )
!                 ( 2.0+0.0i  4.0+0.0i 10.0+0.0i  6.0+0.0i  9.0+0.0i )
!
!             B = ( 1.0+5.0i 12.0-6.0i  1.0-16.0i -3.0-3.0i 25.0+16.0i )
!
      DATA A/(0.0,0.0), (2.0,0.0), (-1.0,1.0), (4.0, 0.0), (1.0,2.0),&
            (10.0,0.0), (0.0,4.0), (6.0,0.0), (1.0,1.0), (9.0,0.0)/
      DATA B/(1.0,5.0), (12.0,-6.0), (1.0,-16.0), (-3.0,-3.0),&
            (25.0,16.0)/
!                                 Solve A*X = B
      CALL LSAQH (A, NCODA, B, X)
!                                 Print results
      CALL WRCRN ('X', X, 1, N, 1)
!
      END
```

Output

```
                                     X
              1                  2                  3                  4
  ( 2.000, 1.000)  ( 3.000, 0.000)  (-1.000,-1.000)  ( 0.000,-2.000)
              5
  ( 3.000, 2.000)
```

LSLQH

Solves a complex Hermitian positive definite system of linear equations in band Hermitian storage mode without iterative refinement.

Required Arguments

A — Complex NCODA + 1 by N array containing the N by N positive definite band Hermitian coefficient matrix in band Hermitian storage mode. (Input)

NCODA — Number of upper or lower codiagonals of A. (Input)

B — Complex vector of length N containing the right-hand side of the linear system. (Input)

X — Complex vector of length N containing the solution to the linear system. (Output)

Optional Arguments

N — Number of equations. (Input)
Default: N = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

FORTRAN 90 Interface

Generic: CALL LSLQH (A, NCODA, B, X [, …])

Specific: The specific interface names are S_LSLQH and D_LSLQH.

FORTRAN 77 Interface

Single: CALL LSLQH (N, A, LDA, NCODA, B, X)

Double: The double precision name is DLSLQH.

Description

Routine LSLQH solves a system of linear algebraic equations having a complex Hermitian positive definite band coefficient matrix. It first uses the routine LFCQH to compute an $R^H R$ Cholesky factorization of the coefficient matrix and to estimate the condition number of the matrix. R is an upper triangular band matrix. The solution of the linear system is then found using the routine LFSQH.

LSLQH fails if any submatrix of R is not positive definite or if R has a zero diagonal element. These errors occur only if A either is very close to a singular matrix or is a matrix that is not positive definite.

If the estimated condition number is greater than $1/\varepsilon$ (where ε is machine precision), a warning error is issued. This indicates that very small changes in A can cause very large changes in the solution x. If the coefficient matrix is ill-conditioned or poorly sealed, it is recommended that LSAQH be used.

Comments

1. Workspace may be explicitly provided, if desired, by use of L2LQH/DL2LQH The reference is:

   CALL L2LQH (N, A, LDA, NCODA, B, X, FACT, WK)

   The additional arguments are as follows:

   FACT — (NCODA + 1) × N complex work array containing the $R^H R$ factorization of A in band Hermitian storage form on output. If A is not needed, A and FACT can share the same storage locations.

   WK — Complex work vector of length N.

2. Informational errors

Type	Code	Description
3	3	The input matrix is too ill-conditioned. The solution might not be accurate.
3	4	The input matrix is not Hermitian. It has a diagonal entry with a small imaginary part.
4	2	The input matrix is not positive definite.
4	4	The input matrix is not Hermitian. It has a diagonal entry with an imaginary part.

3. *Integer Options* with *Chapter 11* Options Manager

   16 This option uses four values to solve memory bank conflict (access inefficiency) problems. In routine L2LQH the leading dimension of FACT is increased by IVAL(3) when N is a multiple of IVAL(4). The values IVAL(3) and IVAL(4) are temporarily replaced by IVAL(1) and IVAL(2), respectively, in LSLQH. Additional memory allocation for FACT and option value restoration are done automatically in LSLQH. Users directly calling L2LQH can allocate additional space for `FACT` and set `IVAL`(3) and `IVAL`(4) so that memory bank conflicts no longer cause inefficiencies. There is no requirement that users change existing applications that use `LSLQH` or `L2LQH`. Default values for the option are `IVAL(*)` = 1, 16, 0, 1.

17 This option has two values that determine if the L_1 condition number is to be computed. Routine `LSLQH` temporarily replaces `IVAL`(2) by `IVAL`(1). The routine `L2CQH` computes the condition number if `IVAL`(2) = 2. Otherwise `L2CQH` skips this computation. `LSLQH` restores the option. Default values for the option are `IVAL(*)` = 1, 2.

Example

A system of five linear equations is solved. The coefficient matrix has complex Hermitian positive definite band form with one codiagonal and the right-hand-side vector *b* has five elements.

```
      USE LSLQH_INT
      USE WRCRN_INT
!                                 Declare variables
      INTEGER    N, NCODA, LDA
      PARAMETER  (N=5, NCODA=1, LDA=NCODA+1)
      COMPLEX    A(LDA,N), B(N), X(N)
!
!             Set values for A in band Hermitian form, and B
!
!             A = ( 0.0+0.0i -1.0+1.0i  1.0+2.0i  0.0+4.0i  1.0+1.0i )
!                 ( 2.0+0.0i  4.0+0.0i 10.0+0.0i  6.0+0.0i  9.0+0.0i )
!
!             B = ( 1.0+5.0i 12.0-6.0i  1.0-16.0i -3.0-3.0i 25.0+16.0i )
!
      DATA A/(0.0,0.0), (2.0,0.0), (-1.0,1.0), (4.0, 0.0), (1.0,2.0),&
            (10.0,0.0), (0.0,4.0), (6.0,0.0), (1.0,1.0), (9.0,0.0)/
      DATA B/(1.0,5.0), (12.0,-6.0), (1.0,-16.0), (-3.0,-3.0),&
            (25.0,16.0)/
!                                 Solve A*X = B
      CALL LSLQH (A, NCODA, B, X)
!                                 Print results
      CALL WRCRN ('X', X, 1, N, 1)
!
      END
```

Output

```
                                    X
               1                  2                  3                  4
 ( 2.000, 1.000)  ( 3.000, 0.000)  (-1.000,-1.000)  ( 0.000,-2.000)

               5
 ( 3.000, 2.000)
```

LSLQB

Computes the $R^H DR$ Cholesky factorization of a complex Hermitian positive-definite matrix *A* in codiagonal band Hermitian storage mode. Solve a system *Ax* = *b*.

Required Arguments

A — Array containing the N by N positive-definite band coefficient matrix and the right hand side in codiagonal band Hermitian storage mode. (Input/Output)
The number of array columns must be at least 2 * NCODA + 3. The number of columns is not an input to this subprogram.

NCODA — Number of upper codiagonals of matrix A. (Input)
Must satisfy NCODA ≥ 0 and NCODA < N.

U — Array of flags that indicate any singularities of A, namely loss of positive-definiteness of a leading minor. (Output)
A value U(I) = 0. means that the leading minor of dimension I is not positive-definite. Otherwise, U(I) = 1.

Optional Arguments

N — Order of the matrix. (Input)
Must satisfy N > 0.
Default: N = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Must satisfy LDA ≥ N + NCODA.
Default: LDA = size (A,1).

IJOB — flag to direct the desired factorization or solving step. (Input)
Default: IJOB = 1.

IJOBMeaning

1 factor the matrix A and solve the system A*x* = *b*; where the real part of *b* is stored in column 2 * NCODA + 2 and the imaginary part of *b* is stored in column 2 * NCODA + 3 of array A. The real and imaginary parts of *b* are overwritten by the real and imaginary parts of *x*.

2 solve step only. Use the real part of *b* as column 2 * NCODA + 2 and the imaginary part of *b* as column 2 * NCODA + 3 of A. (The factorization step has already been done.) The real and imaginary parts of *b* are overwritten by the real and imaginary parts of *x*.

3 factor the matrix A but do not solve a system.

4,5,6 same meaning as with the value IJOB − 3. For efficiency, no error checking is done on values LDA, N, NCODA, and U(*).

FORTRAN 90 Interface

Generic: CALL LSLQB (A, NCODA, U [, …])

Specific: The specific interface names are S_LSLQB and D_LSLQB.

FORTRAN 77 Interface

Single: CALL LSLQB (N, A, LDA, NCODA, IJOB, U)

Double: The double precision name is DLSLQB.

Description

Routine LSLQB factors and solves the Hermitian positive definite banded linear system $Ax = b$. The matrix is factored so that $A = R^H DR$, where R is unit upper triangular and D is diagonal and real. The reciprocals of the diagonal entries of D are computed and saved to make the solving step more efficient. Errors will occur if D has a nonpositive diagonal element. Such events occur only if A is very close to a singular matrix or is not positive definite.

LSLQB is efficient for problems with a small band width. The particular cases NCODA = 0, 1 are done with special loops within the code. These cases will give good performance. See Hanson (1989) for more on the algorithm. When solving tridiagonal systems, NCODA = 1, the cyclic reduction code LSLCQ should be considered as an alternative. The expectation is that LSLCQ will outperform LSLQB on vector or parallel computers. It may be inferior on scalar computers or even parallel computers with non-optimizing compilers.

Comments

1. Workspace may be explicitly provided, if desired, by use of L2LQB/DL2LQB The reference is:

   CALL L2LQB (N, A, LDA, NCODA, IJOB, U, WK1, WK2)

   The additional arguments are as follows:

   WK1 — Work vector of length NCODA.

   WK2 — Work vector of length NCODA.

2. Informational error

Type	Code	Description
4	2	The input matrix is not positive definite.

Example

A system of five linear equations is solved. The coefficient matrix has real positive definite codiagonal Hermitian band form and the right-hand-side vector *b* has five elements.

```
      USE LSLQB_INT
      USE WRRRN_INT
      INTEGER    LDA, N, NCODA
      PARAMETER  (N=5, NCODA=1, LDA=N+NCODA)
!
      INTEGER    I, IJOB, J
      REAL       A(LDA,2*NCODA+3), U(N)
!
!                                 Set values for A and right hand side
!                                 in codiagonal band Hermitian form:
!
!                           (  *     *     *     *     * )
!                           ( 2.0    *     *    1.0   5.0)
!                  A   =    ( 4.0  -1.0   1.0  12.0  -6.0)
!                           (10.0   1.0   2.0   1.0 -16.0)
!                           ( 6.0   0.0   4.0  -3.0  -3.0)
!                           ( 9.0   1.0   1.0  25.0  16.0)
!
      DATA ((A(I+NCODA,J),I=1,N),J=1,2*NCODA+3)/2.0, 4.0, 10.0, 6.0,&
          9.0, 0.0, -1.0, 1.0, 0.0, 1.0, 0.0, 1.0, 2.0, 4.0, 1.0,&
          1.0, 12.0, 1.0, -3.0, 25.0, 5.0, -6.0, -16.0, -3.0, 16.0/
!
!                                 Factor and solve A*x = b.
!
      IJOB = 1
      CALL LSLQB (A, NCODA, U)
!
!                                 Print results
!
      CALL WRRRN ('REAL(X)', A((NCODA+1):,(2*NCODA+2):), 1, N, 1)
      CALL WRRRN ('IMAG(X)', A((NCODA+1):,(2*NCODA+3):), 1, N, 1)
      END
```

Output

```
                  REAL(X)
    1        2        3        4        5
2.000    3.000   -1.000    0.000    3.000

                 IMAG(X)
    1        2        3        4        5
1.000    0.000   -1.000   -2.000    2.000
```

LFCQH

Computes the $R^H R$ factorization of a complex Hermitian positive definite matrix in band Hermitian storage mode and estimate its L_1 condition number.

Required Arguments

A — Complex `NCODA` + 1 by `N` array containing the `N` by `N` positive definite band Hermitian matrix to be factored in band Hermitian storage mode. (Input)

NCODA — Number of upper or lower codiagonals of `A`. (Input)

FACT — Complex `NCODA` + 1 by `N` array containing the $R^H R$ factorization of the matrix `A`. (Output)
If `A` is not needed, `A` and `FACT` can share the same storage locations.

RCOND — Scalar containing an estimate of the reciprocal of the L_1 condition number of `A`. (Output)

Optional Arguments

N — Order of the matrix. (Input)
Default: `N` = size (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = size (`A`,1).

LDFACT — Leading dimension of `FACT` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDFACT` = size (`FACT`,1).

FORTRAN 90 Interface

Generic: `CALL LFCQH` (`A`, `NCODA`, `FACT`, `RCOND` `[, …]`)

Specific: The specific interface names are `S_LFCQH` and `D_LFCQH`.

FORTRAN 77 Interface

Single: `CALL LFCQH` (`N`, `A`, `LDA`, `NCODA`, `FACT`, `LDFACT`, `RCOND`)

Double: The double precision name is `DLFCQH`.

Description

Routine LFCQH computes an $R^H R$ Cholesky factorization and estimates the condition number of a complex Hermitian positive definite band coefficient matrix. R is an upper triangular band matrix.

The L_1 condition number of the matrix A is defined to be $\kappa(A) = \|A\|_1 \|A^{-1}\|_1$. Since it is expensive to compute $\|A^{-1}\|_1$, the condition number is only estimated. The estimation algorithm is the same as used by LINPACK and is described by Cline et al. (1979).

If the estimated condition number is greater than $1/\varepsilon$ (where ε is machine precision), a warning error is issued. This indicates that very small changes in A can cause very large changes in the solution x. Iterative refinement can sometimes find the solution to such a system.

LFCQH fails if any submatrix of R is not positive definite or if R has a zero diagonal element. These errors occur only if A either is very close to a singular matrix or is a matrix which is not positive definite.

The $R^H R$ factors are returned in a form that is compatible with routines LFIQH, LFSQH and LFDQH. To solve systems of equations with multiple right-hand-side vectors, use LFCQH followed by either LFIQH or LFSQH called once for each right-hand side. The routine LFDQH can be called to compute the determinant of the coefficient matrix after LFCQH has performed the factorization.

LFCQH is based on the LINPACK routine CPBCO; see Dongarra et al. (1979).

Comments

1. Workspace may be explicitly provided, if desired, by use of L2CQH/DL2CQH. The reference is:

   CALL L2CQH (N, A, LDA, NCODA, FACT, LDFACT, RCOND, WK)

   The additional argument is:

   WK — Complex work vector of length N.

2. Informational errors

Type	Code	Description
3	1	The input matrix is algorithmically singular.
3	4	The input matrix is not Hermitian. It has a diagonal entry with a small imaginary part.
4	2	The input matrix is not positive definite.
4	4	The input matrix is not Hermitian. It has a diagonal entry with an imaginary part

Example

The inverse of a 5 × 5 band Hermitian matrix with one codiagonal is computed. LFCQH is called to factor the matrix and to check for nonpositive definiteness or ill-conditioning. LFIQH is called to determine the columns of the inverse.

```
      USE LFCQH_INT
      USE LFIQH_INT
      USE UMACH_INT
      USE WRCRN_INT
!                                 Declare variables
      INTEGER    N, NCODA, LDA, LDFACT, NOUT
      PARAMETER  (N=5, NCODA=1, LDA=NCODA+1, LDFACT=LDA)
      REAL       RCOND
      COMPLEX    A(LDA,N), AINV(N,N), FACT(LDFACT,N), RES(N), RJ(N)
!
!             Set values for A in band Hermitian form
!
!             A = ( 0.0+0.0i -1.0+1.0i  1.0+2.0i  0.0+4.0i  1.0+1.0i )
!                 ( 2.0+0.0i  4.0+0.0i 10.0+0.0i  6.0+0.0i  9.0+0.0i )
!
      DATA A/(0.0,0.0), (2.0,0.0), (-1.0,1.0), (4.0, 0.0), (1.0,2.0), &
            (10.0,0.0), (0.0,4.0), (6.0,0.0), (1.0,1.0), (9.0,0.0)/
!                                 Factor the matrix A
      CALL LFCQH (A, NCODA, FACT, RCOND)
!                                 Set up the columns of the identity
!                                 matrix one at a time in RJ
      RJ = (0.0E0,0.0E0)
      DO 10  J=1, N
         RJ(J) = (1.0E0,0.0E0)
!                                 RJ is the J-th column of the identity
!                                 matrix so the following LFIQH
!                                 reference places the J-th column of
!                                 the inverse of A in the J-th column
!                                 of AINV
         CALL LFIQH (A, NCODA, FACT, RJ, AINV(:,J), RES)
         RJ(J) = (0.0E0,0.0E0)
   10 CONTINUE
!                                 Print the results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) RCOND, 1.0E0/RCOND
      CALL WRCRN ('AINV', AINV)
!
99999 FORMAT ('  RCOND = ',F5.3,/,'  L1 Condition number = ',F6.3)
      END
```

Output

```
RCOND = 0.067
L1 Condition number = 14.961

                                     AINV
                    1                     2                     3                  4
1 ( 0.7166, 0.0000)  ( 0.2166,-0.2166)  (-0.0899,-0.0300) (-0.0207, 0.0622)
2 ( 0.2166, 0.2166)  ( 0.4332, 0.0000)  (-0.0599,-0.1198) (-0.0829, 0.0415)
3 (-0.0899, 0.0300)  (-0.0599, 0.1198)  ( 0.1797, 0.0000) ( 0.0000,-0.1244)
4 (-0.0207,-0.0622)  (-0.0829,-0.0415)  ( 0.0000, 0.1244) ( 0.2592, 0.0000)
5 ( 0.0092, 0.0046)  ( 0.0138,-0.0046)  (-0.0138,-0.0138) (-0.0288, 0.0288)
                     5
1  ( 0.0092,-0.0046)
2  ( 0.0138, 0.0046)
3  (-0.0138, 0.0138)
```

```
 4  (-0.0288,-0.0288)
 5  ( 0.1175, 0.0000)
```

LFTQH

Computes the $R^H R$ factorization of a complex Hermitian positive definite matrix in band Hermitian storage mode.

Required Arguments

A — Complex NCODA + 1 by N array containing the N by N positive definite band Hermitian matrix to be factored in band Hermitian storage mode. (Input)

NCODA — Number of upper or lower codiagonals of A. (Input)

FACT — Complex NCODA + 1 by N array containing the $R^H R$ factorization of the matrix A. (Output)
If A is not needed, A and FACT can share the same storage locations.

Optional Arguments

N — Order of the matrix. (Input)
Default: N = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

LDFACT — Leading dimension of FACT exactly as specified in the dimension statement of the calling program. (Input)
Default: LDFACT = size (FACT,1).

FORTRAN 90 Interface

Generic: CALL LFTQH (A, NCODA, FACT [, …])

Specific: The specific interface names are S_LFTQH and D_LFTQH.

FORTRAN 77 Interface

Single: CALL LFTQH (N, A, LDA, NCODA, FACT, LDFACT)

Double: The double precision name is DLFTQH.

Description

Routine LFTQH computes an $R^H R$ Cholesky factorization of a complex Hermitian positive definite band coefficient matrix. R is an upper triangular band matrix.

LFTQH fails if any submatrix of R is not positive definite or if R has a zero diagonal element. These errors occur only if A either is very close to a singular matrix or is a matrix which is not positive definite.

The $R^H R$ factors are returned in a form that is compatible with routines LFIQH, LFSQH and LFDQH. To solve systems of equations with multiple right-hand-side vectors, use LFTQH followed by either LFIQH or LFSQH called once for each right-hand side. The routine LFDQH can be called to compute the determinant of the coefficient matrix after LFTQH has performed the factorization.

LFTQH is based on the LINPACK routine SPBFA; see Dongarra et al. (1979).

Comments

Informational errors

Type	Code	Description
3	4	The input matrix is not Hermitian. It has a diagonal entry with a small imaginary part.
4	2	The input matrix is not positive definite.
4	4	The input matrix is not Hermitian. It has a diagonal entry with an imaginary part.

Example

The inverse of a 5 × 5 band Hermitian matrix with one codiagonal is computed. LFTQH is called to factor the matrix and to check for nonpositive definiteness. LFSQH is called to determine the columns of the inverse.

```
      USE LFTQH_INT
      USE LFSQH_INT
      USE WRCRN_INT
!                                 Declare variables
      INTEGER    LDA, LDFACT, N, NCODA
      PARAMETER  (LDA=2, LDFACT=2, N=5, NCODA=1)
      COMPLEX    A(LDA,N), AINV(N,N), FACT(LDFACT,N), RJ(N)
!
!            Set values for A in band Hermitian form
!
!            A = ( 0.0+0.0i -1.0+1.0i  1.0+2.0i  0.0+4.0i  1.0+1.0i )
!                ( 2.0+0.0i  4.0+0.0i 10.0+0.0i  6.0+0.0i  9.0+0.0i )
!
      DATA A/(0.0,0.0), (2.0,0.0), (-1.0,1.0), (4.0, 0.0), (1.0,2.0),&
            (10.0,0.0), (0.0,4.0), (6.0,0.0), (1.0,1.0), (9.0,0.0)/
!                                 Factor the matrix A
```

```
      CALL LFTQH (A, NCODA, FACT)
!                                   Set up the columns of the identity
!                                   matrix one at a time in RJ
      RJ = (0.0E0,0.0E0)
      DO 10  J=1, N
         RJ(J) = (1.0E0,0.0E0)
!                                   RJ is the J-th column of the identity
!                                   matrix so the following LFSQH
!                                   reference places the J-th column of
!                                   the inverse of A in the J-th column
!                                   of AINV
         CALL LFSQH (FACT, NCODA, RJ, AINV(:,J))
         RJ(J) = (0.0E0,0.0E0)
   10 CONTINUE
!                                   Print the results
      CALL WRCRN ('AINV', AINV)
!
      END
```

Output

```
                                        AINV
                  1                   2                   3                 4
1 ( 0.7166, 0.0000) ( 0.2166,-0.2166)  (-0.0899,-0.0300)  (-0.0207, 0.0622)
2 ( 0.2166, 0.2166) ( 0.4332, 0.0000)  (-0.0599,-0.1198)  (-0.0829, 0.0415)
3 (-0.0899, 0.0300) (-0.0599, 0.1198)  ( 0.1797, 0.0000)  ( 0.0000,-0.1244)
4 (-0.0207,-0.0622) (-0.0829,-0.0415)  ( 0.0000, 0.1244)  ( 0.2592, 0.0000)
5 ( 0.0092, 0.0046) ( 0.0138,-0.0046)  (-0.0138,-0.0138)  (-0.0288, 0.0288)
                   5
1  ( 0.0092,-0.0046)
2  ( 0.0138, 0.0046)
3  (-0.0138, 0.0138)
4  (-0.0288,-0.0288)
5  ( 0.1175, 0.0000)
```

LFSQH

Solves a complex Hermitian positive definite system of linear equations given the factorization of the coefficient matrix in band Hermitian storage mode.

Required Arguments

FACT — Complex NCODA + 1 by N array containing the $R^H R$ factorization of the Hermitian positive definite band matrix A. (Input)
FACT is obtained as output from routine LFCQH/DLFCQH or LFTQH/DLFTQH .

NCODA — Number of upper or lower codiagonals of A. (Input)

B — Complex vector of length N containing the right-hand-side of the linear system. (Input)

X — Complex vector of length N containing the solution to the linear system. (Output)
If B is not needed, B and X can share the same storage locations.

Optional Arguments

N — Number of equations. (Input)
Default: N = size (FACT,2).

LDFACT — Leading dimension of FACT exactly as specified in the dimension statement of the calling program. (Input)
Default: LDFACT = size (FACT,1).

FORTRAN 90 Interface

Generic: CALL LFSQH (FACT, NCODA, B, X [, …])

Specific: The specific interface names are S_LFSQH and D_LFSQH.

FORTRAN 77 Interface

Single: CALL LFSQH (N, FACT, LDFACT, NCODA, B, X)

Double: The double precision name is DLFSQH.

Description

Routine LFSQH computes the solution for a system of linear algebraic equations having a complex Hermitian positive definite band coefficient matrix. To compute the solution, the coefficient matrix must first undergo an $R^H R$ factorization. This may be done by calling either IMSL routine LFCQH or LFTQH. R is an upper triangular band matrix.

The solution to $Ax = b$ is found by solving the triangular systems $R^H y = b$ and $Rx = y$.

LFSQH and LFIQH both solve a linear system given its $R^H R$ factorization. LFIQH generally takes more time and produces a more accurate answer than LFSQH. Each iteration of the iterative refinement algorithm used by LFIQH calls LFSQH.

LFSQH is based on the LINPACK routine CPBSL; see Dongarra et al. (1979).

Comments

Informational error

Type	Code	Description
4	1	The factored matrix has a diagonal element close to zero.

Example

A set of linear systems is solved successively. LFTQH is called to factor the coefficient matrix. LFSQH is called to compute the three solutions for the three right-hand sides. In this case the coefficient matrix is assumed to be well-conditioned and correctly scaled. Otherwise, it would be better to call LFCQH to perform the factorization, and LFIQH to compute the solutions.

```
      USE LFSQH_INT
      USE LFTQH_INT
      USE WRCRN_INT
!                                 Declare variables
      INTEGER    LDA, LDFACT, N, NCODA
      PARAMETER  (LDA=2, LDFACT=2, N=5, NCODA=1)
      COMPLEX    A(LDA,N), B(N,3), FACT(LDFACT,N), X(N,3)
!
!             Set values for A in band Hermitian form, and B
!
!             A = ( 0.0+0.0i -1.0+1.0i  1.0+2.0i  0.0+4.0i  1.0+1.0i )
!                 ( 2.0+0.0i  4.0+0.0i 10.0+0.0i  6.0+0.0i  9.0+0.0i )
!
!             B = (  3.0+3.0i   4.0+0.0i   29.0-9.0i  )
!                 (  5.0-5.0i  15.0-10.0i -36.0-17.0i )
!                 (  5.0+4.0i -12.0-56.0i -15.0-24.0i )
!                 (  9.0+7.0i -12.0+10.0i -23.0-15.0i )
!                 (-22.0+1.0i   3.0-1.0i  -23.0-28.0i )
!
```

```
      DATA A/(0.0,0.0), (2.0,0.0), (-1.0,1.0), (4.0, 0.0), (1.0,2.0),&
            (10.0,0.0), (0.0,4.0), (6.0,0.0), (1.0,1.0), (9.0,0.0)/
      DATA B/(3.0,3.0), (5.0,-5.0), (5.0,4.0), (9.0,7.0), (-22.0,1.0),&
            (4.0,0.0), (15.0,-10.0), (-12.0,-56.0), (-12.0,10.0),&
            (3.0,-1.0), (29.0,-9.0), (-36.0,-17.0), (-15.0,-24.0),&
            (-23.0,-15.0), (-23.0,-28.0)/
!                                 Factor the matrix A
      CALL LFTQH (A, NCODA, FACT)
!                                 Compute the solutions
      DO 10  I=1, 3
         CALL LFSQH (FACT, NCODA, B(:,I), X(:,I))
   10 CONTINUE
!                                 Print solutions
      CALL WRCRN ('X', X)
      END
```

Output

```
                            X
                  1                  2                  3
1  (  1.00,  0.00)  (  3.00, -1.00)  ( 11.00, -1.00)
2  (  1.00, -2.00)  (  2.00,  0.00)  ( -7.00,  0.00)
3  (  2.00,  0.00)  ( -1.00, -6.00)  ( -2.00, -3.00)
4  (  2.00,  3.00)  (  2.00,  1.00)  ( -2.00, -3.00)
5  ( -3.00,  0.00)  (  0.00,  0.00)  ( -2.00, -3.00)
```

LFIQH

Uses iterative refinement to improve the solution of a complex Hermitian positive definite system of linear equations in band Hermitian storage mode.

Required Arguments

A — Complex NCODA + 1 by N array containing the N by N positive definite band Hermitian coefficient matrix in band Hermitian storage mode. (Input)

NCODA — Number of upper or lower codiagonals of A. (Input)

FACT — Complex NCODA + 1 by N array containing the $R^H R$ factorization of the matrix A as output from routine LFCQH/DLFCQH or LFTQH/DLFTQH. (Input)

B — Complex vector of length N containing the right-hand side of the linear system. (Input)

X — Complex vector of length N containing the solution to the linear system. (Output)

RES — Complex vector of length N containing the residual vector at the improved solution. (Output)

Optional Arguments

N — Number of equations. (Input)
Default: N = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

LDFACT — Leading dimension of FACT exactly as specified in the dimension statement of the calling program. (Input)
Default: LDFACT = size (FACT,1).

FORTRAN 90 Interface

Generic: CALL LFIQH (A, NCODA, FACT, B, X, RES [, …])

Specific: The specific interface names are S_LFIQH and D_LFIQH.

FORTRAN 77 Interface

Single: CALL LFIQH (N, A, LDA, NCODA, FACT, LDFACT, B, X, RES)

Double: The double precision name is DLFIQH.

Description

Routine LFIQH computes the solution for a system of linear algebraic equations having a complex Hermitian positive definite band coefficient matrix. To compute the solution, the coefficient matrix must first undergo an $R^H R$ factorization. This may be done by calling either IMSL routine LFCQH or LFTQH. R is an upper triangular band matrix.

The solution to $Ax = b$ is found by solving the triangular systems $R^H y = b$ and $Rx = y$.

LFSQH and LFIQH both solve a linear system given its $R^H R$ factorization. LFIQH generally takes more time and produces a more accurate answer than LFSQH. Each iteration of the iterative refinement algorithm used by LFIQH calls LFSQH.

Comments

Informational error

Type	Code	Description
4	1	The factored matrix has a diagonal element close to zero.

Example

A set of linear systems is solved successively. The right-hand side vector is perturbed after solving the system each of the fisrt two times by adding $(1 + i)/2$ to the second element.

```
      USE IMSL_LIBRARIES
!                                 Declare variables
      INTEGER    LDA, LDFACT, N, NCODA
      PARAMETER  (LDA=2, LDFACT=2, N=5, NCODA=1)
      REAL       RCOND
      COMPLEX    A(LDA,N), B(N), FACT(LDFACT,N), RES(N,3), X(N,3)
!
!             Set values for A in band Hermitian form, and B
!
!             A = ( 0.0+0.0i -1.0+1.0i  1.0+2.0i  0.0+4.0i  1.0+1.0i )
!                 ( 2.0+0.0i  4.0+0.0i 10.0+0.0i  6.0+0.0i  9.0+0.0i )
!
!             B = (  3.0+3.0i 5.0-5.0i  5.0+4.0i 9.0+7.0i -22.0+1.0i )
!
      DATA A/(0.0,0.0), (2.0,0.0), (-1.0,1.0), (4.0, 0.0), (1.0,2.0),&
            (10.0,0.0), (0.0,4.0), (6.0,0.0), (1.0,1.0), (9.0,0.0)/
```

```
      DATA B/(3.0,3.0), (5.0,-5.0), (5.0,4.0), (9.0,7.0), (-22.0,1.0)/
!                                Factor the matrix A
      CALL LFCQH (A, NCODA, FACT, RCOND=RCOND)
!                                Print the estimated condition number
      CALL UMACH (2, NOUT)
      WRITE (NOUT, 99999) RCOND, 1.0E0/RCOND
!                                Compute the solutions
      DO 10  I=1, 3
         CALL LFIQH (A, NCODA, FACT,  B, X(:,I), RES(:,I))
         B(2) = B(2) + (0.5E0, 0.5E0)
   10 CONTINUE
!                                Print solutions
      CALL WRCRN ('X', X)
      CALL WRCRN ('RES', RES)
99999 FORMAT ('  RCOND = ', F5.3, /, '  L1 Condition number = ', F6.3)
      END
```

Output

```
                           X
                 1                 2                 3
1  (  1.00,  0.00)  (  3.00, -1.00)  ( 11.00, -1.00)
2  (  1.00, -2.00)  (  2.00,  0.00)  ( -7.00,  0.00)
3  (  2.00,  0.00)  ( -1.00, -6.00)  ( -2.00, -3.00)
4  (  2.00,  3.00)  (  2.00,  1.00)  ( -2.00, -3.00)
5  ( -3.00,  0.00)  (  0.00,  0.00)  ( -2.00, -3.00)
```

LFDQH

Computes the determinant of a complex Hermitian positive definite matrix given the $R^H R$ Cholesky factorization in band Hermitian storage mode.

Required Arguments

FACT — Complex NCODA + 1 by N array containing the $R^H R$ factorization of the Hermitian positive definite band matrix A. (Input)
FACT is obtained as output from routine LFCQH/DLFCQH or LFTQH/DLFTQH.

NCODA — Number of upper or lower codiagonals of A. (Input)

DET1 — Scalar containing the mantissa of the determinant. (Output)
The value DET1 is normalized so that 1.0 ≤ |DET1| < 10.0 or DET1 = 0.0.

DET2 — Scalar containing the exponent of the determinant. (Output)
The determinant is returned in the form det (*A*) = DET1 * 10^{DET2}.

Optional Arguments

N — Number of equations. (Input)
Default: N = size (FACT,2).

LDFACT — Leading dimension of FACT exactly as specified in the dimension statement of the calling program. (Input)
Default: LDFACT = size (FACT,1).

FORTRAN 90 Interface

Generic: CALL LFDQH (FACT, NCODA, DET1, DET2 [, …])

Specific: The specific interface names are S_LFDQH and D_LFDQH.

FORTRAN 77 Interface

Single: CALL LFDQH (N, FACT, LDFACT, NCODA, DET1, DET2)

Double: The double precision name is DLFDQH.

Description

Routine LFDQH computes the determinant of a complex Hermitian positive definite band coefficient matrix. To compute the determinant, the coefficient matrix must first undergo an $R^H R$ factorization. This may be done by calling either LFCQH or LFTQH. The formula $\det A = \det R^H \det R = (\det R)^2$ is used to compute the determinant. Since the determinant of a triangular matrix is the product of the diagonal elements,

$$\det R = \prod_{i=1}^{N} R_{ii}$$

LFDQH is based on the LINPACK routine CPBDI; see Dongarra et al. (1979).

Example

The determinant is computed for a 5 × 5 complex Hermitian positive definite band matrix with one codiagonal.

```
      USE LFDQH_INT
      USE LFTQH_INT
      USE UMACH_INT
!                                 Declare variables
      INTEGER    LDA, LDFACT, N, NCODA, NOUT
      PARAMETER  (LDA=2, N=5, LDFACT=2, NCODA=1)
      REAL       DET1, DET2
      COMPLEX    A(LDA,N), FACT(LDFACT,N)
!
!             Set values for A in band Hermitian form
!
!             A = ( 0.0+0.0i -1.0+1.0i  1.0+2.0i  0.0+4.0i  1.0+1.0i )
!                 ( 2.0+0.0i  4.0+0.0i 10.0+0.0i  6.0+0.0i  9.0+0.0i )
!
      DATA A/(0.0,0.0), (2.0,0.0), (-1.0,1.0), (4.0, 0.0), (1.0,2.0),&
            (10.0,0.0), (0.0,4.0), (6.0,0.0), (1.0,1.0), (9.0,0.0)/
!                                 Factor the matrix
      CALL LFTQH (A, NCODA, FACT)
!                                 Compute the determinant
      CALL LFDQH (FACT, NCODA, DET1, DET2)
!                                 Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) DET1, DET2
!
99999 FORMAT (' The determinant of A is ',F6.3,' * 10**',F2.0)
      END
```

Output

```
The determinant of A is  1.736 * 10**3.
```

LSLXG

Solves a sparse system of linear algebraic equations by Gaussian elimination.

NOTE: Additional sparse solvers are available in the *Sparse Matrix Computations* section.

Required Arguments

A — Vector of length NZ containing the nonzero coefficients of the linear system. (Input)

IROW — Vector of length NZ containing the row numbers of the corresponding elements in A. (Input)

JCOL — Vector of length NZ containing the column numbers of the corresponding elements in A. (Input)

B — Vector of length N containing the right-hand side of the linear system. (Input)

X — Vector of length N containing the solution to the linear system. (Output)

Optional Arguments

N — Number of equations. (Input)
Default: N = size (B,1).

NZ — The number of nonzero coefficients in the linear system. (Input)
Default: NZ = size (A,1).

IPATH — Path indicator. (Input)
IPATH = 1 means the system $Ax = b$ is solved.
IPATH = 2 means the system $A^T x = b$ is solved.
Default: IPATH = 1.

IPARAM — Parameter vector of length 6. (Input/Output)
Set IPARAM(1) to zero for default values of IPARAM and RPARAM.
Default: IPARAM(1) = 0.
See Comment 3.

RPARAM — Parameter vector of length 5. (Input/Output)
See Comment 3.

FORTRAN 90 Interface

Generic: `CALL LSLXG (A, IROW, JCOL, B, X [, …])`

Specific: The specific interface names are `S_LSLXG` and `D_LSLXG`.

FORTRAN 77 Interface

Single: `CALL LSLXG (N, NZ, A, IROW, JCOL, B, IPATH, IPARAM, RPARAM, X)`

Double: The double precision name is `DLSLXG`.

Description

Consider the linear equation

$$Ax = b$$

where *A* is a $n \times n$ sparse matrix. The sparse coordinate format for the matrix *A* requires one real and two integer vectors. The real array `a` contains all the nonzeros in *A*. Let the number of nonzeros be `nz`. The two integer arrays `irow` and `jcol`, each of length `nz`, contain the row and column numbers for these entries in *A*. That is

$$A_{\mathrm{irow}(i),\mathrm{icol}(i)} = a(i),\ i = 1, \ldots, \mathtt{nz}$$

with all other entries in *A* zero.

The routine `LSLXG` solves a system of linear algebraic equations having a real sparse coefficient matrix. It first uses the routine `LFTXG` to perform an *LU* factorization of the coefficient matrix. The solution of the linear system is then found using `LFSXG`.

The routine `LFTXG` by default uses a *symmetric Markowitz strategy* (Crowe et al. 1990) to choose pivots that most likely would reduce fill-ins while maintaining numerical stability. Different strategies are also provided as options for row oriented or column oriented problems. The algorithm can be expressed as

$$\mathrm{P\,AQ} = \mathrm{LU}$$

where *P* and *Q* are the row and column permutation matrices determined by the Markowitz strategy (Duff et al. 1986), and *L* and *U* are lower and upper triangular matrices, respectively.

Finally, the solution *x* is obtained by the following calculations:

$$1)\ Lz = Pb$$

$$2)\ Uy = z$$

$$3)\ x = Qy$$

Comments

1. Workspace may be explicitly provided, if desired, by use of L2LXG/DL2LXG. The reference is:

   CALL L2LXG (N, NZ, A, IROW, JCOL, B, IPATH, IPARAM, RPARAM, X, WK, LWK, IWK, LIWK)

   The additional arguments are as follows:

   WK — Real work vector of length LWK.

   LWK — The length of WK, LWK should be at least 2N + MAXNZ.

   IWK — Integer work vector of length LIWK.

   LIWK — The length of IWK, LIWK should be at least 17N + 4 * MAXNZ.

   MAXNZ is the maximal number of nonzero elements at any stage of the Gaussian elimination. In the absence of other information, setting MAXNZ equal to 3 * NZ is recommended. Higher or lower values may be used depending on fill-in. See also IPARAM(5) in Comment 3.

2. Informational errors

Type	Code	Description
3	1	The coefficient matrix is numerically singular.
3	2	The growth factor is too large to continue.
3	3	The matrix is too ill-conditioned for iterative refinement.

3. If the default parameters are desired for LSLXG, then set IPARAM(1) to zero and call the routine LSLXG. Otherwise, if any nondefault parameters are desired for IPARAM or RPARAM. then the following steps should be taken before calling LSLXG.

   CALL L4LXG (IPARAM, RPARAM)

   Set nondefault values for desired IPARAM, RPARAM elements.

Note that the call to L4LXG will set IPARAM and RPARAM to their default values, so only nondefault values need to be set above.

IPARAM — Integer vector of length 6.

IPARAM(1) = Initialization flag.

IPARAM(2) = The pivoting strategy

IPARAM(2)	Action
1	Markowitz row search
2	Markowitz column search
3	Symmetric Markowitz search

Default: 3.

IPARAM(3) = The number of rows which have least numbers of nonzero elements that will be searched for a pivotal element.
Default: 3.

IPARAM(4) = The maximal number of nonzero elements in A at any stage of the Gaussian elimination. (Output)

IPARAM(5) = The workspace limit.

IPARAM(5)	Action
0	Default limit. For single precision, 19N + 5 * MAXNZ. For double precision, 21N + 6 * MAXNZ. See comment 1 for the definition of MAXNZ.
integer	This integer value replaces the default workspace limit.

When L2LXG is called, the values of LWK and LIWK are used instead of IPARAM(5).
Default: 0.

IPARAM(6) = Iterative refinement is done when this is nonzero.
Default: 0.

RPARAM — Real vector of length 5.

RPARAM(1) = The upper limit on the growth factor. The computation stops when the growth factor exceeds the limit.
Default: 10^{16}

RPARAM(2) = The stability factor. The absolute value of the pivotal element must be bigger than the largest element in absolute value in its row divided by RPARAM(2).
Default: 10.0.

RPARAM(3) = Drop-tolerance. Any element in the lower triangular factor L will be removed if its absolute value becomes smaller than the drop-tolerance at any stage of the Gaussian elimination.
Default: 0.0.

RPARAM(4) = The growth factor. It is calculated as the largest element in absolute value in A at any stage of the Gaussian elimination divided by the largest element in absolute value in the original A matrix. (Output)
Large value of the growth factor indicates that an appreciable error in the computed solution is possible.

RPARAM(5) = The value of the smallest pivotal element in absolute value. (Output)

If double precision is required, then DL4LXG is called and RPARAM is declared double precision.

Example

As an example consider the 6×6 linear system:

$$A = \begin{bmatrix} 10 & 0 & 0 & 0 & 0 & 0 \\ 0 & 10 & -3 & -1 & 0 & 0 \\ 0 & 0 & 15 & 0 & 0 & 0 \\ -2 & 0 & 0 & 10 & -1 & 0 \\ -1 & 0 & 0 & -5 & 1 & -3 \\ -1 & -2 & 0 & 0 & 0 & 6 \end{bmatrix}$$

Let $x^T = (1, 2, 3, 4, 5, 6)$ so that $Ax = (10, 7, 45, 33, -34, 31)^T$. The number of nonzeros in A is `nz` = 15. The sparse coordinate form for A is given by:

irow	6	2	3	2	4	4	5	5	5	5	1	6	6	2	4
jcol	6	2	3	3	4	5	1	6	4	5	1	1	2	4	1
a	6	10	15	−3	10	−1	−1	−3	−5	1	10	−1	−2	−1	−2

```
      USE LSLXG_INT
      USE WRRRN_INT
      USE L4LXG_INT
      INTEGER    N, NZ
      PARAMETER  (N=6, NZ=15)
!
      INTEGER    IPARAM(6), IROW(NZ), JCOL(NZ)
      REAL       A(NZ), B(N), RPARAM(5), X(N)
!
      DATA A/6., 10., 15., -3., 10., -1., -1., -3., -5., 1., 10., -1.,&
          -2., -1., -2./
      DATA B/10., 7., 45., 33., -34., 31./
      DATA IROW/6, 2, 3, 2, 4, 4, 5, 5, 5, 5, 1, 6, 6, 2, 4/
      DATA JCOL/6, 2, 3, 3, 4, 5, 1, 6, 4, 5, 1, 1, 2, 4, 1/
!
!                                Change a default parameter
      CALL L4LXG (IPARAM, RPARAM)
      IPARAM(5) = 203
!                                Solve for X
      CALL LSLXG (A, IROW, JCOL, B, X, IPARAM=IPARAM)
!
      CALL WRRRN (' x ', X, 1, N, 1)
      END
```

Output

```
                        x
     1       2       3       4       5       6
 1.000   2.000   3.000   4.000   5.000   6.000
```

LFTXG

Computes the *LU* factorization of a real general sparse matrix.

NOTE: Additional sparse solvers are available in the *Sparse Matrix Computations* section.

Required Arguments

A — Vector of length `NZ` containing the nonzero coefficients of the linear system. (Input)

IROW — Vector of length `NZ` containing the row numbers of the corresponding elements in `A`. (Input)

JCOL — Vector of length `NZ` containing the column numbers of the corresponding elements in `A`. (Input)

NL — The number of nonzero coefficients in the triangular matrix *L* excluding the diagonal elements. (Output)

NFAC — On input, the dimension of vector `FACT`. (Input/Output)
On output, the number of nonzero coefficients in the triangular matrix *L* and *U*.

FACT — Vector of length `NFAC` containing the nonzero elements of *L* (excluding the diagonals) in the first `NL` locations and the nonzero elements of *U* in `NL` + 1 to `NFAC` locations. (Output)

IRFAC — Vector of length `NFAC` containing the row numbers of the corresponding elements in `FACT`. (Output)

JCFAC — Vector of length `NFAC` containing the column numbers of the corresponding elements in `FACT`. (Output)

IPVT — Vector of length `N` containing the row pivoting information for the *LU* factorization. (Output)

JPVT — Vector of length `N` containing the column pivoting information for the *LU* factorization. (Output)

Optional Arguments

N — Number of equations. (Input)
Default: `N` = size (`IPVT`,1).

NZ — The number of nonzero coefficients in the linear system. (Input)
Default: `NZ` = size (`A`,1).

IPARAM — Parameter vector of length 6. (Input/Output)
Set IPARAM(1) to zero for default values of IPARAM and RPARAM.
Default: IPARAM(1) = 0.
See Comment 3.

RPARAM — Parameter vector of length 5. (Input/Output)
See Comment 3.

FORTRAN 90 Interface

Generic: CALL LFTXG (A, IROW, JCOL, NL, NFAC, FACT, IRFAC, JCFAC, IPVT, JPVT [, …])

Specific: The specific interface names are S_LFTXG and D_LFTXG.

FORTRAN 77 Interface

Single: CALL LFTXG (N, NZ, A, IROW, JCOL, IPARAM, RPARAM, NFAC, NL, FACT, IRFAC, JCFAC, IPVT, JPVT)

Double: The double precision name is DLFTXG.

Description

Consider the linear equation

$$Ax = b$$

where A is a $n \times n$ sparse matrix. The sparse coordinate format for the matrix A requires one real and two integer vectors. The real array a contains all the nonzeros in A. Let the number of nonzeros be nz. The two integer arrays irow and jcol, each of length nz, contain the row and column numbers for these entries in A. That is

$$A_{\mathrm{irow}(i),\, \mathrm{icol}(i)} = a(i),\ i = 1, \ldots, \mathrm{nz}$$

with all other entries in A zero.

The routine LFTXG performs an LU factorization of the coefficient matrix A. It by default uses a *symmetric Markowitz strategy* (Crowe et al. 1990) to choose pivots that most likely would reduce fillins while maintaining numerical stability. Different strategies are also provided as options for row oriented or column oriented problems. The algorithm can be expressed as

$$PAQ = LU$$

where P and Q are the row and column permutation matrices determined by the Markowitz strategy (Duff et al. 1986), and L and U are lower and upper triangular matrices, respectively.

Finally, the solution x is obtained using LFSXG by the following calculations:

$$1)\ Lz = Pb$$

$$2)\ Uy = z$$

$$3)\ x = Qy$$

Comments

1.Workspace may be explicitly provided, if desired, by use of L2TXG/DL2TXG. The reference is:

CALL L2TXG (N, NZ, A, IROW, JCOL, IPARAM, RPARAM, NFAC, NL, FACT, IRFAC, JCFAC, IPVT, JPVT, WK, LWK, IWK, LIWK)

The additional arguments are as follows:

WK — Real work vector of length LWK.

LWK — The length of WK, LWK should be at least MAXNZ.

IWK — Integer work vector of length LIWK.

LIWK — The length of IWK, LIWK should be at least 15N + 4 * MAXNZ.

The workspace limit is determined by MAXNZ, where

MAXNZ = MIN0(LWK, INT(0.25(LIWK-15N)))

2. Informational errors

Type	Code	Description
3	1	The coefficient matrix is numerically singular.
3	2	The growth factor is too large to continue.

3. If the default parameters are desired for LFTXG, then set IPARAM(1) to zero and call the routine LFTXG. Otherwise, if any nondefault parameters are desired for IPARAM or RPARAM, then the following steps should be taken before calling LFTXG.

CALL L4LXG (IPARAM, RPARAM)

Set nondefault values for desired IPARAM, RPARAM elements.

Note that the call to L4LXG will set IPARAM and RPARAM to their default values, so only nondefault values need to be set above.

The arguments are as follows:

IPARAM — Integer vector of length 6.

IPARAM(1) = Initialization flag.

IPARAM(2) = The pivoting strategy.

IPARAM(2)	Action
1	Markowitz row search
2	Markowitz column search
3	Symmetric Markowitz search

Default: 3.

IPARAM(3) = The number of rows which have least numbers of nonzero elements that will be searched for a pivotal element.
Default: 3.

IPARAM(4) = The maximal number of nonzero elements in A at any stage of the Gaussian elimination. (Output)

IPARAM(5) = The workspace limit.

IPARAM(5)	Action
0	Default limit, see Comment 1.
integer	This integer value replaces the default workspace limit.

When L2TXG is called, the values of LWK and LIWK are used instead of IPARAM(5).

IPARAM(6) = Not used in LFTXG.

RPARAM — Real vector of length 5.

RPARAM(1) = The upper limit on the growth factor. The computation stops when the growth factor exceeds the limit.
Default: 10.

RPARAM(2) = The stability factor. The absolute value of the pivotal element must be bigger than the largest element in absolute value in its row divided by RPARAM(2).
Default: 10.0.

RPARAM(3) = Drop-tolerance. Any element in the lower triangular factor L will be removed if its absolute value becomes smaller than the drop-tolerance at any stage of the Gaussian elimination.
Default: 0.0.

RPARAM(4) = The growth factor. It is calculated as the largest element in absolute value in A at any stage of the Gaussian elimination divided by the largest element in absolute value in the original A matrix. (Output)
Large value of the growth factor indicates that an appreciable error in the computed solution is possible.

RPARAM(5) = The value of the smallest pivotal element in absolute value. (Output)

If double precision is required, then DL4LXG is called and RPARAM is declared double precision.

Example

As an example, consider the 6×6 matrix of a linear system:

$$A = \begin{bmatrix} 10 & 0 & 0 & 0 & 0 & 0 \\ 0 & 10 & -3 & -1 & 0 & 0 \\ 0 & 0 & 15 & 0 & 0 & 0 \\ -2 & 0 & 0 & 10 & -1 & 0 \\ -1 & 0 & 0 & -5 & 1 & -3 \\ -1 & -2 & 0 & 0 & 0 & 6 \end{bmatrix}$$

The sparse coordinate form for *A* is given by:

irow	6	2	3	2	4	4	5	5	5	5	1	6	6	2	4
jcol	6	2	3	3	4	5	1	6	4	5	1	1	2	4	1
a	6	10	15	−3	10	−1	−1	−3	−5	1	10	−1	−2	−1	−2

```
      USE LFTXG_INT
      USE WRRRN_INT
      USE WRIRN_INT
      INTEGER     N, NZ
      PARAMETER   (N=6, NZ=15)
      INTEGER     IROW(NZ), JCOL(NZ), NFAC, NL,&
                  IRFAC(3*NZ), JCFAC(3*NZ), IPVT(N), JPVT(N)
      REAL        A(NZ), FACT(3*NZ)
!
      DATA A/6., 10., 15., -3., 10., -1., -1., -3., -5., 1., 10., -1.,&
            -2., -1., -2./
      DATA IROW/6, 2, 3, 2, 4, 4, 5, 5, 5, 5, 1, 6, 6, 2, 4/
      DATA JCOL/6, 2, 3, 3, 4, 5, 1, 6, 4, 5, 1, 1, 2, 4, 1/
!
      NFAC = 3*NZ
!                                  Use default options
      CALL LFTXG (A, IROW, JCOL, NL, NFAC, FACT, IRFAC, JCFAC, IPVT, JPVT)
!
      CALL WRRRN (' fact ', FACT, 1, NFAC, 1)
      CALL WRIRN (' irfac ', IRFAC, 1, NFAC, 1)
      CALL WRIRN (' jcfac ', JCFAC, 1, NFAC, 1)
      CALL WRIRN (' p ', IPVT, 1, N, 1)
      CALL WRIRN (' q ', JPVT, 1, N, 1)

!
      END
```

Output

```
                                        fact
    1       2       3       4       5       6       7       8       9     10
-0.10  -5.00  -0.20  -0.10  -0.10  -1.00  -0.20   4.90  -5.10   1.00
   11      12      13      14      15      16
-1.00   30.00    6.00   -2.00   10.00   15.00

                                 irfac
1   2   3   4   5   6   7   8   9  10  11  12  13  14  15  16
3   4   4   5   5   6   6   6   5   5   4   4   3   3   2   1
```

```
                              jcfac
 1   2   3   4   5   6   7   8   9  10  11  12  13  14  15  16
 2   3   1   4   2   5   2   6   6   5   6   4   4   3   2   1

             p
 1   2   3   4   5   6
 3   1   6   2   5   4

             q
 1   2   3   4   5   6
 3   1   2   6   5   4
```

LFSXG

Solves a sparse system of linear equations given the *LU* factorization of the coefficient matrix.

NOTE: Additional sparse solvers are available in the *Sparse Matrix Computations* section.

Required Arguments

NFAC — The number of nonzero coefficients in `FACT` as output from subroutine `LFTXG/DLFTXG`. (Input)

NL — The number of nonzero coefficients in the triangular matrix *L* excluding the diagonal elements as output from subroutine `LFTXG/DLFTXG`. (Input)

FACT — Vector of length `NFAC` containing the nonzero elements of *L* (excluding the diagonals) in the first `NL` locations and the nonzero elements of *U* in `NL` + 1 to `NFAC` locations as output from subroutine `LFTXG/DLFTXG`. (Input)

IRFAC — Vector of length `NFAC` containing the row numbers of the corresponding elements in `FACT` as output from subroutine `LFTXG/DLFTXG`. (Input)

JCFAC — Vector of length `NFAC` containing the column numbers of the corresponding elements in `FACT` as output from subroutine `LFTXG/DLFTXG`. (Input)

IPVT — Vector of length `N` containing the row pivoting information for the *LU* factorization as output from subroutine `LFTXG/DLFTXG`. (Input)

JPVT — Vector of length `N` containing the column pivoting information for the *LU* factorization as output from subroutine `LFTXG/DLFTXG`. (Input)

B — Vector of length `N` containing the right-hand side of the linear system. (Input)

X — Vector of length `N` containing the solution to the linear system. (Output)

Optional Arguments

N — Number of equations. (Input)
Default: `N` = size (`B`,1).

IPATH — Path indicator. (Input)
`IPATH` = 1 means the system $Ax = B$ is solved.
`IPATH` = 2 means the system $A^T x = B$ is solved.
Default: `IPATH` = 1.

FORTRAN 90 Interface

Generic: CALL LFSXG (NFAC, NL, FACT, IRFAC, JCFAC, IPVT, JPVT, B, X [, …])

Specific: The specific interface names are S_LFSXG and D_LFSXG.

FORTRAN 77 Interface

Single: CALL LFSXG (N, NFAC, NL, FACT, IRFAC, JCFAC, IPVT, JPVT, B, IPATH, X)

Double: The double precision name is DLFSXG.

Description

Consider the linear equation

$$Ax = b$$

where A is a $n \times n$ sparse matrix. The sparse coordinate format for the matrix A requires one real and two integer vectors. The real array a contains all the nonzeros in A. Let the number of nonzeros be nz. The two integer arrays irow and jcol, each of length nz, contain the row and column numbers for these entries in A. That is

$$A_{\text{irow}(i),\, \text{icol}(i)} = a(i),\ i = 1, \ldots, \text{nz}$$

with all other entries in A zero. The routine LFSXG computes the solution of the linear equation given its LU factorization. The factorization is performed by calling LFTXG. The solution of the linear system is then found by the forward and backward substitution. The algorithm can be expressed as

$$P\,AQ = LU$$

where P and Q are the row and column permutation matrices determined by the Markowitz strategy (Duff et al. 1986), and L and U are lower and upper triangular matrices, respectively. Finally, the solution x is obtained by the following calculations:

$$1)\ Lz = Pb$$
$$2)\ Uy = z$$
$$3)\ x = Qy$$

For more details, see Crowe et al. (1990).

Example

As an example, consider the 6 × 6 linear system:

$$A = \begin{bmatrix} 10 & 0 & 0 & 0 & 0 & 0 \\ 0 & 10 & -3 & -1 & 0 & 0 \\ 0 & 0 & 15 & 0 & 0 & 0 \\ -2 & 0 & 0 & 10 & -1 & 0 \\ -1 & 0 & 0 & -5 & 1 & -3 \\ -1 & -2 & 0 & 0 & 0 & 6 \end{bmatrix}$$

Let

$$x_1^{\boldsymbol{T}} = (1,2,3,4,5,6)$$

so that Ax_1 = (10, 7, 45, 33, −34, 31)$^{\boldsymbol{T}}$, and

$$x_2^{\boldsymbol{T}} = (6,5,4,3,2,1)$$

so that Ax_2 = (60, 35, 60, 16, −22, 10)$^{\boldsymbol{T}}$. The sparse coordinate form for A is given by:

irow	6	2	3	2	4	4	5	5	5	5	1	6	6	2	4
jcol	6	2	3	3	4	5	1	6	4	5	1	1	2	4	1
a	6	10	15	−3	10	−1	−1	−3	−5	1	10	−1	−2	−1	−2

```
      USE LFSXG_INT
      USE WRRRL_INT
      USE LFTXG_INT
      INTEGER     N, NZ
      PARAMETER  (N=6, NZ=15)
      INTEGER    IPATH, IROW(NZ), JCOL(NZ), NFAC,&
                 NL, IRFAC(3*NZ), JCFAC(3*NZ), IPVT(N), JPVT(N)
      REAL       X(N), A(NZ), B(N,2), FACT(3*NZ)
      CHARACTER  TITLE(2)*2, RLABEL(1)*4, CLABEL(1)*6
      DATA RLABEL(1)/'NONE'/, CLABEL(1)/'NUMBER'/
!
      DATA A/6., 10., 15., -3., 10., -1., -1., -3., -5., 1., 10., -1.,&
            -2., -1., -2./
      DATA B/10., 7., 45., 33., -34., 31.,&
            60., 35., 60., 16., -22., -10./
      DATA IROW/6, 2, 3, 2, 4, 4, 5, 5, 5, 5, 1, 6, 6, 2, 4/
      DATA JCOL/6, 2, 3, 3, 4, 5, 1, 6, 4, 5, 1, 1, 2, 4, 1/
      DATA TITLE/'x1', 'x2'/
!
      NFAC = 3*NZ
!                                 Perform LU factorization
      CALL LFTXG (A, IROW, JCOL, NL, NFAC, FACT, IRFAC, JCFAC, IPVT, JPVT)
!
      DO 10 I = 1, 2
!                                 Solve A * X(i) = B(i)
         CALL LFSXG (NFAC, NL, FACT, IRFAC, JCFAC, IPVT, JPVT, B(:,I), X)
!
         CALL WRRRL (TITLE(I), X,  RLABEL, CLABEL, 1, N, 1)
   10 CONTINUE
      END
```

Output

```
                    x1
   1      2      3      4      5      6
 1.0    2.0    3.0    4.0    5.0    6.0

                    x2
   1      2      3      4      5      6
 6.0    5.0    4.0    3.0    2.0    1.0
```

LSLZG

Solves a complex sparse system of linear equations by Gaussian elimination.

NOTE: Additional sparse solvers are available in the *Sparse Matrix Computations* section.

Required Arguments

A — Complex vector of length NZ containing the nonzero coefficients of the linear system. (Input)

IROW — Vector of length NZ containing the row numbers of the corresponding elements in A. (Input)

JCOL — Vector of length NZ containing the column numbers of the corresponding elements in A. (Input)

B — Complex vector of length N containing the right-hand side of the linear system. (Input)

X — Complex vector of length N containing the solution to the linear system. (Output)

Optional Arguments

N — Number of equations. (Input)
Default: N = size (B,1).

NZ — The number of nonzero coefficients in the linear system. (Input)
Default: NZ = size (A,1).

IPATH — Path indicator. (Input)
IPATH = 1 means the system Ax = b is solved.
IPATH = 2 means the system A^H x = b is solved.
Default: IPATH =1.

IPARAM — Parameter vector of length 6. (Input/Output)
Set IPARAM(1) to zero for default values of IPARAM and RPARAM. See Comment 3.
Default: IPARAM = 0.

RPARAM — Parameter vector of length 5. (Input/Output)
See Comment 3

FORTRAN 90 Interface

Generic: CALL LSLZG (A, IROW, JCOL, B, X [, …])

Specific: The specific interface names are `S_LSLZG` and `D_LSLZG`.

FORTRAN 77 Interface

Single: `CALL LSLZG (N, NZ, A, IROW, JCOL, B, IPATH, IPARAM, RPARAM, X)`

Double: The double precision name is `DLSLZG`.

Description

Consider the linear equation

$$Ax = b$$

where *A* is a $n \times n$ complex sparse matrix. The sparse coordinate format for the matrix *A* requires one complex and two integer vectors. The complex array `a` contains all the nonzeros in *A*. Let the number of nonzeros be `nz`. The two integer arrays `irow` and `jcol`, each of length `nz`, contain the row and column numbers for these entries in *A*. That is

$$A_{\mathrm{irow}(i),\ \mathrm{icol}(i)} = a(i),\ i = 1, \ldots, \mathtt{nz}$$

with all other entries in *A* zero.

The subroutine `LSLZG` solves a system of linear algebraic equations having a complex sparse coefficient matrix. It first uses the routine `LFTZG` to perform an *LU* factorization of the coefficient matrix. The solution of the linear system is then found using `LFSZG`. The routine `LFTZG` by default uses a *symmetric Markowitz strategy* (Crowe et al. 1990) to choose pivots that most likely would reduce fill-ins while maintaining numerical stability. Different strategies are also provided as options for row oriented or column oriented problems. The algorithm can be expressed as

$$\mathrm{P\,AQ = LU}$$

where *P* and *Q* are the row and column permutation matrices determined by the Markowitz strategy (Duff et al. 1986), and *L* and *U* are lower and upper triangular matrices, respectively. Finally, the solution *x* is obtained by the following calculations:

$$1)\ Lz = Pb$$

$$2)\ Uy = z$$

$$3)\ x = Qy$$

Comments

1. Workspace may be explicitly provided, if desired, by use of `L2LZG/DL2LZG`. The reference is:

   `CALL L2LZG (N, NZ, A, IROW, JCOL, B, IPATH, IPARAM, RPARAM, X, WK, LWK, IWK, LIWK)`

The additional arguments are as follows:

WK — Complex work vector of length `LWK`.

LWK — The length of `WK`, `LWK` should be at least 2`N`+ `MAXNZ`.

IWK — Integer work vector of length `LIWK`.

LIWK — The length of `IWK`, `LIWK` should be at least 17`N` + 4 * `MAXNZ`.

The workspace limit is determined by `MAXNZ`, where

`MAXNZ = MIN0(LWK-2N, INT(0.25(LIWK-17N)))`

2. Informational errors

Type	Code	Description
3	1	The coefficient matrix is numerically singular.
3	2	The growth factor is too large to continue.
3	3	The matrix is too ill-conditioned for iterative refinement.

3. If the default parameters are desired for `LSLZG`, then set `IPARAM`(1) to zero and call the routine `LSLZG`. Otherwise, if any nondefault parameters are desired for `IPARAM` or `RPARAM`. then the following steps should be taken before calling `LSLZG`.

`CALL L4LZG (IPARAM, RPARAM)`

Set nondefault values for desired `IPARAM`, `RPARAM` elements.

Note that the call to `L4LZG` will set `IPARAM` and `RPARAM` to their default values, so only nondefault values need to be set above. The arguments are as follows:

IPARAM — Integer vector of length 6.

`IPARAM`(1) = Initialization flag.

`IPARAM`(2) = The pivoting strategy.

IPARAM(2)	**Action**
1	Markowitz row search
2	Markowitz column search
3	Symmetric Markowitz search

Default: 3.

`IPARAM`(3) = The number of rows which have least numbers of nonzero elements that will be searched for a pivotal element.
Default: 3.

`IPARAM`(4) = The maximal number of nonzero elements in *A* at any stage of the Gaussian elimination. (Output)

IPARAM(5) = The workspace limit.

IPARAM(5)	Action
0	Default limit, see Comment 1.
integer	This integer value replaces the default workspace limit.

When L2LZG is called, the values of LWK and LIWK are used instead of IPARAM(5).
Default: 0.

IPARAM(6) = Iterative refinement is done when this is nonzero.
Default: 0.

RPARAM — Real vector of length 5.

RPARAM(1) = The upper limit on the growth factor. The computation stops when the growth factor exceeds the limit.
Default: 10.

RPARAM(2) = The stability factor. The absolute value of the pivotal element must be bigger than the largest element in absolute value in its row divided by RPARAM(2).
Default: 10.0.

RPARAM(3) = Drop-tolerance. Any element in A will be removed if its absolute value becomes smaller than the drop-tolerance at any stage of the Gaussian elimination.
Default: 0.0.

RPARAM(4) = The growth factor. It is calculated as the largest element in absolute value in A at any stage of the Gaussian elimination divided by the largest element in absolute value in the original A matrix. (Output)
Large value of the growth factor indicates that an appreciable error in the computed solution is possible.

RPARAM(5) = The value of the smallest pivotal element in absolute value. (Output)

If double precision is required, then DL4LZG is called and RPARAM is declared double precision.

Example

As an example, consider the 6×6 linear system:

$$A = \begin{bmatrix} 10+7i & 0 & 0 & 0 & 0 & 0 \\ 0 & 3+2i & -3+0i & -1+2i & 0 & 0 \\ 0 & 0 & 4+2i & 0 & 0 & 0 \\ -2-4i & 0 & 0 & 1+6i & -1+3i & 0 \\ -5+4i & 0 & 0 & -5+0i & 12+2i & -7+7i \\ -1+12i & -2+8i & 0 & 0 & 0 & 3+7i \end{bmatrix}$$

Let

$$x^T = (1 + i, 2 + 2i, 3 + 3i, 4 + 4i, 5 + 5i, 6 + 6i)$$

so that

$$Ax = (3 + 17i, -19 + 5i, 6 + 18i, -38 + 32i, -63 + 49i, -57 + 83i)^T$$

The number of nonzeros in *A* is `nz` = 15. The sparse coordinate form for *A* is given by:

irow	6	2	2	4	3	1	5	4	6	5	5	6	4	2	5
jcol	6	2	3	5	3	1	1	4	1	4	5	2	1	4	6

```
      USE LSLZG_INT
      USE WRCRN_INT
      INTEGER    N, NZ
      PARAMETER  (N=6, NZ=15)
!
      INTEGER    IROW(NZ), JCOL(NZ)
      COMPLEX    A(NZ), B(N), X(N)
!
      DATA A/(3.0,7.0), (3.0,2.0), (-3.0,0.0), (-1.0,3.0), (4.0,2.0),&
          (10.0,7.0), (-5.0,4.0), (1.0,6.0), (-1.0,12.0), (-5.0,0.0),&
          (12.0,2.0), (-2.0,8.0), (-2.0,-4.0), (-1.0,2.0), (-7.0,7.0)/
      DATA B/(3.0,17.0), (-19.0,5.0), (6.0,18.0), (-38.0,32.0),&
          (-63.0,49.0), (-57.0,83.0)/
      DATA IROW/6, 2, 2, 4, 3, 1, 5, 4, 6, 5, 5, 6, 4, 2, 5/
      DATA JCOL/6, 2, 3, 5, 3, 1, 1, 4, 1, 4, 5, 2, 1, 4, 6/
!
!                                 Use default options
      CALL LSLZG (A, IROW, JCOL, B, X)
!
      CALL WRCRN ('X', X)
      END
```

Output

```
           X
1  ( 1.000, 1.000)
2  ( 2.000, 2.000)
3  ( 3.000, 3.000)
4  ( 4.000, 4.000)
5  ( 5.000, 5.000)
6  ( 6.000, 6.000)
```

LFTZG

Computes the *LU* factorization *of a* complex general sparse matrix.

NOTE: Additional sparse solvers are available in the *Sparse Matrix Computations* section.

Required Arguments

A — Complex vector of length `NZ` containing the nonzero coefficients of the linear system. (Input)

IROW — Vector of length `NZ` containing the row numbers of the corresponding elements in `A`. (Input)

JCOL — Vector of length `NZ` containing the column numbers of the corresponding elements in `A`. (Input)

NFAC — On input, the dimension of vector `FACT`. (Input/Output)
On output, the number of nonzero coefficients in the triangular matrix *L* and *U*.

NL — The number of nonzero coefficients in the triangular matrix *L* excluding the diagonal elements. (Output)

FACT — Complex vector of length `NFAC` containing the nonzero elements of *L* (excluding the diagonals) in the first `NL` locations and the nonzero elements of *U* in `NL` + 1 to `NFAC` locations. (Output)

IRFAC — Vector of length `NFAC` containing the row numbers of the corresponding elements in `FACT`. (Output)

JCFAC — Vector of length `NFAC` containing the column numbers of the corresponding elements in `FACT`. (Output)

IPVT — Vector of length `N` containing the row pivoting information for the *LU* factorization. (Output)

JPVT — Vector of length `N` containing the column pivoting information for the *LU* factorization. (Output)

Optional Arguments

N — Number of equations. (Input)
Default: `N` = size (`IPVT`,1).

NZ — The number of nonzero coefficients in the linear system. (Input)
Default: `NZ` = size (`A`,1).

IPARAM — Parameter vector of length 6. (Input/Output)
Set IPARAM(1) to zero for default values of IPARAM and RPARAM. See Comment 3.
Default: IPARAM = 0.

RPARAM — Parameter vector of length 5. (Input/Output)
See Comment 3.

FORTRAN 90 Interface

Generic: CALL LFTZG (A, IROW, JCOL, NFAC, NL, FACT, IRFAC, JCFAC, IPVT, JPVT [, …])

Specific: The specific interface names are S_LFTZG and D_LFTZG.

FORTRAN 77 Interface

Single: CALL LFTZG (N, NZ, A, IROW, JCOL, IPARAM, RPARAM, NFAC, NL, FACT, IRFAC, JCFAC, IPVT, JPVT)

Double: The double precision name is DLFTZG.

Description

Consider the linear equation

$$Ax = b$$

where *A* is a complex $n \times n$ sparse matrix. The sparse coordinate format for the matrix *A* requires one complex and two integer vectors. The complex array a contains all the nonzeros in *A*. Let the number of nonzeros be nz. The two integer arrays irow and jcol, each of length nz, contain the row and column indices for these entries in *A*. That is

$$A_{\mathrm{irow}(i),\, \mathrm{icol}(i)} = a(i),\ i = 1, \ldots, \mathtt{nz}$$

with all other entries in *A* zero.

The routine LFTZG performs an *LU* factorization of the coefficient matrix *A*. It uses by default a *symmetric Markowitz strategy* (Crowe et al. 1990) to choose pivots that most likely would reduce fill-ins while maintaining numerical stability. Different strategies are also provided as options for row oriented or column oriented problems. The algorithm can be expressed as

$$PAQ = LU$$

where *P* and *Q* are the row and column permutation matrices determined by the Markowitz strategy (Duff et al. 1986), and *L* and *U* are lower and upper triangular matrices, respectively.

Finally, the solution *x* is obtained using LFSZG by the following calculations:

$$1)\ Lz = Pb$$
$$2)\ Uy = z$$
$$3)\ x = Qy$$

Comments

1. Workspace may be explicitly provided, if desired, by use of L2TZG/DL2TZG. The reference is:

   CALL L2TZG (N, NZ, A, IROW, JCOL, IPARAM, RPARAM, NFAC, NL, FACT, IRFAC, JCFAC, IPVT, JPVT, WK, LWK, IWK, LIWK)

   The additional arguments are as follows:

   WK — Complex work vector of length LWK.

   LWK — The length of WK, LWK should be at least MAXNZ.

   IWK — Integer work vector of length LIWK.

   LIWK — The length of IWK, LIWK should be at least 15N + 4 * MAXNZ.

   The workspace limit is determined by MAXNZ, where

   MAXNZ = MIN0 (LWK, INT (0.25 (LIWK-15N)))

2. Informational errors

Type	Code	Description
3	1	The coefficient matrix is numerically singular.
3	2	The growth factor is too large to continue.

3. If the default parameters are desired for LFTZG, then set IPARAM(1) to zero and call the routine LFTZG. Otherwise, if any nondefault parameters are desired for IPARAM or RPARAM. then the following steps should be taken before calling LFTZG:

   CALL L4LZG (IPARAM, RPARAM)

   Set nondefault values for desired IPARAM, RPARAM elements.

Note that the call to L4LZG will set IPARAM and RPARAM to their default values so only nondefault values need to be set above. The arguments are as follows:

IPARAM — Integer vector of length 6.

IPARAM(1) = Initialization flag.

IPARAM(2) = The pivoting strategy.

IPARAM(2)	Action
1	Markowitz row search

2	Markowitz column search
3	Symmetric Markowitz search

IPARAM(3) = The number of rows which have least numbers of nonzero elements that will be searched for a pivotal element.

Default: 3.

IPARAM(4) = The maximal number of nonzero elements in A at any stage of the Gaussian elimination. (Output)

IPARAM(5) = The workspace limit.

IPARAM(5)	Action
0	Default limit, see Comment 1.
integer	This integer value replaces the default workspace limit. When L2TZG is called, the values of LWK and LIWK are used instead of IPARAM(5).

Default: 0.

IPARAM(6) = Not used in LFTZG.

RPARAM — Real vector of length 5.

RPARAM(1) = The upper limit on the growth factor. The computation stops when the growth factor exceeds the limit.

Default: 10.

RPARAM(2) = The stability factor. The absolute value of the pivotal element must be bigger than the largest element in absolute value in its row divided by RPARAM(2).

Default: 10.0.

RPARAM(3) = Drop-tolerance. Any element in the lower triangular factor *L* will be removed if its absolute value becomes smaller than the drop-tolerance at any stage of the Gaussian elimination.

Default: 0.0.

RPARAM(4) = The growth factor. It is calculated as the largest element in absolute value in A at any stage of the Gaussian elimination divided by the largest element in absolute value in the original A matrix. (Output)
Large value of the growth factor indicates that an appreciable error in the computed solution is possible.

RPARAM(5) = The value of the smallest pivotal element in absolute value. (Output)

If double precision is required, then DL4LZG is called and RPARAM is declared double precision.

Example

As an example, the following 6×6 matrix is factorized, and the outcome is printed:

$$A = \begin{bmatrix} 10+7i & 0 & 0 & 0 & 0 & 0 \\ 0 & 3+2i & -3+0i & -1+2i & 0 & 0 \\ 0 & 0 & 4+2i & 0 & 0 & 0 \\ -2-4i & 0 & 0 & 1+6i & -1+3i & 0 \\ -5+4i & 0 & 0 & -5+0i & 12+2i & -7+7i \\ -1+12i & -2+8i & 0 & 0 & 0 & 3+7i \end{bmatrix}$$

The sparse coordinate form for *A* is given by:

$$\begin{array}{cccccccccccccccc} irow & 6 & 2 & 2 & 4 & 3 & 1 & 5 & 4 & 6 & 5 & 5 & 6 & 4 & 2 & 5 \\ jcol & 6 & 2 & 3 & 5 & 3 & 1 & 1 & 4 & 1 & 4 & 5 & 2 & 1 & 4 & 6 \end{array}$$

```
      USE LFTZG_INT
      USE WRCRN_INT
      USE WRIRN_INT
      INTEGER     N, NFAC, NZ
      PARAMETER  (N=6, NZ=15)
!                                 SPECIFICATIONS FOR LOCAL VARIABLES
      INTEGER    IPVT(N), IRFAC(45), IROW(NZ), JCFAC(45),&
                 JCOL(NZ), JPVT(N), NL
      COMPLEX    A(NZ), FAC(45)
!
      DATA A/(3.0,7.0), (3.0,2.0), (-3.0,0.0), (-1.0,3.0), (4.0,2.0),&
          (10.0,7.0), (-5.0,4.0), (1.0,6.0), (-1.0,12.0), (-5.0,0.0),&
          (12.0,2.0), (-2.0,8.0), (-2.0,-4.0), (-1.0,2.0), (-7.0,7.0)/
      DATA IROW/6, 2, 2, 4, 3, 1, 5, 4, 6, 5, 5, 6, 4, 2, 5/
      DATA JCOL/6, 2, 3, 5, 3, 1, 1, 4, 1, 4, 5, 2, 1, 4, 6/
      DATA NFAC/45/
!                                 Use default options
      CALL LFTZG (A, IROW, JCOL, NFAC, NL, FACT, IRFAC, JCFAC, IPVT, JPVT)
!
      CALL WRCRN ('fact',FACT, 1, NFAC, 1)
      CALL WRIRN (' irfac ',IRFAC, 1, NFAC, 1)
      CALL WRIRN (' jcfac ',JCFAC, 1, NFAC, 1)
      CALL WRIRN (' p ',IPVT, 1, N, 1)
      CALL WRIRN (' q ',JPVT, 1, N, 1)
!
      END
```

Output

```
           fact
  1  (  0.50,  0.85)
  2  (  0.15, -0.41)
  3  ( -0.60,  0.30)
  4  (  2.23, -1.97)
  5  ( -0.15,  0.50)
  6  ( -0.04,  0.26)
  7  ( -0.32, -0.17)
  8  ( -0.92,  7.46)
  9  ( -6.71, -6.42)
 10  ( 12.00,  2.00)
 11  ( -1.00,  2.00)
```

```
 12  ( -3.32,  0.21)
 13  (  3.00,  7.00)
 14  ( -2.00,  8.00)
 15  ( 10.00,  7.00)
 16  (  4.00,  2.00)

                                   irfac
 1   2   3   4   5   6   7   8   9  10  11  12  13  14  15  16
 3   4   4   5   5   6   6   6   5   5   4   4   3   3   2   1



                                   jcfac
 1   2   3   4   5   6   7   8   9  10  11  12  13  14  15  16
 2   3   1   4   2   5   2   6   6   5   6   4   4   3   2   1

             p
 1   2   3   4   5   6
 3   1   6   2   5   4

             q
 1   2   3   4   5   6
 3   1   2   6   5   4
```

LFSZG

Solves a complex sparse system of linear equations given the *LU* factorization of the coefficient matrix.

NOTE: Additional sparse solvers are available in the *Sparse Matrix Computations* section.

Required Arguments

NFAC — The number of nonzero coefficients in `FACT` as output from subroutine `LFTZG`/`DLFTZG`. (Input)

NL — The number of nonzero coefficients in the triangular matrix *L* excluding the diagonal elements as output from subroutine `LFTZG`/`DLFTZG`. (Input)

FACT — Complex vector of length `NFAC` containing the nonzero elements of *L* (excluding the diagonals) in the first `NL` locations and the nonzero elements of *U* in `NL`+ 1 to `NFAC` locations as output from subroutine `LFTZG`/`DLFTZG`. (Input)

IRFAC — Vector of length `NFAC` containing the row numbers of the corresponding elements in `FACT` as output from subroutine `LFTZG`/`DLFTZG`. (Input)

JCFAC — Vector of length `NFAC` containing the column numbers of the corresponding elements in `FACT` as output from subroutine `LFTZG`/`DLFTZG`. (Input)

IPVT — Vector of length `N` containing the row pivoting information for the *LU* factorization as output from subroutine `LFTZG`/`DLFTZG`. (Input)

JPVT — Vector of length `N` containing the column pivoting information for the *LU* factorization as output from subroutine `LFTZG`/`DLFTZG`. (Input)

B — Complex vector of length `N` containing the right-hand side of the linear system. (Input)

X — Complex vector of length `N` containing the solution to the linear system. (Output)

Optional Arguments

N — Number of equations. (Input)
Default: `N` = size (`B`,1).

IPATH — Path indicator. (Input)
`IPATH` = 1 means the system Ax = b is solved.
`IPATH` = 2 means the system A^{H} x = b is solved.
Default: `IPATH` = 1.

FORTRAN 90 Interface

Generic: `CALL LFSZG (NFAC, NL, FACT, IRFAC, JCFAC, IPVT, JPVT, B, X [, …])`

Specific: The specific interface names are `S_LFSZG` and `D_LFSZG`.

FORTRAN 77 Interface

Single: `CALL LFSZG (N, NFAC, NL, FACT, IRFAC, JCFAC, IPVT, JPVT, B, IPATH, X)`

Double: The double precision name is `DLFSZG`.

Description

Consider the linear equation

$$Ax = b$$

where *A* is a complex *n* × *n* sparse matrix. The sparse coordinate format for the matrix *A* requires one complex and two integer vectors. The complex array `a` contains all the nonzeros in *A*. Let the number of nonzeros be `nz`. The two integer arrays `irow` and `jcol`, each of length `nz`, contain the row and column numbers for these entries in *A*. That is

$$A_{\mathrm{irow}(i),\ \mathrm{icol}(i)} = a(i),\ i = 1, \ldots, \mathtt{nz}$$

with all other entries in *A* zero.

The routine `LFSZG` computes the solution of the linear equation given its *LU* factorization. The factorization is performed by calling `LFTZG`. The solution of the linear system is then found by the forward and backward substitution. The algorithm can be expressed as

$$\mathrm{P\,AQ = LU}$$

where *P* and *Q* are the row and column permutation matrices determined by the Markowitz strategy (Duff et al. 1986), and *L* and *U* are lower and upper triangular matrices, respectively.

Finally, the solution *x* is obtained by the following calculations:

$$1)\ Lz = Pb$$

$$2)\ Uy = z$$

$$3)\ x = Qy$$

For more details, see Crowe et al. (1990).

Example

As an example, consider the 6 × 6 linear system:

$$A = \begin{bmatrix} 10+7i & 0 & 0 & 0 & 0 & 0 \\ 0 & 3+2i & -3+0i & -1+2i & 0 & 0 \\ 0 & 0 & 4+2i & 0 & 0 & 0 \\ -2-4i & 0 & 0 & 1+6i & -1+3i & 0 \\ -5+4i & 0 & 0 & -5+0i & 12+2i & -7+7i \\ -1+12i & -2+8i & 0 & 0 & 0 & 3+7i \end{bmatrix}$$

Let

$$x_1{}^T = (1+i, 2+2i, 3+3i, 4+4i, 5+5i, 6+6i)$$

so that

$$Ax_1 = (3+17i, -19+5i, 6+18i, -38+32i, -63+49i, -57+83i)^T$$

and

$$x_2{}^T = (6+6i, 5+5i, 4+4i, 3+3i, 2+2i, 1+i)$$

so that

$$Ax_2 = (18+102i, -16+16i, 8+24i, -11-11i, -63+7i, -132+106i)^T$$

The sparse coordinate form for *A* is given by:

$$\begin{array}{cccccccccccccccc} irow & 6 & 2 & 2 & 4 & 3 & 1 & 5 & 4 & 6 & 5 & 5 & 6 & 4 & 2 & 5 \\ jcol & 6 & 2 & 3 & 5 & 3 & 1 & 1 & 4 & 1 & 4 & 5 & 2 & 1 & 4 & 6 \end{array}$$

```
      USE LFSZG_INT
      USE WRCRN_INT
      USE LFTZG_INT
      INTEGER     N, NZ
      PARAMETER   (N=6, NZ=15)
!
      INTEGER     IPATH, IPVT(N), IRFAC(3*NZ), IROW(NZ),&
                  JCFAC(3*NZ), JCOL(NZ), JPVT(N), NFAC, NL
      COMPLEX     A(NZ), B(N,2), FACT(3*NZ), X(N)
      CHARACTER   TITLE(2)*2
!
      DATA A/(3.0,7.0), (3.0,2.0), (-3.0,0.0), (-1.0,3.0), (4.0,2.0),&
          (10.0,7.0), (-5.0,4.0), (1.0,6.0), (-1.0,12.0), (-5.0,0.0),&
          (12.0,2.0), (-2.0,8.0), (-2.0,-4.0), (-1.0,2.0), (-7.0,7.0)/
      DATA B/(3.0,17.0), (-19.0,5.0), (6.0,18.0), (-38.0,32.0),&
          (-63.0,49.0), (-57.0,83.0), (18.0,102.0), (-16.0,16.0),&
          (8.0,24.0), (-11.0,-11.0), (-63.0,7.0), (-132.0,106.0)/
      DATA IROW/6, 2, 2, 4, 3, 1, 5, 4, 6, 5, 5, 6, 4, 2, 5/
      DATA JCOL/6, 2, 3, 5, 3, 1, 1, 4, 1, 4, 5, 2, 1, 4, 6/
```

```
      DATA TITLE/'x1','x2'/
!
      NFAC = 3*NZ
!                                   Perform LU factorization
      CALL LFTZG (A, IROW, JCOL, NFAC, NL, FACT, IRFAC, JCFAC, IPVT, JPVT)
!
      IPATH = 1
      DO 10 I = 1,2
!                                   Solve A * X(i) = B(i)
         CALL LFSZG (NFAC, NL, FACT, IRFAC, JCFAC, IPVT, JPVT,&
                     B(:,I),  X)
         CALL WRCRN (TITLE(I), X)
   10 CONTINUE
!
      END
```

Output

```
            x1
1   ( 1.000, 1.000)
2   ( 2.000, 2.000)
3   ( 3.000, 3.000)
4   ( 4.000, 4.000)
5   ( 5.000, 5.000)
6   ( 6.000, 6.000)

           x2
1   ( 6.000, 6.000)
2   ( 5.000, 5.000)
3   ( 4.000, 4.000)
4   ( 3.000, 3.000)
5   ( 2.000, 2.000)
6   ( 1.000, 1.000)
```

LSLXD

Solves a sparse system of symmetric positive definite linear algebraic equations by Gaussian elimination.

Required Arguments

A — Vector of length `NZ` containing the nonzero coefficients in the lower triangle of the linear system. (Input)
The sparse matrix has nonzeroes only in entries (`IROW` (i), `JCOL`(i)) for i = 1 to `NZ`, and at this location the sparse matrix has value `A`(i).

IROW — Vector of length `NZ` containing the row numbers of the corresponding elements in the lower triangle of `A`. (Input)
Note `IROW`(i) ≥ `JCOL`(i), since we are only indexing the lower triangle.

JCOL — Vector of length `NZ` containing the column numbers of the corresponding elements in the lower triangle of `A`. (Input)

B — Vector of length `N` containing the right-hand side of the linear system. (Input)

X — Vector of length `N` containing the solution to the linear system. (Output)

Optional Arguments

N — Number of equations. (Input)
Default: `N` = size (`B`,1).

NZ — The number of nonzero coefficients in the lower triangle of the linear system. (Input)
Default: `NZ` = size (`A`,1).

ITWKSP — The total workspace needed. (Input)
If the default is desired, set `ITWKSP` to zero.
Default: `ITWKSP` = 0.

FORTRAN 90 Interface

Generic: `CALL LSLXD (A, IROW, JCOL, B, X [, …])`

Specific: The specific interface names are `S_LSLXD` and `D_LSLXD`.

FORTRAN 77 Interface

Single: CALL LSLXD (N, NZ, A, IROW, JCOL, B, ITWKSP, X)

Double: The double precision name is DLSLXD.

Description

Consider the linear equation

$$Ax = b$$

where *A* is sparse, positive definite and symmetric. The sparse coordinate format for the matrix *A* requires one real and two integer vectors. The real array a contains all the nonzeros in the *lower triangle* of *A* including the diagonal. Let the number of nonzeros be nz. The two integer arrays irow and jcol, each of length nz, contain the row and column indices for these entries in *A*. That is

$$A_{\mathrm{irow}(i),\ \mathrm{icol}(i)} = a(i),\ i = 1, \dots, \mathtt{nz}$$

$$\mathtt{irow}(i) \geq \mathtt{jcol}(i) \quad i = 1, \dots, \mathtt{nz}$$

with all other entries in the lower triangle of *A* zero.

The routine LSLXD solves a system of linear algebraic equations having a real, sparse and positive definite coefficient matrix. It first uses the routine LSCXD to compute a symbolic factorization of a permutation of the coefficient matrix. It then calls LNFXD to perform the numerical factorization. The solution of the linear system is then found using LFSXD.

The routine LSCXD computes a minimum degree ordering or uses a user-supplied ordering to set up the sparse data structure for the Cholesky factor, *L*. Then the routine LNFXD produces the numerical entries in *L* so that we have

$$\mathrm{P\,AP}^{T} = \mathrm{LL}^{T}$$

Here *P* is the permutation matrix determined by the ordering.

The numerical computations can be carried out in one of two ways. The first method performs the factorization using a multifrontal technique. This option requires more storage but in certain cases will be faster. The multifrontal method is based on the routines in Liu (1987). For detailed description of this method, see Liu (1990), also Duff and Reid (1983, 1984), Ashcraft (1987), Ashcraft et al. (1987), and Liu (1986, 1989). The second method is fully described in George and Liu (1981). This is just the standard factorization method based on the sparse compressed storage scheme.

Finally, the solution *x* is obtained by the following calculations:

$$1)\ Ly_1 = Pb$$

$$2)\ L^{T}y_2 = y_1$$

$$3)\ x = P^T y_2$$

The routine LFSXD accepts b and the permutation vector which determines P. It then returns x.

Comments

1. Workspace may be explicitly provided, if desired, by use of L2LXD/DL2LXD. The reference is:

   CALL L2LXD (N, NZ, A, IROW, JCOL, B, X, IPER, IPARAM, RPARAM, WK, LWK, IWK, LIWK)

   The additional arguments are as follows:

   IPER — Vector of length N containing the ordering.

   IPARAM — Integer vector of length 4. See Comment 3.

   RPARAM — Real vector of length 2. See Comment 3.

   WK — Real work vector of length LWK.

   LWK — The length of WK, LWK should be at least 2N + 6NZ.

   IWK — Integer work vector of length LIWK.

   LIWK — The length of IWK, LIWK should be at least 15N + 15NZ + 9.

   Note that the parameter ITWKSP is not an argument to this routine.

2. Informational errors

Type	Code	Description
4	1	The coefficient matrix is not positive definite.
4	2	A column without nonzero elements has been found in the coefficient matrix.

3. If the default parameters are desired for L2LXD, then set IPARAM(1) to zero and call the routine L2LXD. Otherwise, if any nondefault parameters are desired for IPARAM or RPARAM, then the following steps should be taken before calling L2LXD.

   CALL L4LXD (IPARAM, RPARAM)

   Set nondefault values for desired IPARAM, RPARAM elements.

Note that the call to L4LXD will set IPARAM and RPARAM to their default values, so only nondefault values need to be set above. The arguments are as follows:

IPARAM — Integer vector of length 4.

IPARAM(1) = Initialization flag.

IPARAM(2) = The numerical factorization method.

IPARAM(2)	Action
0	Multifrontal
1	Markowitz column search

Default: 0.

IPARAM(3) = The ordering option.

IPARAM(3)	Action
0	Minimum degree ordering
1	User's ordering specified in IPER

Default: 0.

IPARAM(4) = The total number of nonzeros in the factorization matrix.

RPARAM — Real vector of length 2.

RPARAM(1) = The value of the largest diagonal element in the Cholesky factorization.

RPARAM(2) = The value of the smallest diagonal element in the Cholesky factorization.

If double precision is required, then DL4LXD is called and RPARAM is declared double precision.

Example

As an example consider the 5× 5 linear system:

$$A = \begin{bmatrix} 10 & 0 & 1 & 0 & 2 \\ 0 & 20 & 0 & 0 & 3 \\ 1 & 0 & 30 & 4 & 0 \\ 0 & 0 & 4 & 40 & 5 \\ 2 & 3 & 0 & 5 & 50 \end{bmatrix}$$

Let $x^T = (1, 2, 3, 4, 5)$ so that $Ax = (23, 55, 107, 197, 278)^T$. The number of nonzeros in the lower triangle of A is nz = 10. The sparse coordinate form for the lower triangle of A is given by:

irow	1	2	3	3	4	4	5	5	5	5
jcol	1	2	1	3	3	4	1	2	4	5
a	10	20	1	30	4	40	2	3	5	50

or equivalently by

irow	4	5	5	5	1	2	3	3	4	5
jcol	4	1	2	4	1	2	1	3	3	5
a	40	2	3	5	10	20	1	30	4	50

```
      USE LSLXD_INT
      USE WRRRN_INT
      INTEGER     N, NZ
      PARAMETER  (N=5, NZ=10)
!
      INTEGER    IROW(NZ), JCOL(NZ)
      REAL       A(NZ), B(N), X(N)
!
      DATA A/10., 20., 1., 30., 4., 40., 2., 3., 5., 50./
      DATA B/23., 55., 107., 197., 278./
      DATA IROW/1, 2, 3, 3, 4, 4, 5, 5, 5, 5/
      DATA JCOL/1, 2, 1, 3, 3, 4, 1, 2, 4, 5/
!                                  Solve A * X = B
      CALL LSLXD (A, IROW, JCOL, B, X)
!                                  Print results
      CALL WRRRN (’ x ’, X, 1, N, 1)
      END
```

Output

```
                     x
    1        2        3        4        5
1.000    2.000    3.000    4.000    5.000
```

LSCXD

Performs the symbolic Cholesky factorization for a sparse symmetric matrix using a minimum degree ordering or a user-specified ordering, and set up the data structure for the numerical Cholesky factorization

Required Arguments

IROW — Vector of length NZ containing the row subscripts of the nonzeros in the lower triangular part of the matrix including the nonzeros on the diagonal. (Input)

JCOL — Vector of length NZ containing the column subscripts of the nonzeros in the lower triangular part of the matrix including the nonzeros on the diagonal. (Input)
(IROW (K), JCOL(K)) gives the row and column indices of the *k*-th nonzero element of the matrix stored in coordinate form. Note, IROW(K) ≥ JCOL(K).

NZSUB — Vector of length MAXSUB containing the row subscripts for the off-diagonal nonzeros in the Cholesky factor in compressed format. (Output)

INZSUB — Vector of length N + 1 containing pointers for NZSUB. The row subscripts for the off-diagonal nonzeros in column J are stored in NZSUB from location INZSUB (J) to INZSUB(J + (ILNZ (J + 1) − ILNZ(J) − 1). (Output)

MAXNZ — Total number of off-diagonal nonzeros in the Cholesky factor. (Output)

ILNZ — Vector of length N + 1 containing pointers to the Cholesky factor. The off-diagonal nonzeros in column J of the factor are stored from location ILNZ (J) to ILNZ(J + 1) − 1. (Output)
(ILNZ, NZSUB, INZSUB) sets up the data structure for the off-diagonal nonzeros of the Cholesky factor in column ordered form using compressed subscript format.

INVPER — Vector of length N containing the inverse permutation. (Output)
INVPER (K) = I indicates that the original row K is the new row I.

Optional Arguments

N — Number of equations. (Input)
Default: N = size (INVPER,1).

NZ — Total number of the nonzeros in the lower triangular part of the symmetric matrix, including the nonzeros on the diagonal. (Input)
Default: NZ = size (IROW,1).

IJOB — Integer parameter selecting an ordering to permute the matrix symmetrically. (Input)

IJOB = 0 selects the user ordering specified in IPER and reorders it so that the multifrontal method can be used in the numerical factorization.

IJOB = 1 selects the user ordering specified in IPER.

IJOB = 2 selects a minimum degree ordering.

IJOB = 3 selects a minimum degree ordering suitable for the multifrontal method in the numerical factorization.

Default: IJOB = 3.

ITWKSP — The total workspace needed. (Input)

If the default is desired, set ITWKSP to zero.

Default: ITWKSP = 0.

MAXSUB — Number of subscripts contained in array NZSUB. (Input/Output)

On input, MAXSUB gives the size of the array NZSUB. Note that when default workspace (ITWKSP = 0) is used, set MAXSUB = 3 * NZ. Otherwise (ITWKSP > 0), set MAXSUB = (ITWKSP – 10 * N – 7) / 4. On output, MAXSUB gives the number of subscripts used by the compressed subscript format.

Default: MAXSUB = 3 * NZ.

IPER — Vector of length N containing the ordering specified by IJOB. (Input/Output)

IPER(I) = K indicates that the original row K is the new row I.

ISPACE — The storage space needed for stack of frontal matrices. (Output)

FORTRAN 90 Interface

Generic:	Because the Fortran compiler cannot determine the precision desired from the required arguments, there is no generic Fortran 90 Interface for this routine. The specific Fortran 90 Interfaces are:
Single:	CALL LSCXD (IROW, JCOL, NZSUB, INZSUB, MAXNZ, ILNZ, INVPER [, …])
	Or
	CALL S_LSCXD (IROW, JCOL, NZSUB, INZSUB, MAXNZ, ILNZ, INVPER [, …])
Double:	CALL DLSCXD (IROW, JCOL, NZSUB, INZSUB, MAXNZ, ILNZ, INVPER [, …])
	Or
	CALL D_LSCXD (IROW, JCOL, NZSUB, INZSUB, MAXNZ, ILNZ, INVPER [, …])

FORTRAN 77 Interface

Single: CALL LSCXD (N, NZ, IROW, JCOL, IJOB, ITWKSP, MAXSUB, NZSUB, INZSUB, MAXNZ, ILNZ, IPER, INVPER, ISPACE)

Double: The double precision name is DLSCXD.

Description

Consider the linear equation

$$Ax = b$$

where *A* is sparse, positive definite and symmetric. The sparse coordinate format for the matrix *A* requires one real and two integer vectors. The real array a contains all the nonzeros in the *lower triangle* of *A* including the diagonal. Let the number of nonzeros be nz. The two integer arrays irow and jcol, each of length nz, contain the row and column indices for these entries in *A*. That is

$$A_{\mathrm{irow}(i),\,\mathrm{icol}(i)} = a(i),\ i = 1, \ldots, \mathtt{nz}$$

$$\mathtt{irow}(i) \geq \mathtt{jcol}(i) \quad i = 1, \ldots, \mathtt{nz}$$

with all other entries in the lower triangle of *A* zero.

The routine LSCXD computes a minimum degree ordering or uses a user-supplied ordering to set up the sparse data structure for the Cholesky factor, *L*. Then the routine LNFXD produces the numerical entries in *L* so that we have

$$\mathrm{P\,AP}^{T} = \mathrm{LL}^{T}$$

Here, *P* is the permutation matrix determined by the ordering.

The numerical computations can be carried out in one of two ways. The first method performs the factorization using a multifrontal technique. This option requires more storage but in certain cases will be faster. The multifrontal method is based on the routines in Liu (1987). For detailed description of this method, see Liu (1990), also Duff and Reid (1983, 1984), Ashcraft (1987), Ashcraft et al. (1987), and Liu (1986, 1989). The second method is fully described in George and Liu (1981). This is just the standard factorization method based on the sparse compressed storage scheme.

Comments

1. Workspace may be explicitly provided, if desired, by use of L2CXD. The reference is:

   CALL L2CXD (N, NZ, IROW, JCOL, IJOB, MAXSUB, NZSUB, INZSUB, MAXNZ, ILNZ, IPER, INVPER, ISPACE, LIWK, IWK)

   The additional arguments are as follows:

LIWK — The length of IWK, LIWK should be at least 10N + 12NZ + 7. Note that the argument MAXSUB should be set to (LIWK − 10N − 7) / 4.

IWK — Integer work vector of length LIWK.

Note that the parameter ITWKSP is not an argument to this routine.

2. Informational errors

Type	Code	Description
4	1	The matrix is structurally singular.

Example

As an example, the following matrix is symbolically factorized, and the result is printed:

$$A = \begin{bmatrix} 10 & 0 & 1 & 0 & 2 \\ 0 & 20 & 0 & 0 & 3 \\ 1 & 0 & 30 & 4 & 0 \\ 0 & 0 & 4 & 40 & 5 \\ 2 & 3 & 0 & 5 & 50 \end{bmatrix}$$

The number of nonzeros in the lower triangle of *A* is nz = 10. The sparse coordinate form for the lower triangle of *A* is given by:

irow	1	2	3	3	4	4	5	5	5	5
jcol	1	2	1	3	3	4	1	2	4	5

or equivalently by

irow	4	5	5	5	1	2	3	3	4	5
jcol	4	1	2	4	1	2	1	3	3	5

```
      USE LSCXD_INT
      USE WRIRN_INT
      INTEGER    N, NZ
      PARAMETER  (N=5, NZ=10)
!
      INTEGER    ILNZ(N+1), INVPER(N), INZSUB(N+1), IPER(N),&
                 IROW(NZ), ISPACE, JCOL(NZ), MAXNZ, MAXSUB,&
                 NZSUB(3*NZ)
!
      DATA IROW/1, 2, 3, 3, 4, 4, 5, 5, 5, 5/
      DATA JCOL/1, 2, 1, 3, 3, 4, 1, 2, 4, 5/
      MAXSUB = 3 * NZ
      CALL LSCXD (IROW, JCOL, NZSUB, INZSUB, MAXNZ, ILNZ, INVPER,&
                 MAXSUB=MAXSUB, IPER=IPER)
!                                  Print results
      CALL WRIRN (' iper ', IPER, 1, N, 1)
      CALL WRIRN (' invper ',INVPER, 1, N, 1)
      CALL WRIRN (' nzsub ', NZSUB, 1, MAXSUB, 1)
      CALL WRIRN (' inzsub ', INZSUB, 1, N+1, 1)
      CALL WRIRN (' ilnz ', ILNZ, 1, N+1, 1)
```

```
        END
```

Output

```
            iper
  1   2   3   4   5
  2   1   5   4   3

          invper
  1   2   3   4   5
  2   1   5   4   3

        nzsub
  1   2   3   4
  3   5   4   5
            inzsub
  1   2   3   4   5   6
  1   1   3   4   4   4

             ilnz
  1   2   3   4   5   6
  1   2   4   6   7   7
```

LNFXD

Computes the numerical Cholesky factorization of a sparse symmetrical matrix *A*.

Required Arguments

A — Vector of length `NZ` containing the nonzero coefficients of the lower triangle of the linear system. (Input)

IROW — Vector of length `NZ` containing the row numbers of the corresponding elements in the lower triangle of `A`. (Input)

JCOL — Vector of length `NZ` containing the column numbers of the corresponding elements in the lower triangle of `A`. (Input)

MAXSUB — Number of subscripts contained in array `NZSUB` as output from subroutine `LSCXD/DLSCXD`. (Input)

NZSUB — Vector of length `MAXSUB` containing the row subscripts for the nonzeros in the Cholesky factor in compressed format as output from subroutine `LSCXD/DLSCXD`. (Input)

INZSUB — Vector of length `N` + 1 containing pointers for `NZSUB` as output from subroutine `LSCXD/DLSCXD`. (Input)
The row subscripts for the nonzeros in column `J` are stored from location `INZSUB` (`J`) to `INZSUB`(`J` + 1) − 1.

MAXNZ — Length of `RLNZ` as output from subroutine `LSCXD/DLSCXD`. (Input)

ILNZ — Vector of length `N` + 1 containing pointers to the Cholesky factor as output from subroutine `LSCXD/DLSCXD`. (Input)
The row subscripts for the nonzeros in column `J` of the factor are stored from location `ILNZ`(`J`) to `ILNZ`(`J` + 1) − 1. (`ILNZ`, `NZSUB`, `INZSUB`) sets up the compressed data structure in column ordered form for the Cholesky factor.

IPER — Vector of length `N` containing the permutation as output from subroutine `LSCXD/DLSCXD`. (Input)

INVPER — Vector of length `N` containing the inverse permutation as output from subroutine `LSCXD/DLSCXD`. (Input)

ISPACE — The storage space needed for the stack of frontal matrices as output from subroutine `LSCXD/DLSCXD`. (Input)

DIAGNL — Vector of length `N` containing the diagonal of the factor. (Output)

RLNZ — Vector of length `MAXNZ` containing the strictly lower triangle nonzeros of the Cholesky factor. (Output)

RPARAM — Parameter vector containing factorization information. (Output)
`RPARAM`(1) = smallest diagonal element.
`RPARAM`(2) = largest diagonal element.

Optional Arguments

N — Number of equations. (Input)
Default: `N` = size (`IPER`,1).

NZ — The number of nonzero coefficients in the linear system. (Input)
Default: `NZ` = size (`A`,1).

IJOB — Integer parameter selecting factorization method. (Input)
`IJOB` = 1 yields factorization in sparse column format.
`IJOB` = 2 yields factorization using multifrontal method.
Default: `IJOB` = 1.

ITWKSP — The total workspace needed. (Input)
If the default is desired, set `ITWKSP` to zero.
Default: `ITWKSP` = 0.

FORTRAN 90 Interface

Generic: `CALL LNFXD (A, IROW, JCOL, MAXSUB, NZSUB, INZSUB, MAXNZ, ILNZ, IPER, INVPER, ISPACE, DIAGNL, RLNZ, RPARAM [, …])`

Specific: The specific interface names are `S_LNFXD` and `D_LNFXD`.

FORTRAN 77 Interface

Single: `CALL LNFXD (N, NZ, A, IROW, JCOL, IJOB, ITWKSP, MAXSUB, NZSUB, INZSUB, MAXNZ, ILNZ, IPER, INVPER, ISPACE, ITWKSP, DIAGNL, RLNZ, RPARAM)`

Double: The double precision name is `DLNFXD`.

Description

Consider the linear equation

$$Ax = b$$

where *A* is sparse, positive definite and symmetric. The sparse coordinate format for the matrix *A* requires one real and two integer vectors. The real array a contains all the nonzeros in the *lower triangle* of *A* including the diagonal. Let the number of nonzeros be nz. The two integer arrays irow and jcol, each of length nz, contain the row and column indices for these entries in *A*. That is

$$A_{\mathrm{irow}(i),\, \mathrm{icol}(i)} = a(i),\ i = 1, \ldots, \mathrm{nz}$$

$$\mathrm{irow}(i) \geq \mathrm{jcol}(i) \quad i = 1, \ldots, \mathrm{nz}$$

with all other entries in the lower triangle of *A* zero. The routine LNFXD produces the Cholesky factorization of PAP^T given the symbolic factorization of *A* which is computed by LSCXD. That is, this routine computes *L* which satisfies

$$PAP^T = LL^T$$

The diagonal of *L* is stored in DIAGNL and the strictly lower triangular part of *L* is stored in compressed subscript form in *R* = RLNZ as follows. The nonzeros in the *j*-th column of *L* are stored in locations *R*(*i*), …, *R*(*i* + *k*) where *i* = ILNZ(*j*) and *k* = ILNZ(*j* + 1) − ILNZ(*j*) − 1. The row subscripts are stored in the vector NZSUB from locations INZSUB(*j*) to INZSUB(*j*) + *k*.

The numerical computations can be carried out in one of two ways. The first method (when IJOB = 2) performs the factorization using a multifrontal technique. This option requires more storage but in certain cases will be faster. The multifrontal method is based on the routines in Liu (1987). For detailed description of this method, see Liu (1990), also Duff and Reid (1983, 1984), Ashcraft (1987), Ashcraft et al. (1987), and Liu (1986, 1989). The second method (when IJOB = 1) is fully described in George and Liu (1981). This is just the standard factorization method based on the sparse compressed storage scheme.

Comments

1. Workspace may be explicitly provided by use of L2FXD/DL2FXD . The reference is:

   CALL L2FXD (N, NZ, A, IROW, JCOL, IJOB, MAXSUB, NZSUB, INZSUB, MAXNZ, ILNZ, IPER, INVPER, ISPACE, DIAGNL, RLNZ, RPARAM, WK, LWK, IWK, LIWK)

   The additional arguments are as follows:

   WK — Real work vector of length LWK.

   LWK — The length of WK, LWK should be at least N + 3NZ.

   IWK — Integer work vector of length LIWK.

   LIWK — The length of IWK, LIWK should be at least 2N.

   Note that the parameter ITWKSP is not an argument to this routine.

2. Informational errors

Type	Code	Description
4	1	The coefficient matrix is not positive definite.
4	2	A column without nonzero elements has been found in the coefficient matrix.

Example

As an example, consider the 5 × 5 linear system:

$$A = \begin{bmatrix} 10 & 0 & 1 & 0 & 2 \\ 0 & 20 & 0 & 0 & 3 \\ 1 & 0 & 30 & 4 & 0 \\ 0 & 0 & 4 & 40 & 5 \\ 2 & 3 & 0 & 5 & 50 \end{bmatrix}$$

The number of nonzeros in the lower triangle of *A* is `nz` = 10. The sparse coordinate form for the lower triangle of *A* is given by:

irow	1	2	3	3	4	4	5	5	5	5
jcol	1	2	1	3	3	4	1	2	4	5
a	10	20	1	30	4	40	2	3	5	50

or equivalently by

irow	4	5	5	5	1	2	3	3	4	5
jcol	4	1	2	4	1	2	1	3	3	5
a	40	2	3	5	10	20	1	30	4	50

We first call `LSCXD` to produce the symbolic information needed to pass on to `LNFXD`. Then call `LNFXD` to factor this matrix. The results are displayed below.

```
      USE LNFXD_INT
      USE LSCXD_INT
      USE WRRRN_INT
      INTEGER    N, NZ, NRLNZ
      PARAMETER  (N=5, NZ=10, NRLNZ=10)
!
      INTEGER    IJOB, ILNZ(N+1), INVPER(N), INZSUB(N+1), IPER(N),&
                 IROW(NZ), ISPACE, JCOL(NZ), MAXNZ, MAXSUB,&
                 NZSUB(3*NZ)
      REAL       A(NZ), DIAGNL(N), RLNZ(NRLNZ), RPARAM(2) , R(N,N)
!
      DATA A/10., 20., 1., 30., 4., 40., 2., 3., 5., 50./
      DATA IROW/1, 2, 3, 3, 4, 4, 5, 5, 5, 5/
      DATA JCOL/1, 2, 1, 3, 3, 4, 1, 2, 4, 5/
!                                 Select minimum degree ordering
!                                 for multifrontal method
      IJOB = 3
!                                 Use default workspace
```

```
      MAXSUB = 3*NZ
      CALL LSCXD (IROW, JCOL, NZSUB, INZSUB, MAXNZ, ILNZ, INVPER, &
                  MAXSUB=MAXSUB)
!                                  Check if NRLNZ is large enough
      IF (NRLNZ .GE. MAXNZ) THEN
!                                  Choose multifrontal method
         IJOB = 2
         CALL LNFXD (A, IROW, JCOL, MAXSUB, NZSUB, INZSUB, MAXNZ, &
                     ILNZ,IPER, INVPER, ISPACE, DIAGNL, RLNZ, RPARAM, &
                     IJOB=IJOB)
!                                  Print results
         CALL WRRRN (' diagnl ', DIAGNL,  NRA=1, NCA=N, LDA=1)
         CALL WRRRN (' rlnz ', RLNZ,  NRA= 1,  NCA= MAXNZ,  LDA= 1)
      END IF
!
!                                 Construct L matrix
      DO I=1,N
!                                 Diagonal
        R(I,I) = DIAG(I)
        IF (ILNZ(I) .GT. MAXNZ) GO TO 50
!                                 Find elements of RLNZ for this column
        ISTRT = ILNZ(I)
        ISTOP = ILNZ(I+1) - 1
!                                 Get starting index for NZSUB
        K = INZSUB(I)
        DO J=ISTRT, ISTOP
!                                 NZSUB(K) is the row for this element of
                                  RLNZ
           R((NZSUB(K)),I) = RLNZ(J)
           K = K + 1
        END DO
      END DO
  50  CONTINUE
      CALL WRRRN ('L', R, NRA=N, NCA=N)
      END
```

Output

```
                  diagnl
    1       2       3       4       5
4.472   3.162   7.011   6.284   5.430

                           rlnz
     1         2         3         4         5         6
0.6708    0.6325    0.3162    0.7132   -0.0285    0.6398

                                L
         1       2       3       4       5
 1   4.472   0.000   0.000   0.000   0.000
 2   0.000   3.162   0.000   0.000   0.000
 3   0.671   0.632   7.011   0.000   0.000
 4   0.000   0.000   0.713   6.284   0.000
 5   0.000   0.316  -0.029   0.640   5.430
```

LFSXD

Solves a real sparse symmetric positive definite system of linear equations, given the Cholesky factorization of the coefficient matrix.

Required Arguments

N — Number of equations. (Input)

MAXSUB — Number of subscripts contained in array NZSUB as output from subroutine LSCXD/DLSCXD. (Input)

NZSUB — Vector of length MAXSUB containing the row subscripts for the off-diagonal nonzeros in the factor as output from subroutine LSCXD/DLSCXD. (Input)

INZSUB — Vector of length N + 1 containing pointers for NZSUB as output from subroutine LSCXD/DLSCXD. (Input)
The row subscripts of column J are stored from location INZSUB(J) to INZSUB(J + 1) − 1.

MAXNZ — Total number of off-diagonal nonzeros in the Cholesky factor as output from subroutine LSCXD/DLSCXD. (Input)

RLNZ — Vector of length MAXNZ containing the off-diagonal nonzeros in the factor in column ordered format as output from subroutine LNFXD/DLNFXD. (Input)

ILNZ — Vector of length N + 1 containing pointers to RLNZ as output from subroutine LSCXD/DLSCXD. The nonzeros in column J of the factor are stored from location ILNZ(J) to ILNZ(J + 1) − 1. (Input)
The values (RLNZ, ILNZ, NZSUB, INZSUB) give the off-diagonal nonzeros of the factor in a compressed subscript data format.

DIAGNL — Vector of length N containing the diagonals of the Cholesky factor as output from subroutine LNFXD/DLNFXD. (Input)

IPER — Vector of length N containing the ordering as output from subroutine LSCXD/DLSCXD. (Input)
IPER(I) = K indicates that the original row K is the new row I.

B — Vector of length N containing the right-hand side. (Input)

X — Vector of length N containing the solution. (Output)

FORTRAN 90 Interface

Generic: CALL LFSXD (N, MAXSUB, NZSUB, INZSUB, MAXNZ, RLNZ, ILNZ, DIAGNL, IPER, B, X)

Specific: The specific interface names are S_LFSXD and D_LFSXD.

FORTRAN 77 Interface

Single: CALL LFSXD (N, MAXSUB, NZSUB, INZSUB, MAXNZ, RLNZ, ILNZ, DIAGNL, IPER, B, X)

Double: The double precision name is DLFSXD.

Description

Consider the linear equation

$$Ax = b$$

where *A* is sparse, positive definite and symmetric. The sparse coordinate format for the matrix *A* requires one real and two integer vectors. The real array a contains all the nonzeros in the *lower triangle* of *A* including the diagonal. Let the number of nonzeros be nz. The two integer arrays irow and jcol, each of length nz, contain the row and column indices for these entries in *A*. That is

$$A_{\mathrm{irow}(i),\ \mathrm{icol}(i)} = a(i),\ i = 1, \ldots, \mathrm{nz}$$

$$\mathrm{irow}(i) \geq \mathrm{jcol}(i) \quad i = 1, \ldots, \mathrm{nz}$$

with all other entries in the lower triangle of *A* zero.

The routine LFSXD computes the solution of the linear system given its Cholesky factorization. The factorization is performed by calling LSCXD followed by LNFXD. The routine LSCXD computes a minimum degree ordering or uses a user-supplied ordering to set up the sparse data structure for the Cholesky factor, *L*. Then the routine LNFXD produces the numerical entries in *L* so that we have

$$P\,AP^T = LL^T$$

Here *P* is the permutation matrix determined by the ordering.

The numerical computations can be carried out in one of two ways. The first method performs the factorization using a multifrontal technique. This option requires more storage but in certain cases will be faster. The multifrontal method is based on the routines in Liu (1987). For detailed description of this method, see Liu (1990), also Duff and Reid (1983, 1984), Ashcraft (1987), Ashcraft et al. (1987), and Liu (1986, 1989). The second method is fully described in George and Liu (1981). This is just the standard factorization method based on the sparse compressed storage scheme.

Finally, the solution *x* is obtained by the following calculations:

$$1)\ Ly_1 = Pb$$

$$2)\ L^T y_2 = y_1$$

$$3)\ x = P^T y_2$$

Comments

Informational error

Type	Code	Description
4	1	The input matrix is numerically singular.

Example

As an example, consider the 5 × 5 linear system:

$$A = \begin{bmatrix} 10 & 0 & 1 & 0 & 2 \\ 0 & 20 & 0 & 0 & 3 \\ 1 & 0 & 30 & 4 & 0 \\ 0 & 0 & 4 & 40 & 5 \\ 2 & 3 & 0 & 5 & 50 \end{bmatrix}$$

Let

$$x_1{}^T = (1,2,3,4,5)$$

so that $Ax_1 = (23, 55, 107, 197, 278)^T$, and

$$x_2{}^T = (5,4,3,2,1)$$

so that $Ax_2 = (55, 83, 103, 97, 82)^T$. The number of nonzeros in the lower triangle of A is `nz` = 10. The sparse coordinate form for the lower triangle of A is given by:

irow	1	2	3	3	4	4	5	5	5	5
jcol	1	2	1	3	3	4	1	2	4	5
a	10	20	1	30	4	40	2	3	5	50

or equivalently by

irow	4	5	5	5	1	2	3	3	4	5
jcol	4	1	2	4	1	2	1	3	3	5
a	40	2	3	5	10	20	1	30	4	50

```
      USE LFSXD_INT
      USE LNFXD_INT
      USE LSCXD_INT
      USE WRRRN_INT
      INTEGER     N, NZ, NRLNZ
      PARAMETER  (N=5, NZ=10, NRLNZ=10)
!
      INTEGER    IJOB, ILNZ(N+1), INVPER(N), INZSUB(N+1), IPER(N),&
                IROW(NZ), ISPACE, ITWKSP, JCOL(NZ), MAXNZ, MAXSUB,&
                NZSUB(3*NZ)
      REAL       A(NZ), B1(N), B2(N), DIAGNL(N), RLNZ(NRLNZ), RPARAM(2),&
                X(N)
!
      DATA A/10., 20., 1., 30., 4., 40., 2., 3., 5., 50./
      DATA B1/23., 55., 107., 197., 278./
      DATA B2/55., 83., 103., 97., 82./
      DATA IROW/1, 2, 3, 3, 4, 4, 5, 5, 5, 5/
      DATA JCOL/1, 2, 1, 3, 3, 4, 1, 2, 4, 5/
!                                Select minimum degree ordering
!                                for multifrontal method
      IJOB = 3
!                                Use default workspace
      ITWKSP = 0
      MAXSUB = 3*NZ
      CALL LSCXD (IROW, JCOL, NZSUB, INZSUB, MAXNZ, ILNZ, INVPER, &
                  MAXSUB=MAXSUB, IPER=IPER, ISPACE=ISPACE)
!                                Check if NRLNZ is large enough
      IF (NRLNZ .GE. MAXNZ) THEN
!                                Choose multifrontal method
         IJOB = 2
      CALL LNFXD (A, IROW, JCOL, MAXSUB, NZSUB, INZSUB, MAXNZ, ILNZ,&
              IPER, INVPER,ISPACE, DIAGNL, RLNZ, RPARAM, IJOB=IJOB)
!                                Solve A * X1 = B1
      CALL LFSXD (N, MAXSUB, NZSUB, INZSUB, MAXNZ, RLNZ, ILNZ, DIAGNL,&
                     IPER, B1, X)
!                                Print X1
      CALL WRRRN (' x1 ', X, 1, N, 1)
!                                Solve A * X2 = B2
      CALL LFSXD (N, MAXSUB, NZSUB, INZSUB, MAXNZ, RLNZ, ILNZ, &
                     DIAGNL, IPER, B2, X)
!                                Print X2
      CALL WRRRN (' x2 ' X, 1, N, 1)


      END IF
!
      END
```

Output

```
                    x1
    1       2       3       4       5
1.000   2.000   3.000   4.000   5.000

                    x2
    1       2       3       4       5
5.000   4.000   3.000   2.000   1.000
```

LSLZD

Solves a complex sparse Hermitian positive definite system of linear equations by Gaussian elimination.

Required Arguments

A — Complex vector of length NZ containing the nonzero coefficients in the lower triangle of the linear system. (Input)
The sparse matrix has nonzeroes only in entries (IROW(*i*), JCOL(*i*)) for *i* = 1 to NZ, and at this location the sparse matrix has value A(*i*).

IROW — Vector of length NZ containing the row numbers of the corresponding elements in the lower triangle of A. (Input)
Note IROW(*i*) ≥ JCOL(*i*), since we are only indexing the lower triangle.

JCOL — Vector of length NZ containing the column numbers of the corresponding elements in the lower triangle of A. (Input)

B — Complex vector of length N containing the right-hand side of the linear system. (Input)

X — Complex vector of length N containing the solution to the linear system. (Output)

Optional Arguments

N — Number of equations. (Input)
Default: N = size (B,1).

NZ — The number of nonzero coefficients in the lower triangle of the linear system. (Input)
Default: NZ = size (A,1).

ITWKSP — The total workspace needed. (Input)
If the default is desired, set ITWKSP to zero.
Default: ITWKSP = 0.

FORTRAN 90 Interface

Generic: CALL LSLZD (A, IROW, JCOL, B, X [, …])

Specific: The specific interface names are S_LSLZD and D_LSLZD.

FORTRAN 77 Interface

Single: CALL LSLZD (N, NZ, A, IROW, JCOL, B, ITWKSP, X)

Double: The double precision name is DLSLZD.

Description

Consider the linear equation

$$Ax = b$$

where *A* is sparse, positive definite and Hermitian. The sparse coordinate format for the matrix *A* requires one complex and two integer vectors. The complex array a contains all the nonzeros in the lower triangle of *A* including the diagonal. Let the number of nonzeros be nz. The two integer arrays irow and jcol, each of length nz, contain the row and column indices for these entries in *A*. That is

$$A_{\mathrm{irow}(i),\ \mathrm{icol}(i)} = a(i),\ i = 1, \ldots, \mathtt{nz}$$

$$\mathtt{irow}(i) \geq \mathtt{jcol}(i) \quad i = 1, \ldots, \mathtt{nz}$$

with all other entries in the lower triangle of *A* zero.

The routine LSLZD solves a system of linear algebraic equations having a complex, sparse, Hermitian and positive definite coefficient matrix. It first uses the routine LSCXD to compute a symbolic factorization of a permutation of the coefficient matrix. It then calls LNFZD to perform the numerical factorization. The solution of the linear system is then found using LFSZD.

The routine LSCXD computes a minimum degree ordering or uses a user-supplied ordering to set up the sparse data structure for the Cholesky factor, *L*. Then the routine LNFZD produces the numerical entries in *L* so that we have

$$\mathrm{P\,AP}^{\boldsymbol{T}} = \mathrm{LL}^{\boldsymbol{H}}$$

Here P is the permutation matrix determined by the ordering.

The numerical computations can be carried out in one of two ways. The first method performs the factorization using a multifrontal technique. This option requires more storage but in certain cases will be faster. The multifrontal method is based on the routines in Liu (1987). For detailed description of this method, see Liu (1990), also Duff and Reid (1983, 1984), Ashcraft (1987), Ashcraft et al. (1987), and Liu (1986, 1989). The second method is fully described in George and Liu (1981). This is just the standard factorization method based on the sparse compressed storage scheme.

Finally, the solution *x* is obtained by the following calculations:

$$1)\quad Ly_1 = Pb$$

$$2)\ L^{\boldsymbol{H}} y_2 = y_1$$

3) $x = P^T y_2$

The routine LFSZD accepts b and the permutation vector which determines P . It then returns x.

Comments

1. Workspace may be explicitly provided, if desired, by use of L2LZD/DL2LZD. The reference is:

   CALL L2LZD (N, NZ, A, IROW, JCOL, B, X, IPER, IPARAM, RPARAM, WK, LWK, IWK, LIWK)

   The additional arguments are as follows:

   IPER — Vector of length N containing the ordering.

   IPARAM — Integer vector of length 4. See Comment 3.

   RPARAM — Real vector of length 2. See Comment 3.

   WK — Complex work vector of length LWK.

   LWK — The length of WK, LWK should be at least 2N + 6NZ.

   IWK — Integer work vector of length LIWK.

   LIWK — The length of IWK, LIWK should be at least 15N + 15NZ + 9.

   Note that the parameter ITWKSP is not an argument for this routine.

2. Informational errors

Type	Code	Description
4	1	The coefficient matrix is not positive definite.
4	2	A column without nonzero elements has been found in the coefficient matrix.

3. If the default parameters are desired for L2LZD, then set IPARAM(1) to zero and call the routine L2LZD. Otherwise, if any nondefault parameters are desired for IPARAM or RPARAM, then the following steps should be taken before calling L2LZD.

   CALL L4LZD (IPARAM, RPARAM)

   Set nondefault values for desired IPARAM, RPARAM elements.

Note that the call to L4LZD will set IPARAM and RPARAM to their default values, so only nondefault values need to be set above. The arguments are as follows:

IPARAM — Integer vector of length 4.

IPARAM(1) = Initialization flag.

IPARAM(2) = The numerical factorization method.

IPARAM(2)	Action
0	Multifrontal
1	Sparse column

Default: 0.

IPARAM(3) = The ordering option.

IPARAM(3)	Action
0	Minimum degree ordering
1	User's ordering specified in IPER

Default: 0.

IPARAM(4) = The total number of nonzeros in the factorization matrix.

RPARAM — Real vector of length 2.

RPARAM(1) = The absolute value of the largest diagonal element in the Cholesky factorization.

RPARAM(2) = The absolute value of the smallest diagonal element in the Cholesky factorization.

If double precision is required, then DL4LZD is called and RPARAM is declared double precision.

Example

As an example, consider the 3 × 3 linear system:

$$A = \begin{bmatrix} 2+0i & -1+i & 0 \\ -1-i & 4+0i & 1+2i \\ 0 & 1-2i & 10+0i \end{bmatrix}$$

Let $x^T = (1 + i, 2 + 2i, 3 + 3i)$ so that $Ax = (-2 + 2i, 5 + 15i, 36 + 28i)^T$. The number of nonzeros in the lower triangle of A is nz = 5. The sparse coordinate form for the lower triangle of A is given by:

$$\begin{array}{cccccc} \text{irow} & 1 & 2 & 3 & 2 & 3 \\ \text{jcol} & 1 & 2 & 3 & 1 & 2 \\ \text{a} & 2+0i & 4+0i & 10+0i & -1-i & 1-2i \end{array}$$

or equivalently by

irow	3	2	3	1	2
jcol	3	1	2	1	2
a	$10+0i$	$-1-i$	$1-2i$	$2+0i$	$4+0i$

```
      USE LSLZD_INT
      USE WRCRN_INT
      INTEGER    N, NZ
      PARAMETER  (N=3, NZ=5)
!
      INTEGER    IROW(NZ), JCOL(NZ)
      COMPLEX    A(NZ), B(N), X(N)
!
      DATA A/(2.0,0.0), (4.0,0.0), (10.0,0.0), (-1.0,-1.0), (1.0,-2.0)/
      DATA B/(-2.0,2.0), (5.0,15.0), (36.0,28.0)/
      DATA IROW/1, 2, 3, 2, 3/
      DATA JCOL/1, 2, 3, 1, 2/
!                                 Solve A * X = B
      CALL LSLZD (A, IROW, JCOL, B, X)


!                                 Print results
      CALL WRCRN (' x ', X, 1, N, 1)
      END
```

Output

```
                        x
              1                 2                 3
( 1.000, 1.000)  ( 2.000, 2.000)  ( 3.000, 3.000)
```

LNFZD

Computes the numerical Cholesky factorization of a sparse Hermitian matrix *A*.

Required Arguments

A — Complex vector of length NZ containing the nonzero coefficients of the lower triangle of the linear system. (Input)

IROW — Vector of length NZ containing the row numbers of the corresponding elements in the lower triangle of A. (Input)

JCOL — Vector of length NZ containing the column numbers of the corresponding elements in the lower triangle of A. (Input)

MAXSUB — Number of subscripts contained in array NZSUB as output from subroutine LSCXD/DLSCXD. (Input)

NZSUB — Vector of length MAXSUB containing the row subscripts for the nonzeros in the Cholesky factor in compressed format as output from subroutine LSCXD/DLSCXD. (Input)

INZSUB — Vector of length N + 1 containing pointers for NZSUB as output from subroutine LSCXD/DLSCXD. (Input)
The row subscripts for the nonzeros in column J are stored from location INZSUB(J) to INZSUB(J + 1) − 1.

MAXNZ — Length of RLNZ as output from subroutine LSCXD/DLSCXD. (Input)

ILNZ — Vector of length N + 1 containing pointers to the Cholesky factor as output from subroutine LSCXD/DLSCXD. (Input)
The row subscripts for the nonzeros in column J of the factor are stored from location ILNZ(J) to ILNZ(J + 1) − 1. (ILNZ , NZSUB, INZSUB) sets up the compressed data structure in column ordered form for the Cholesky factor.

IPER — Vector of length N containing the permutation as output from subroutine LSCXD/DLSCXD. (Input)

INVPER — Vector of length N containing the inverse permutation as output from subroutine LSCXD/DLSCXD. (Input)

ISPACE — The storage space needed for the stack of frontal matrices as output from subroutine LSCXD/DLSCXD. (Input)

DIAGNL — Complex vector of length `N` containing the diagonal of the factor. (Output)

RLNZ — Complex vector of length `MAXNZ` containing the strictly lower triangle nonzeros of the Cholesky factor. (Output)

RPARAM — Parameter vector containing factorization information. (Output)
`RPARAM` (1) = smallest diagonal element in absolute value.
`RPARAM` (2) = largest diagonal element in absolute value.

Optional Arguments

N — Number of equations. (Input)
Default: `N` = size (`IPER`,1).

NZ — The number of nonzero coefficients in the linear system. (Input)
Default: `NZ` = size (`A`,1).

IJOB — Integer parameter selecting factorization method. (Input)
`IJOB` = 1 yields factorization in sparse column format.
`IJOB` = 2 yields factorization using multifrontal method.
Default: `IJOB` = 1.

ITWKSP — The total workspace needed. (Input)
If the default is desired, set `ITWKSP` to zero. See Comment 1 for the default.
Default: `ITWKSP` = 0.

FORTRAN 90 Interface

Generic: `CALL LNFZD` (`A`, `IROW`, `JCOL`, `MAXSUB`, `NZSUB`, `INZSUB`, `MAXNZ`, `ILNZ`, `IPER`, `INVPER`, `ISPACE`, `DIAGNL`, `RLNZ`, `RPARAM` [, …])

Specific: The specific interface names are `S_LNFZD` and `D_LNFZD`.

FORTRAN 77 Interface

Single: `CALL LNFZD` (`N`, `NZ`, `A`, `IROW`, `JCOL`, `IJOB`, `MAXSUB`, `NZSUB`, `INZSUB`, `MAXNZ`, `ILNZ`, `IPER`, `INVPER`, `ISPACE`, `ITWKSP`, `DIAGNL`, `RLNZ`, `RPARAM`)

Double: The double precision name is `DLNFZD`.

Description

Consider the linear equation

$$Ax = b$$

where *A* is sparse, positive definite and Hermitian. The sparse coordinate format for the matrix *A* requires one complex and two integer vectors. The complex array `a` contains all the nonzeros in the *lower triangle* of *A* including the diagonal. Let the number of nonzeros be `nz`. The two integer arrays `irow` and `jcol`, each of length `nz`, contain the row and column indices for these entries in *A*. That is

$$A_{\mathrm{irow}(i),\,\mathrm{icol}(i)} = a(i),\ i = 1, \ldots, \mathtt{nz}$$
$$\mathtt{irow}(i) \geq \mathtt{jcol}(i) \quad i = 1, \ldots, \mathtt{nz}$$

with all other entries in the lower triangle of *A* zero.

The routine `LNFZD` produces the Cholesky factorization of PAP^T given the symbolic factorization of *A* which is computed by `LSCXD`. That is, this routine computes *L* which satisfies

$$PAP^T = LL^H$$

The diagonal of *L* is stored in `DIAGNL` and the strictly lower triangular part of *L* is stored in compressed subscript form in *R* = `RLNZ` as follows. The nonzeros in the *j*th column of *L* are stored in locations *R*(*i*), …, *R*(*i* + *k*) where *i* = `ILNZ`(*j*) and *k* = `ILNZ`(*j* + 1)− `ILNZ`(*j*) − 1. The row subscripts are stored in the vector `NZSUB` from locations `INZSUB`(*j*) to `INZSUB`(*j*) + *k*.

The numerical computations can be carried out in one of two ways. The first method (when `IJOB` = 2) performs the factorization using a multifrontal technique. This option requires more storage but in certain cases will be faster. The multifrontal method is based on the routines in Liu (1987). For detailed description of this method, see Liu (1990), also Duff and Reid (1983, 1984), Ashcraft (1987), Ashcraft et al. (1987), and Liu (1986, 1989). The second method (when `IJOB` = 1) is fully described in George and Liu (1981). This is just the standard factorization method based on the sparse compressed storage scheme.

Comments

1. Workspace may be explicitly provided by use of `L2FZD`/`DL2FZD`. The reference is:

   ```
   CALL L2FZD (N, NZ, A, IROW, JCOL, IJOB, MAXSUB, NZSUB, INZSUB, MAXNZ,
       ILNZ, IPER, INVPER, ISPACE, DIAGNL, RLNZ, RPARAM, WK, LWK, IWK, LIWK)
   ```

   The additional arguments are as follows:

   WK — Complex work vector of length `LWK`.

   LWK — The length of `WK`, `LWK` should be at least `N` + 3`NZ`.

   IWK — Integer work vector of length `LIWK`.

LIWK — The length of `IWK`, `LIWK` should be at least 2`N`.

Note that the parameter `ITWKSP` is not an argument to this routine.

2. Informational errors

Type	Code	Description
4	1	The coefficient matrix is not positive definite.
4	2	A column without nonzero elements has been found in the coefficient matrix.

Example

As an example, consider the 3 × 3 linear system:

$$A = \begin{bmatrix} 2+0i & -1+i & 0 \\ -1-i & 4+0i & 1+2i \\ 0 & 1-2i & 10+0i \end{bmatrix}$$

The number of nonzeros in the lower triangle of *A* is `nz` = 5. The sparse coordinate form for the lower triangle of *A* is given by:

$$\begin{array}{cccccc} \text{irow} & 1 & 2 & 3 & 2 & 3 \\ \text{jcol} & 1 & 2 & 3 & 1 & 2 \\ \text{a} & 2+0i & 4+0i & 10+0i & -1-i & 1-2i \end{array}$$

or equivalently by

$$\begin{array}{cccccc} \text{irow} & 3 & 2 & 3 & 1 & 2 \\ \text{jcol} & 3 & 1 & 2 & 1 & 2 \\ \text{a} & 10+0i & -1-i & 1-2i & 2+0i & 4+0i \end{array}$$

We first call `LSCXD` to produce the symbolic information needed to pass on to `LNFZD`. Then call `LNFZD` to factor this matrix. The results are displayed below.

```
      USE LNFZD_INT
      USE LSCXD_INT
      USE WRCRN_INT
      INTEGER    N, NZ, NRLNZ
      PARAMETER  (N=3, NZ=5, NRLNZ=5)
!
      INTEGER    IJOB, ILNZ(N+1), INVPER(N), INZSUB(N+1), IPER(N),&
                 IROW(NZ), ISPACE, JCOL(NZ), MAXNZ, MAXSUB,&
                 NZSUB(3*NZ)
      REAL       RPARAM(2)
      COMPLEX    A(NZ), DIAGNL(N), RLNZ(NRLNZ)
!
      DATA A/(2.0,0.0), (4.0,0.0), (10.0,0.0), (-1.0,-1.0), (1.0,-2.0)/
      DATA IROW/1, 2, 3, 2, 3/
      DATA JCOL/1, 2, 3, 1, 2/
```

```
!                                   Select minimum degree ordering
!                                   for multifrontal method
      IJOB = 3
      MAXSUB = 3*NZ
      CALL LSCXD (IROW, JCOL, NZSUB, INZSUB, MAXNZ, ILNZ, INVPER, &
                  IJOB=IJOB, MAXSUB=MAXSUB)
!                                   Check if NRLNZ is large enough
      IF (NRLNZ .GE. MAXNZ) THEN
!                                   Choose multifrontal method
         IJOB = 2
      CALL LNFZD (A, IROW, JCOL, MAXSUB, NZSUB, INZSUB, MAXNZ, &
                     ILNZ, IPER, INVPER, ISPACE, DIAGNL, RLNZ, RPARAM, &
                     IJOB=IJOB)
!                                   Print results
      CALL WRCRN (' diagnl ', DIAGNL, 1, N, 1)
      CALL WRCRN (' rlnz ', RLNZ, 1, MAXNZ, 1)
      END IF
!
      END
```

Output

```
                          diagnl
              1                  2                  3
( 1.414, 0.000)   ( 1.732, 0.000)   ( 2.887, 0.000)

                    rlnz
              1                  2
(-0.707,-0.707)   ( 0.577,-1.155)
```

LFSZD

Solves a complex sparse Hermitian positive definite system of linear equations, given the Cholesky factorization of the coefficient matrix.

Required Arguments

N — Number of equations. (Input)

MAXSUB — Number of subscripts contained in array NZSUB as output from subroutine LSCXD/DLSCXD. (Input)

NZSUB — Vector of length MAXSUB containing the row subscripts for the off-diagonal nonzeros in the factor as output from subroutine LSCXD/DLSCXD. (Input)

INZSUB — Vector of length N + 1 containing pointers for NZSUB as output from subroutine LSCXD/DLSCXD. (Input)
The row subscripts of column J are stored from location INZSUB(J) to INZSUB(J + 1) − 1.

MAXNZ — Total number of off-diagonal nonzeros in the Cholesky factor as output from subroutine LSCXD/DLSCXD. (Input)

RLNZ — Complex vector of length MAXNZ containing the off-diagonal nonzeros in the factor in column ordered format as output from subroutine LNFZD/DLNFZD. (Input)

ILNZ — Vector of length N +1 containing pointers to RLNZ as output from subroutine LSCXD/DLSCXD. The nonzeros in column J of the factor are stored from location ILNZ(J) to ILNZ(J + 1) − 1. (Input)
The values (RLNZ, ILNZ, NZSUB, INZSUB) give the off-diagonal nonzeros of the factor in a compressed subscript data format.

DIAGNL — Complex vector of length N containing the diagonals of the Cholesky factor as output from subroutine LNFZD/DLNFZD. (Input)

IPER — Vector of length N containing the ordering as output from subroutine LSCXD/DLSCXD. (Input)
IPER(I) = K indicates that the original row K is the new row I.

B — Complex vector of length N containing the right-hand side. (Input)

X — Complex vector of length N containing the solution. (Output)

FORTRAN 90 Interface

Generic: CALL LFSZD (N, MAXZUB, NZSUB, INZSUB, MAXNZ, RLNZ, ILNZ, DIAGNL, IPER, B, X)

Specific: The specific interface names are S_LFSZD and D_LFSZD.

FORTRAN 77 Interface

Single: CALL LFSZD (N, MAXSUB, NZSUB, INZSUB, MAXNZ, RLNZ, ILNZ, DIAGNL, IPER, B, X)

Double: The double precision name is DLFSZD.

Description

Consider the linear equation

$$Ax = b$$

where *A* is sparse, positive definite and Hermitian. The sparse coordinate format for the matrix *A* requires one complex and two integer vectors. The complex array a contains all the nonzeros in the *lower triangle* of *A* including the diagonal. Let the number of nonzeros be nz. The two integer arrays irow and jcol, each of length nz, contain the row and column indices for these entries in *A*. That is

$$A_{\text{irow}(i),\ \text{icol}(i)} = a(i),\ i = 1, \ldots, \text{nz}$$

$$\text{irow}(i) \geq \ \text{jcol}(i) \quad i = 1, \ldots, \text{nz}$$

with all other entries in the lower triangle of *A* zero.

The routine LFSZD computes the solution of the linear system given its Cholesky factorization. The factorization is performed by calling LSCXD followed by LNFZD. The routine LSCXD computes a minimum degree ordering or uses a user-supplied ordering to set up the sparse data structure for the Cholesky factor, *L*. Then the routine LNFZD produces the numerical entries in L so that we have

$$\text{P AP}^{T} = \text{LL}^{H}$$

Here *P* is the permutation matrix determined by the ordering.

The numerical computations can be carried out in one of two ways. The first method performs the factorization using a multifrontal technique. This option requires more storage but in certain cases will be faster. The multifrontal method is based on the routines in Liu (1987). For detailed description of this method, see Liu (1990), also Duff and Reid (1983, 1984), Ashcraft (1987), Ashcraft et al. (1987), and Liu (1986, 1989). The second method is fully described in George and Liu (1981). This is just the standard factorization method based on the sparse compressed storage scheme. Finally, the solution *x* is obtained by the following calculations:

$$1)\ Ly_1 = Pb$$

2) $L^{H} y_2 = y_1$

3) $x = P^{T} y_2$

Comments

Informational error

Type	Code	Description
4	1	The input matrix is numerically singular.

Example

As an example, consider the 3 × 3 linear system:

$$A = \begin{bmatrix} 2+0i & -1+i & 0 \\ -1-i & 4+0i & 1+2i \\ 0 & 1-2i & 10+0i \end{bmatrix}$$

Let

$$x_1^{T} = (1+i, 2+2i, 3+3i)$$

so that $Ax_1 = (-2 + 2i, 5 + 15i, 36 + 28i)^{T}$, and

$$x_2^{T} = (3+3i, 2+2i, 1+i)$$

so that $Ax_2 = (2 + 6i, 7 - 5i, 16 + 8i)^{T}$. The number of nonzeros in the lower triangle of A is `nz` = 5. The sparse coordinate form for the lower triangle of A is given by:

$$\begin{array}{cccccc} \text{irow} & 1 & 2 & 3 & 2 & 3 \\ \text{jcol} & 1 & 2 & 3 & 1 & 2 \\ \text{a} & 2+0i & 4+0i & 10+0i & -1-i & 1-2i \end{array}$$

or equivalently by

$$\begin{array}{cccccc} \text{irow} & 3 & 2 & 3 & 1 & 2 \\ \text{jcol} & 3 & 1 & 2 & 1 & 2 \\ \text{a} & 10+0i & -1-i & 1-2i & 2+0i & 4+0i \end{array}$$

```
      USE IMSL_LIBRARIES
      INTEGER    N, NZ, NRLNZ
      PARAMETER  (N=3, NZ=5, NRLNZ=5)
!
      INTEGER    IJOB, ILNZ(N+1), INVPER(N), INZSUB(N+1), IPER(N),&
                 IROW(NZ), ISPACE, JCOL(NZ), MAXNZ, MAXSUB,&
```

```
                   NZSUB(3*NZ)
      COMPLEX      A(NZ), B1(N), B2(N), DIAGNL(N), RLNZ(NRLNZ), X(N)
      REAL         RPARAM(2)
!
      DATA A/(2.0,0.0), (4.0,0.0), (10.0,0.0), (-1.0,-1.0), (1.0,-2.0)/
      DATA B1/(-2.0,2.0), (5.0,15.0), (36.0,28.0)/
      DATA B2/(2.0,6.0), (7.0,5.0), (16.0,8.0)/
      DATA IROW/1, 2, 3, 2, 3/
      DATA JCOL/1, 2, 3, 1, 2/
!                                  Select minimum degree ordering
!                                  for multifrontal method
      IJOB = 3
!                                  Use default workspace
      MAXSUB = 3*NZ
      CALL LSCXD (IROW, JCOL, NZSUB, INZSUB, MAXNZ, ILNZ, INVPER, &
                  IJOB=IJOB, MAXSUB=MAXSUB, IPER=IPER, ISPACE=ISPACE)
!                                  Check if NRLNZ is large enough
      IF (NRLNZ .GE. MAXNZ) THEN
!                                  Choose multifrontal method
         IJOB = 2
         CALL LNFZD (A, IROW, JCOL, MAXSUB, NZSUB, INZSUB,&
                     MAXNZ, ILNZ, IPER, INVPER, ISPACE, DIAGNL,&
                     RLNZ, RPARAM, IJOB=IJOB)
!                                  Solve A * X1 = B1
         CALL LFSZD (N, MAXSUB, NZSUB, INZSUB, MAXNZ, RLNZ, ILNZ, DIAGNL,&
                     IPER, B1, X)
!                                  Print X1
         CALL WRCRN (' x1 ', X, 1, N,1)
!                                  Solve A * X2 = B2
         CALL LFSZD (N, MAXSUB, NZSUB, INZSUB, MAXNZ, RLNZ, ILNZ, DIAGNL,&
                     IPER, B2, X)
!                                  Print X2
         CALL WRCRN (' x2 ', X, 1, N,1)
      END IF
!
      END
```

Output

```
                          x1
               1                  2                  3
( 1.000, 1.000)   ( 2.000, 2.000)   ( 3.000, 3.000)

                          x2
               1                  2                  3
( 3.000, 3.000)   ( 2.000, 2.000)   ( 1.000, 1.000)
```

LSLTO

Solves a complex sparse Hermitian positive definite system of linear equations, given the Cholesky factorization of the coefficient matrix.

Required Arguments

A — Real vector of length 2N – 1 containing the first row of the coefficient matrix followed by its first column beginning with the second element. (Input)
See Comment 2.

B — Real vector of length N containing the right-hand side of the linear system. (Input)

X — Real vector of length N containing the solution of the linear system. (Output)
If B is not needed then B and X may share the same storage locations.

Optional Arguments

N — Order of the matrix represented by A. (Input)
Default: N = (size (A,1) + 1)/2

IPATH — Integer flag. (Input)
IPATH = 1 means the system $Ax = B$ is solved.
IPATH = 2 means the system $A^T x = B$ is solved.
Default: IPATH =1.

FORTRAN 90 Interface

Generic: CALL LSLTO (A, B, X [, …])

Specific: The specific interface names are S_LSLTO and D_LSLTO.

FORTRAN 77 Interface

Single: CALL LSLTO (N, A, B, IPATH, X)

Double: The double precision name is DLSLTO.

Description

Toeplitz matrices have entries that are constant along each diagonal, for example,

$$A = \begin{bmatrix} p_0 & p_1 & p_2 & p_3 \\ p_{-1} & p_0 & p1 & p_2 \\ p_{-2} & p_{-1} & p_0 & p_1 \\ p_{-3} & p_{-2} & p_{-1} & p_0 \end{bmatrix}$$

The routine LSLTO is based on the routine TSLS in the TOEPLITZ package, see Arushanian et al. (1983). It is based on an algorithm of Trench (1964). This algorithm is also described by Golub and van Loan (1983), pages 125−133.

Comments

1. Workspace may be explicitly provided, if desired, by use of L2LTO/DL2LTO. The reference is:

   CALL L2LTO (N, A, B, IPATH, X, WK)

   The additional argument is:

   WK — Work vector of length 2N − 2.

2. Because of the special structure of Toeplitz matrices, the first row and the first column of a Toeplitz matrix completely characterize the matrix. Hence, only the elements A(1, 1), …, A(1, N), A(2, 1), …, A(N, 1) need to be stored.

Example

A system of four linear equations is solved. Note that only the first row and column of the matrix *A* are entered.

```
      USE LSLTO_INT
      USE WRRRN_INT
!                                 Declare variables
      INTEGER    N
      PARAMETER  (N=4)
      REAL       A(2*N-1), B(N), X(N)
!                                 Set values for  A, and B
!
!                                 A = (  2   -3   -1    6  )
!                                     (  1    2   -3   -1  )
!                                     (  4    1    2   -3  )
!                                     (  3    4    1    2  )
!
!                                 B = ( 16  -29   -7    5  )
!
      DATA A/2.0, -3.0, -1.0, 6.0, 1.0, 4.0, 3.0/
      DATA B/16.0, -29.0, -7.0, 5.0/
!                                 Solve AX = B
      CALL LSLTO (A, B, X)
!                                 Print results
```

```
      CALL WRRRN ('X', X, 1, N, 1)
      END
```

Output

```
                 X
      1       2       3       4
 -2.000  -1.000   7.000   4.000
```

LSLTC

Solves a complex Toeplitz linear system.

Required Arguments

A — Complex vector of length 2N − 1 containing the first row of the coefficient matrix followed by its first column beginning with the second element. (Input)
See Comment 2.

B — Complex vector of length N containing the right-hand side of the linear system. (Input)

X — Complex vector of length N containing the solution of the linear system. (Output)

Optional Arguments

N — Order of the matrix represented by A. (Input)
Default: N = size (A,1).

IPATH — Integer flag. (Input)
IPATH = 1 means the system $Ax = B$ is solved.
IPATH = 2 means the system $A^T x = B$ is solved.
Default: IPATH = 1.

FORTRAN 90 Interface

Generic: CALL LSLTC (A, B, X [, …])

Specific: The specific interface names are S_LSLTC and D_LSLTC.

FORTRAN 77 Interface

Single: CALL LSLTC (N, A, B, IPATH, X)

Double: The double precision name is DLSLTC.

Description

Toeplitz matrices have entries which are constant along each diagonal, for example,

$$A = \begin{bmatrix} p_0 & p_1 & p_2 & p_3 \\ p_{-1} & p_0 & p1 & p_2 \\ p_{-2} & p_{-1} & p_0 & p_1 \\ p_{-3} & p_{-2} & p_{-1} & p_0 \end{bmatrix}$$

The routine LSLTC is based on the routine TSLC in the TOEPLITZ package, see Arushanian et al. (1983). It is based on an algorithm of Trench (1964). This algorithm is also described by Golub and van Loan (1983), pages 125–133.

Comments

1. Workspace may be explicitly provided, if desired, by use of L2LTC/DL2LTC. The reference is:

   CALL L2LTC (N, A, B, IPATH, X, WK)

   The additional argument is

   WK — Complex work vector of length 2N − 2.

2. Because of the special structure of Toeplitz matrices, the first row and the first column of a Toeplitz matrix completely characterize the matrix. Hence, only the elements A(1, 1), …, A(1, N), A(2, 1), …, A(N, 1) need to be stored.

Example

A system of four complex linear equations is solved. Note that only the first row and column of the matrix *A* are entered.

```
      USE LSLTC_INT
      USE WRCRN_INT
!                                 Declare variables
      PARAMETER  (N=4)
      COMPLEX    A(2*N-1), B(N), X(N)
!                                 Set values for  A and B
!
!                                 A = ( 2+2i     -3      1+4i    6-2i )
!                                     (  i       2+2i    -3      1+4i )
!                                     ( 4+2i      i      2+2i    -3   )
!                                     ( 3-4i     4+2i     i      2+2i )
!
!                                 B = ( 6+65i  -29-16i  7+i  -10+i )
!
      DATA A/(2.0,2.0), (-3.0,0.0), (1.0,4.0), (6.0,-2.0), (0.0,1.0),&
            (4.0,2.0), (3.0,-4.0)/
      DATA B/(6.0,65.0), (-29.0,-16.0), (7.0,1.0), (-10.0,1.0)/
!                                 Solve AX = B
      CALL LSLTC (A, B, X)
!                                 Print results
      CALL WRCRN ('X', X, 1, N, 1)
      END
```

Output

```
Output

                                        X
                1                   2                   3                   4
 (-2.000, 0.000)  (-1.000,-5.000)  ( 7.000, 2.000)  ( 0.000, 4.000)
```

LSLCC

more...

Solves a complex circulant linear system.

Required Arguments

A — Complex vector of length `N` containing the first row of the coefficient matrix. (Input)

B — Complex vector of length `N` containing the right-hand side of the linear system. (Input)

X — Complex vector of length `N` containing the solution of the linear system. (Output)

Optional Arguments

N — Order of the matrix represented by `A`. (Input)
Default: `N` = size (`A`,1).

IPATH — Integer flag. (Input)
`IPATH` = 1 means the system Ax = B is solved.
`IPATH` = 2 means the system $A^T x$ = B is solved.
Default: `IPATH` = 1.

FORTRAN 90 Interface

Generic: `CALL LSLCC (A, B, X [, …])`

Specific: The specific interface names are `S_LSLCC` and `D_LSLCC`.

FORTRAN 77 Interface

Single: `CALL LSLCC (N, A, B, IPATH, X)`

Double: The double precision name is `DLSLCC`.

Description

Circulant matrices have the property that each row is obtained by shifting the row above it one place to the right. Entries that are shifted off at the right re-enter at the left. For example,

$$A = \begin{bmatrix} p_1 & p_2 & p_3 & p_4 \\ p_4 & p_1 & p_2 & p_3 \\ p_3 & p_4 & p_1 & p_2 \\ p_2 & p_3 & p_4 & p_1 \end{bmatrix}$$

If $q_{\boldsymbol{k}} = p_{\ -\boldsymbol{k}}$ and the subscripts on p and q are interpreted modulo N, then

$$\left(Ax\right)_j = \sum_{i=1}^{N} p_{i-j+1} x_i = \sum_{i=1}^{N} q_{j-i+1} x_i = \left(q * x\right)_i$$

where $q * x$ is the convolution of q and x. By the convolution theorem, if $q * x = b$, then

$$\hat{q} \otimes \hat{x} = \hat{b}, \text{where } \hat{q}$$

is the discrete Fourier transform of q as computed by the IMSL routine `FFTCF and` ⊗ denotes elementwise multiplication. By division,

$$\hat{x} = \hat{b} \varnothing \hat{q}$$

where ∅ denotes elementwise division. The vector x is recovered from

$$\hat{x}$$

through the use of IMSL routine FFTCB.

To solve $A^{\boldsymbol{T}} x = b$, use the vector p instead of q in the above algorithm.

Comments

1. Workspace may be explicitly provided, if desired, by use of `L2LCC/DL2LCC`. The reference is:

   `CALL L2LCC (N, A, B, IPATH, X, ACOPY, WK)`

   The additional arguments are as follows:

   ACOPY — Complex work vector of length `N`. If `A` is not needed, then `A` and `ACOPY` may be the same.

   WK — Work vector of length 6`N` + 15.

2. Informational error

Type	Code	Description
4	2	The input matrix is singular.

3. Because of the special structure of circulant matrices, the first row of a circulant matrix completely characterizes the matrix. Hence, only the elements A(1, 1), …, A(1, N) need to be stored.

Example

A system of four linear equations is solved. Note that only the first row of the matrix *A* is entered.

```
      USE LSLCC_INT
      USE WRCRN_INT
!                                 Declare variables
      INTEGER    N
      PARAMETER  (N=4)
      COMPLEX    A(N), B(N), X(N)
!                                 Set values for  A, and B
!
!                                 A = ( 2+2i -3+0i  1+4i  6-2i)
!
!                                 B = (6+65i  -41-10i  -8-30i  63-3i)
!
      DATA A/(2.0,2.0), (-3.0,0.0), (1.0,4.0), (6.0,-2.0)/
      DATA B/(6.0,65.0), (-41.0,-10.0), (-8.0,-30.0), (63.0,-3.0)/
!                                 Solve AX = B     (IPATH = 1)
      CALL LSLCC (A, B, X)
!                                 Print results
      CALL WRCRN ('X', X, 1, N, 1)
      END
```

Output

```
               1                 2                 3                 4
(-2.000, 0.000)  (-1.000,-5.000)  ( 7.000, 2.000)  ( 0.000, 4.000)
```

PCGRC

Solves a real symmetric definite linear system using a preconditioned conjugate gradient method with reverse communication.

Required Arguments

IDO — Flag indicating task to be done. (Input/Output)
On the initial call `IDO` must be 0. If the routine returns with `IDO` = 1, then set `Z` = `AP`, where `A` is the matrix, and call `PCGRC` again. If the routine returns with `IDO` = 2, then set `Z` to the solution of the system `MZ` = `R`, where `M` is the preconditioning matrix, and call `PCGRC` again. If the routine returns with `IDO` = 3, then the iteration has converged and `X` contains the solution.

X — Array of length `N` containing the solution. (Input/Output)
On input, `X` contains the initial guess of the solution. On output, `X` contains the solution to the system.

P — Array of length `N`. (Output)
Its use is described under `IDO`.

R — Array of length `N`. (Input/Output)
On initial input, it contains the right-hand side of the linear system. On output, it contains the residual.

Z — Array of length `N`. (Input)
When `IDO` = 1, it contains `AP`, where `A` is the linear system. When `IDO` = 2, it contains the solution of `MZ` = `R`, where `M` is the preconditioning matrix. When `IDO` = 0, it is ignored. Its use is described under `IDO`.

Optional Arguments

N — Order of the linear system. (Input)
Default: `N` = size (`X`,1).

RELERR — Relative error desired. (Input)
Default: `RELERR` = 1.e-5 for single precision and 1.d-10 for double precision.

ITMAX — Maximum number of iterations allowed. (Input)
Default: `ITMAX` = `N`.

FORTRAN 90 Interface

Generic: `CALL PCGRC (IDO, X, P, R, Z [, …])`

Specific: The specific interface names are `S_PCGRC` and `D_PCGRC`.

FORTRAN 77 Interface

Single: `CALL PCGRC (IDO, N, X, P, R, Z, RELERR, ITMAX)`

Double: The double precision name is `DPCGRC`.

Description

Routine `PCGRC` solves the symmetric definite linear system $Ax = b$ using the preconditioned conjugate gradient method. This method is described in detail by Golub and Van Loan (1983, Chapter 10), and in Hageman and Young (1981, Chapter 7).

The *preconditioning matrix*, M, is a matrix that approximates A, and for which the linear system $Mz = r$ is easy to solve. These two properties are in conflict; balancing them is a topic of much current research.

The number of iterations needed depends on the matrix and the error tolerance `RELERR`. As a rough guide, `ITMAX` = $\mathtt{N}^{1/2}$ is often sufficient when `N` >> 1. See the references for further information.

Let M be the preconditioning matrix, let b, p, r, x and z be vectors and let τ be the desired relative error. Then the algorithm used is as follows.

$\lambda = -1$

$p_0 = x_0$

$r_1 = b - Ap$

For $k = 1, \ldots,$ `itmax`

$z_k = M^{-1} r_k$

If $k = 1$ then

$\beta_k = 1$

$p_k = z_k$

Else

$$\beta_k = z_k^T r_k / z_{k-1}^T r_{k-1}$$

$$p_k = z_k + \beta_k p_k$$

End if

$z_k = Ap$

$\alpha_k = z_{k-1}^T r_{k-1} / z_k^T p_k$

$x_k = x_k + \alpha_k p_k$

$r_k = r_k - \alpha_k z_k$

If ($\|z_k\|_2 \le \tau(1 - \lambda)\|x_k\|_2$) Then

Recompute λ

If ($\|z_k\|_2 \le \tau(1 - \lambda)\|x_k\|_2$) Exit

End if

End loop

Here λ is an estimate of $\lambda_{max}(G)$, the largest eigenvalue of the iteration matrix $G = I - M^{-1} A$. The stopping criterion is based on the result (Hageman and Young, 1981, pages 148−151)

$$\frac{\|x_k - x\|_M}{\|x\|_M} \le \frac{1}{1 - \lambda_{\max}(G)} \frac{\|z_k\|_M}{\|x_k\|_M}$$

Where

$$\|x\|_M^2 = x^T M x$$

It is known that

$$\lambda_{\max}\left(T_1\right) \le \lambda_{\max}\left(T_2\right) \le \cdots \le \lambda_{\max}\left(G\right) < 1$$

where the T_n are the symmetric, tridiagonal matrices

$$T_n = \begin{bmatrix} \mu_1 & \omega_2 & & & \\ \omega_2 & \mu_2 & \omega_3 & & \\ & \omega_3 & \mu_3 & \omega_4 & \\ & & \ddots & \ddots & \ddots \end{bmatrix}$$

with

$$\mu_k = 1 - \beta_k / \alpha_{k-1} - 1 / \alpha_k,\ \mu_1 = 1 - 1 / \alpha_1$$

and

$$\omega_k = \sqrt{\beta_k} / \alpha_{k-1}$$

The largest eigenvalue of T_k is found using the routine EVASB. Usually this eigenvalue computation is needed for only a few of the iterations.

Comments

1. Workspace may be explicitly provided, if desired, by use of P2GRC/DP2GRC. The reference is:

   CALL P2GRC (IDO, N, X, P, R, Z, RELERR, ITMAX, TRI, WK, IWK)

   The additional arguments are as follows:

   TRI — Workspace of length 2 * ITMAX containing a tridiagonal matrix (in band symmetric form) whose largest eigenvalue is approximately the same as the largest eigenvalue of the iteration matrix. The workspace arrays TRI, WK and IWK should not be changed between the initial call with IDO = 0 and PCGRC/DPCGRC returning with IDO = 3.

   WK — Workspace of length 5 * ITMAX.

   IWK — Workspace of length ITMAX.

2. Informational errors

Type	Code	Description
4	1	The preconditioning matrix is singular.
4	2	The preconditioning matrix is not definite.
4	3	The linear system is not definite.
4	4	The linear system is singular.
4	5	No convergence after ITMAX iterations.

Examples

Example 1

In this example, the solution to a linear system is found. The coefficient matrix *A* is stored as a full matrix. The preconditioning matrix is the diagonal of *A*. This is called the *Jacobi preconditioner*. It is also used by the IMSL routine JCGRC.

```
      USE PCGRC_INT
      USE MURRV_INT
      USE WRRRN_INT
      USE SCOPY_INT
      INTEGER    LDA, N
      PARAMETER  (N=3, LDA=N)
!
      INTEGER    IDO, ITMAX, J
      REAL       A(LDA,N), B(N), P(N), R(N), X(N), Z(N)
!                            (   1,  -3,   2   )
!                       A =  (  -3,  10,  -5   )
!                            (   2,  -5,   6   )
      DATA A/1.0, -3.0, 2.0, -3.0, 10.0, -5.0, 2.0, -5.0, 6.0/
!                       B =  (   27.0, -78.0, 64.0  )
      DATA B/27.0, -78.0, 64.0/
!                                 Set R to right side
```

```
      CALL SCOPY (N, B, 1, R, 1)
!                                 Initial guess for X is B
      CALL SCOPY (N, B, 1, X, 1)
!
      ITMAX  = 100
      IDO    = 0
   10 CALL PCGRC (IDO, X, P, R, Z, ITMAX=ITMAX)
      IF (IDO .EQ. 1) THEN
!                                 Set z = Ap
         CALL MURRV (A, P, Z)
         GO TO 10
      ELSE IF (IDO .EQ. 2) THEN
!                                 Use diagonal of A as the
!                                 preconditioning matrix M
!                                 and set z = inv(M)*r
         DO 20  J=1, N
            Z(J) = R(J)/A(J,J)
   20    CONTINUE
         GO TO 10
      END IF
!                                 Print the solution
      CALL WRRRN ('Solution', X)
!
      END
```

Output

```
Solution
1   1.001
2  -4.000
3   7.000
```

Example 2

In this example, a more complicated preconditioner is used to find the solution of a linear system which occurs in a finite-difference solution of Laplace's equation on a 4 × 4 grid. The matrix is

$$A = \begin{bmatrix} 4 & -1 & 0 & -1 & & & & & \\ -1 & 4 & -1 & 0 & -1 & & & & \\ 0 & -1 & 4 & -1 & 0 & -1 & & & \\ -1 & 0 & -1 & 4 & -1 & 0 & -1 & & \\ & -1 & 0 & -1 & 4 & -1 & 0 & -1 & \\ & & -1 & 0 & -1 & 4 & -1 & 0 & -1 \\ & & & -1 & 0 & -1 & 4 & -1 & 0 \\ & & & & -1 & 0 & -1 & 4 & -1 \\ & & & & & -1 & 0 & -1 & 4 \end{bmatrix}$$

The preconditioning matrix *M* is the symmetric tridiagonal part of *A*,

$$M = \begin{bmatrix} 4 & -1 & & & & & & & \\ -1 & 4 & -1 & & & & & & \\ & -1 & 4 & -1 & & & & & \\ & & -1 & 4 & -1 & & & & \\ & & & -1 & 4 & -1 & & & \\ & & & & -1 & 4 & -1 & & \\ & & & & & -1 & 4 & -1 & \\ & & & & & & -1 & 4 & -1 \\ & & & & & & & -1 & 4 \end{bmatrix}$$

Note that *M*, called `PRECND` in the program, is factored once.

```
      USE IMSL_LIBRARIES
      INTEGER    LDA, LDPRE, N, NCODA, NCOPRE
      PARAMETER  (N=9, NCODA=3, NCOPRE=1, LDA=2*NCODA+1,&
                 LDPRE=NCOPRE+1)
!
      INTEGER    IDO, ITMAX
      REAL       A(LDA,N), P(N), PRECND(LDPRE,N), PREFAC(LDPRE,N),&
                 R(N), RCOND, RELERR, X(N), Z(N)
!                                  Set A in band form
      DATA A/3*0.0, 4.0, -1.0, 0.0, -1.0, 2*0.0, -1.0, 4.0, -1.0, 0.0,&
          -1.0, 2*0.0, -1.0, 4.0, -1.0, 0.0, -1.0, -1.0, 0.0, -1.0,&
          4.0, -1.0, 0.0, -1.0, -1.0, 0.0, -1.0, 4.0, -1.0, 0.0,&
          -1.0, -1.0, 0.0, -1.0, 4.0, -1.0, 0.0, -1.0, -1.0, 0.0,&
          -1.0, 4.0, -1.0, 2*0.0, -1.0, 0.0, -1.0, 4.0, -1.0, 2*0.0,&
          -1.0, 0.0, -1.0, 4.0, 3*0.0/
!                                  Set PRECND in band symmetric form
      DATA PRECND/0.0, 4.0, -1.0, 4.0, -1.0, 4.0, -1.0, 4.0, -1.0, 4.0,&
          -1.0, 4.0, -1.0, 4.0, -1.0, 4.0, -1.0, 4.0/
!                                  Right side is (1, ..., 1)
      R = 1.0E0
!                                  Initial guess for X is 0
      X = 0.0E0
!                                  Factor the preconditioning matrix
      CALL LFCQS (PRECND, NCOPRE, PREFAC, RCOND)
!
      ITMAX  = 100
      RELERR = 1.0E-4
      IDO    = 0
   10 CALL PCGRC (IDO, X, P, R, Z, RELERR=RELERR, ITMAX=ITMAX)
      IF (IDO .EQ. 1) THEN
!                                  Set z = Ap
         CALL MURBV (A, NCODA, NCODA, P, Z)
         GO TO 10
      ELSE IF (IDO .EQ. 2) THEN
!                                  Solve PRECND*z = r for r
         CALL LSLQS (PREFAC, NCOPRE, R, Z)
         GO TO 10
      END IF
!                                  Print the solution
      CALL WRRRN ('Solution', X)
!
      END
```

Output

```
Solution
1   0.955
2   1.241
```

```
  3   1.349
  4   1.578
  5   1.660
  6   1.578
  7   1.349
  8   1.241
  9   0.955
```

JCGRC

Solves a real symmetric definite linear system using the Jacobi-preconditioned conjugate gradient method with reverse communication.

Required Arguments

IDO — Flag indicating task to be done. (Input/Output)
On the initial call IDO must be 0. If the routine returns with IDO = 1, then set
Z = A * P, where A is the matrix, and call JCGRC again. If the routine returns with IDO = 2, then the iteration has converged and X contains the solution.

DIAGNL — Vector of length N containing the diagonal of the matrix. (Input)
Its elements must be all strictly positive or all strictly negative.

X — Array of length N containing the solution. (Input/Output)
On input, X contains the initial guess of the solution. On output, X contains the solution to the system.

P — Array of length N. (Output)
Its use is described under IDO.

R — Array of length N. (Input/Output)
On initial input, it contains the right-hand side of the linear system. On output, it contains the residual.

Z — Array of length N. (Input)
When IDO = 1, it contains AP, where A is the linear system. When IDO = 0, it is ignored. Its use is described under IDO.

Optional Arguments

N — Order of the linear system. (Input)
Default: N = size (X,1).

RELERR — Relative error desired. (Input)
Default: RELERR = 1.e-5 for single precision and 1.d-10 for double precision.

ITMAX — Maximum number of iterations allowed. (Input)
Default: ITMAX = 100.

FORTRAN 90 Interface

Generic: CALL JCGRC (IDO, DIAGNL, X, P, R, Z [, …])

Specific: The specific interface names are S_JCGRC and D_JPCGRC.

FORTRAN 77 Interface

Single: CALL JCGRC (IDO, N, DIAGNL, X, P, R, Z, RELERR, ITMAX)

Double: The double precision name is DJCGRC.

Description

Routine JCGRC solves the symmetric definite linear system $Ax = b$ using the Jacobi conjugate gradient method. This method is described in detail by Golub and Van Loan (1983, Chapter 10), and in Hageman and Young (1981, Chapter 7).

This routine is a special case of the routine PCGRC, with the diagonal of the matrix A used as the preconditioning matrix. For details of the algorithm see PCGRC.

The number of iterations needed depends on the matrix and the error tolerance RELERR. As a rough guide, ITMAX = N is often sufficient when $N \gg 1$. See the references for further information.

Comments

1. Workspace may be explicitly provided, if desired, by use of J2GRC/DJ2GRC. The reference is:

   CALL J2GRC (IDO, N, DIAGNL, X, P, R, Z, RELERR, ITMAX, TRI, WK, IWK)

   The additional arguments are as follows:

   TRI — Workspace of length 2 * ITMAX containing a tridiagonal matrix (in band symmetric form) whose largest eigenvalue is approximately the same as the largest eigenvalue of the iteration matrix. The workspace arrays TRI, WK and IWK should not be changed between the initial call with IDO = 0 and JCGRC/DJCGRC returning with IDO = 2.

   WK — Workspace of length 5 * ITMAX.

   IWK — Workspace of length ITMAX.

2. Informational errors

Type	**Code**	**Description**
4	1	The diagonal contains a zero.
4	2	The diagonal elements have different signs.

Type	Code	Description
4	3	No convergence after ITMAX iterations.
4	4	The linear system is not definite.
4	5	The linear system is singular.

Example

In this example, the solution to a linear system is found. The coefficient matrix *A* is stored as a full matrix.

```
      USE IMSL_LIBRARIES
      INTEGER    LDA, N
      PARAMETER  (LDA=3, N=3)
!
      INTEGER    IDO, ITMAX
      REAL       A(LDA,N), B(N), DIAGNL(N), P(N), R(N), X(N), &
                 Z(N)
!                                (   1,  -3,   2   )
!                          A =   (  -3,  10,  -5   )
!                                (   2,  -5,   6   )
      DATA A/1.0, -3.0, 2.0, -3.0, 10.0, -5.0, 2.0, -5.0, 6.0/
!                          B =   (   27.0, -78.0, 64.0  )
      DATA B/27.0, -78.0, 64.0/
!                                Set R to right side
      CALL SCOPY (N, B, 1, R, 1)
!                                Initial guess for X is B
      CALL SCOPY (N, B, 1, X, 1)
!                                Copy diagonal of A to DIAGNL
      CALL SCOPY (N, A(:, 1), LDA+1, DIAGNL, 1)
!                                Set parameters
      ITMAX  = 100
      IDO    = 0
   10 CALL JCGRC (IDO, DIAGNL, X, P, R, Z, ITMAX=ITMAX)
      IF (IDO .EQ. 1) THEN
!                                Set z = Ap
         CALL MURRV (A, P, Z)
         GO TO 10
      END IF
!                                Print the solution
      CALL WRRRN ('Solution', X)
!
      END
```

Output

```
Solution
1   1.001
2  -4.000
3   7.000
```

GMRES

Uses the Generalized Minimal Residual Method with reverse communication to generate an approximate solution of $Ax = b$.

Required Arguments

IDO— Flag indicating task to be done. (Input/Output)
On the initial call `IDO` must be 0. If the routine returns with `IDO` = 1, then set $Z = AP$, where A is the matrix, and call `GMRES` again. If the routine returns with `IDO` = 2, then set Z to the solution of the system $MZ = P$, where M is the preconditioning matrix, and call `GMRES` again. If the routine returns with `IDO` = 3, set `Z` = $AM^{-1}P$, and call `GMRES` again. If the routine returns with `IDO` = 4, the iteration has converged, and `X` contains the approximate solution to the linear system.

X — Array of length `N` containing an approximate solution. (Input/Output)
On input, `X` contains an initial guess of the solution. On output, `X` contains the approximate solution.

P — Array of length `N`. (Output)
Its use is described under `IDO`.

R — Array of length `N`. (Input/Output)
On initial input, it contains the right-hand side of the linear system. On output, it contains the residual, $b - Ax$.

Z — Array of length `N`. (Input)
When `IDO` = 1, it contains AP, where A is the coefficient matrix. When `IDO` = 2, it contains $M^{-1}P$. When `IDO` = 3, it contains $AM^{-1}P$. When `IDO` = 0, it is ignored.

TOL — Stopping tolerance. (Input/Output)
The algorithm attempts to generate a solution x such that $|b - Ax| \leq$ `TOL*`$|b|$. On output, `TOL` contains the final residual norm.

Optional Arguments

N — Order of the linear system. (Input)
Default: `N` = size (`X`,1).

FORTRAN 90 Interface

Generic: `CALL GMRES (IDO, X, P, R, Z, TOL [, …])`

Specific: The specific interface names are `S_GMRES` and `D_GMRES`.

FORTRAN 77 Interface

Single: `CALL GMRES (IDO, N, X, P, R, Z, TOL)`

Double: The double precision name is `DGMRES`.

Description

The routine `GMRES` implements restarted `GMRES` with reverse communication to generate an approximate solution to $Ax = b$. It is based on GMRESD by Homer Walker.

There are four distinct `GMRES` implementations, selectable through the parameter vector `INFO`. The first Gram-Schmidt implementation, `INFO(1)` = 1, is essentially the original algorithm by Saad and Schultz (1986). The second Gram-Schmidt implementation, developed by Homer Walker and Lou Zhou, is simpler than the first implementation. The least squares problem is constructed in upper-triangular form and the residual vector updating at the end of a `GMRES` cycle is cheaper. The first Householder implementation is algorithm 2.2 of Walker (1988), but with more efficient correction accumulation at the end of each `GMRES` cycle. The second Householder implementation is algorithm 3.1 of Walker (1988). The products of Householder transformations are expanded as sums, allowing most work to be formulated as large scale matrix-vector operations. Although BLAS are used wherever possible, extensive use of Level 2 BLAS in the second Householder implementation may yield a performance advantage on certain computing environments.

The Gram-Schmidt implementations are less expensive than the Householder, the latter requiring about twice as much arithmetic beyond the coefficient matrix/vector products. However, the Householder implementations may be more reliable near the limits of residual reduction. See Walker (1988) for details. Issues such as the cost of coefficient matrix/vector products, availability of effective preconditioners, and features of particular computing environments may serve to mitigate the extra expense of the Householder implementations.

Comments

1. Workspace may be explicitly provided, if desired, by use of `G2RES/DG2RES`. The reference is:

   `CALL G2RES (IDO, N, X, P, R, Z, TOL, INFO, USRNPR, USRNRM, WORK)`

   The additional arguments are as follows:

   INFO — Integer vector of length 10 used to change parameters of `GMRES`. (Input/Output).

For any components INFO(1) ... INFO(7) with value zero on input, the default value is used.

INFO(1) = IMP, the flag indicating the desired implementation.

IMP	Action
1	first Gram-Schmidt implementation
2	second Gram-Schmidt implementation
3	first Householder implementation
4	second Householder implementation

Default: IMP = 1

INFO(2) = KDMAX, the maximum Krylor subspace dimension, i.e., the maximum allowable number of GMRES iterations before restarting. It must satisfy 1 ≤ KDMAX ≤ N.
Default: KDMAX = min(N, 20)

INFO(3) = ITMAX, the maximum number of GMRES iterations allowed.
Default: ITMAX = 1000

INFO(4) = IRP, the flag indicating whether right preconditioning is used.
If IRP = 0, no right preconditioning is performed. If IRP = 1, right preconditioning is performed. If IRP = 0, then IDO = 2 or 3 will not occur.
Default: IRP = 0

INFO(5) = IRESUP, the flag that indicates the desired residual vector updating prior to restarting or on termination.

IRESUP	Action
1	update by linear combination, restarting only
2	update by linear combination, restarting and termination
3	update by direct evaluation, restarting only
4	update by direct evaluation, restarting and termination

Updating by direct evaluation requires an otherwise unnecessary matrix-vector product. The alternative is to update by forming a linear combination of various available vectors. This may or may not be cheaper and may be less reliable if the residual vector has been greatly reduced. If IRESUP = 2 or 4, then the residual vector is returned in WORK(1), ..., WORK(N). This is useful in some applications but costs another unnecessary residual update. It is recommended that IRESUP = 1 or 2 be used, unless matrix-vector products are inexpensive or great residual reduction is required. In this case use IRESUP = 3 or 4. The meaning of “inexpensive” varies with IMP as follows:

IMP	≤
1	(KDMAX + 1) *N flops
2	N flops
3	(2*KDMAX + 1) *N flops
4	(2*KDMAX + 1) *N flops

"Great residual reduction" means that TOL is only a few orders of magnitude larger than machine epsilon.
Default: IRESUP = 1

INFO(6) = flag for indicating the inner product and norm used in the Gram-Schmidt implementations. If INFO(6) = 0, sdot and snrm2, from BLAS, are used. If INFO(6) = 1, the user must provide the routines, as specified under arguments USRNPR and USRNRM.
Default: INFO(6) = 0

INFO(7) = IPRINT, the print flag. If IPRINT = 0, no printing is performed. If IPRINT = 1, print the iteration numbers and residuals. If IPRINT = 2, additionally print the intermediate solution vector X row-wise at the end of each GMRES cycle.
Default: IPRINT = 0

INFO(8) = the total number of GMRES iterations on output.

INFO(9) = the total number of matrix-vector products in GMRES on output.

INFO(10) = the total number of right preconditioner solves in GMRES on output if IRP = 1.

USRNPR — User-supplied FUNCTION to use as the inner product in the Gram-Schmidt implementation, if INFO(6) = 1. If INFO(6) = 0, the dummy function G8RES/DG8RES may be used. The usage is

REAL FUNCTION USRNPR (N, SX, INCX, SY, INCY)

N — Length of vectors X and Y. (Input)

SX — Real vector of length MAX(N*IABS(INCX),1). (Input)

INCX — Displacement between elements of SX. (Input)
X(I) is defined to be SX(1+(I-1)*INCX) if INCX is greater than 0, or SX(1+(I-N)*INCX) if INCX is less than 0.

SY — Real vector of length MAX(N*IABS(INXY),1). (Input)

INCY — Displacement between elements of SY. (Input)
Y(I) is defined to be SY(1+(I-1)*INCY) if INCY is greater than 0, or SY(1+(I-N)*INCY) if INCY is less than zero.

USRNPR must be declared EXTERNAL in the calling program.

USRNRM — User-supplied FUNCTION to use as the norm ||*X*|| in the Gram-Schmidt implementation, if INFO(6) = 1. If INFO(6) = 0, the dummy function G9RES/DG9RES may be used.The usage is

REAL FUNCTION USRNRM (N, SX, INCX)

N — Length of vectors X and Y. (Input)

SX — Real vector of length MAX(N*IABS(INCX),1). (Input)

INCX — Displacement between elements of SX. (Input)
X(I) is defined to be SX(1+(I-1)*INCX) if INCX is greater than 0, or SX(1+(I-N)*INCX) if INCX is less than 0.

USRNRM must be declared EXTERNAL in the calling program.

WORK — Work array whose length is dependent on the chosen implementation.

IMP	length of ***WORK***
1	N*(KDMAX + 2) + KDMAX**2 + 3 *KDMAX + 2
2	N*(KDMAX + 2) + KDMAX**2 + 2 *KDMAX + 1
3	N*(KDMAX + 2) + 3 *KDMAX + 2
4	N*(KDMAX + 2) + KDMAX**2 + 2 *KDMAX + 2

Examples

Example 1

This is a simple example of GMRES usage. A solution to a small linear system is found. The coefficient matrix *A* is stored as a full matrix, and no preconditioning is used. Typically, preconditioning is required to achieve convergence in a reasonable number of iterations.

```
      USE IMSL_LIBRARIES
!                Declare variables
      INTEGER    LDA, N
      PARAMETER  (N=3, LDA=N)
!                                 Specifications for local variables
      INTEGER    IDO, NOUT
      REAL       P(N), TOL, X(N), Z(N)
      REAL       A(LDA,N), R(N)
      SAVE       A, R
!                                 Specifications for intrinsics
      INTRINSIC  SQRT
      REAL       SQRT
!                                 ( 33.0  16.0  72.0)
!                             A = (-24.0 -10.0 -57.0)
!                                 ( 18.0 -11.0   7.0)
!
!                             B = (129.0 -96.0   8.5)
!
      DATA A/33.0, -24.0, 18.0, 16.0, -10.0, -11.0, 72.0, -57.0, 7.0/
      DATA R/129.0, -96.0, 8.5/
!
      CALL UMACH (2, NOUT)
!
!                                 Initial guess = (0 ... 0)
!
      X = 0.0E0
```

```
!                                   Set stopping tolerance to
!                                   square root of machine epsilon
      TOL = AMACH(4)
      TOL = SQRT(TOL)
      IDO = 0
   10 CONTINUE
      CALL GMRES (IDO, X, P, R, Z, TOL)
      IF (IDO .EQ. 1) THEN
!                                   Set z = A*p
        CALL MURRV (A, P, Z)
         GO TO 10
      END IF
!
      CALL WRRRN ('Solution', X, 1, N, 1)
      WRITE (NOUT,'(A11, E15.5)') 'Residual = ', TOL
      END
```

Output

```
      Solution
    1       2       3
1.000   1.500   1.000
Residual =      0.29746E-05
```

Example 2

This example solves a linear system with a coefficient matrix stored in coordinate form, the same problem as in the document example for LSLXG. Jacobi preconditioning is used, i.e. the preconditioning matrix M is the diagonal matrix with $M_{ii} = A_{ii}$, for $i = 1, \ldots, n$.

```
      USE IMSL_LIBRARIES
      INTEGER    N, NZ

      PARAMETER  (N=6, NZ=15)
!                                   Specifications for local variables
      INTEGER    IDO, INFO(10), NOUT
      REAL       P(N), TOL, WORK(1000), X(N), Z(N)
      REAL       DIAGIN(N), R(N)
!                                   Specifications for intrinsics
      INTRINSIC  SQRT
      REAL       SQRT
!                                   Specifications for subroutines
      EXTERNAL   AMULTP
!                                   Specifications for functions
      EXTERNAL   G8RES, G9RES
!
      DATA DIAGIN/0.1, 0.1, 0.0666667, 0.1, 1.0, 0.16666667/
      DATA R/10.0, 7.0, 45.0, 33.0, -34.0, 31.0/
!
      CALL UMACH (2, NOUT)
!
                                    Initial guess = (1 ... 1)
      X = 1.0E0
!                                   Set up the options vector INFO
!                                   to use preconditioning
      INFO = 0
      INFO(4) = 1
!                                   Set stopping tolerance to
!                                   square root of machine epsilon
      TOL = AMACH(4)
      TOL = SQRT(TOL)
      IDO = 0
```

```
   10 CONTINUE
      CALL G2RES (IDO, N, X, P, R, Z, TOL, INFO, G8RES, G9RES, WORK)
      IF (IDO .EQ. 1) THEN
!                                  Set z = A*p
         CALL AMULTP (P, Z)
         GO TO 10
      ELSE IF (IDO .EQ. 2) THEN
!
!                                  Set z = inv(M)*p
!                                  The diagonal of inv(M) is stored
!                                  in DIAGIN
!
         CALL SHPROD (N, DIAGIN, 1, P, 1, Z, 1)
         GO TO 10
      ELSE IF (IDO .EQ. 3) THEN
!
!                                  Set z = A*inv(M)*p
!
         CALL SHPROD (N, DIAGIN, 1, P, 1, Z, 1)
         P = Z
         CALL AMULTP (P, Z)
         GO TO 10
      END IF
!
      CALL WRRRN ('Solution', X)
      WRITE (NOUT,'(A11, E15.5)') 'Residual = ', TOL
      END
!
      SUBROUTINE AMULTP (P, Z)
      USE IMSL_LIBRARIES
      INTEGER    NZ
      PARAMETER  (NZ=15)
!                                  SPECIFICATIONS FOR ARGUMENTS
      REAL       P(*), Z(*)
!                                  SPECIFICATIONS FOR PARAMETERS
      INTEGER    N
      PARAMETER  (N=6)
!                                  SPECIFICATIONS FOR LOCAL VARIABLES
      INTEGER    I
      INTEGER    IROW(NZ), JCOL(NZ)
      REAL       A(NZ)
      SAVE       A, IROW, JCOL
!                                  SPECIFICATIONS FOR SUBROUTINES
!                                  Define the matrix A
!
      DATA A/6.0, 10.0, 15.0, -3.0, 10.0, -1.0, -1.0, -3.0, -5.0, 1.0, &
          10.0, -1.0, -2.0, -1.0, -2.0/
      DATA IROW/6, 2, 3, 2, 4, 4, 5, 5, 5, 5, 1, 6, 6, 2, 4/
      DATA JCOL/6, 2, 3, 3, 4, 5, 1, 6, 4, 5, 1, 1, 2, 4, 1/
!
      CALL SSET(N, 0.0, Z, 1)
!                                  Accumulate the product A*p in z
      DO 10  I=1, NZ
         Z(IROW(I)) = Z(IROW(I)) + A(I)*P(JCOL(I))
   10 CONTINUE
      RETURN
      END
```

Output

```
 Solution
1   1.000
2   2.000
3   3.000
4   4.000
```

```
 5   5.000
 6   6.000
 Residual =      0.25882E-05
```

Example 3

The coefficient matrix in this example corresponds to the five-point discretization of the 2-d Poisson equation with the Dirichlet boundary condition. Assuming the natural ordering of the unknowns, and moving all boundary terms to the right hand side, we obtain the block tridiagonal matrix

$$A = \begin{bmatrix} T & -I & & \\ -I & \ddots & \ddots & \\ & \ddots & \ddots & -I \\ & & -I & T \end{bmatrix}$$

where

$$T = \begin{bmatrix} 4 & -1 & & \\ -1 & \ddots & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 4 \end{bmatrix}$$

and I is the identity matrix. Discretizing on a $k \times k$ grid implies that T and I are both $k \times k$, and thus the coefficient matrix A is $k^2 \times k^2$.

The problem is solved twice, with discretization on a 50×50 grid. During both solutions, use the second Householder implementation to take advantage of the large scale matrix/vector operations done in Level 2 BLAS. Also choose to update the residual vector by direct evaluation since the small tolerance will require large residual reduction.

The first solution uses no preconditioning. For the second solution, we construct a block diagonal preconditioning matrix

$$M = \begin{bmatrix} T & & \\ & \ddots & \\ & & T \end{bmatrix}$$

M is factored once, and these factors are used in the forward solves and back substitutions necessary when `GMRES` returns with `IDO` = 2 or 3.

Timings are obtained for both solutions, and the ratio of the time for the solution with no preconditioning to the time for the solution with preconditioning is printed. Though the exact results are machine dependent, we see that the savings realized by faster convergence from using a preconditioner exceed the cost of factoring `M` and performing repeated forward and back solves.

```
      USE IMSL_LIBRARIES
```

```
      INTEGER    K, N
      PARAMETER  (K=50, N=K*K)
!                                 Specifications for local variables
      INTEGER    IDO, INFO(10), IR(20), IS(20), NOUT
      REAL       A(2*N), B(2*N), C(2*N), G8RES, G9RES, P(2*N), R(N), &
                TNOPRE, TOL, TPRE, U(2*N), WORK(100000), X(N), &
                Y(2*N), Z(2*N)
!                                 Specifications for subroutines
      EXTERNAL   AMULTP, G8RES, G9RES
!                                 Specifications for functions
      CALL UMACH (2, NOUT)
!                                 Right hand side and initial guess
!                                 to (1 ... 1)
      R = 1.0E0
      X = 1.0E0
!                                 Use the 2nd Householder
!                                 implementation and update the
!                                 residual by direct evaluation
      INFO = 0
      INFO(1) = 4
      INFO(5) = 3
      TOL     = AMACH(4)
      TOL     = 100.0*TOL
      IDO     = 0
!                                 Time the solution with no
!                                 preconditioning
      TNOPRE  = CPSEC()
   10 CONTINUE
      CALL G2RES (IDO, N, X, P, R, Z, TOL, INFO, G8RES, G9RES, WORK)
      IF (IDO .EQ. 1) THEN
!
!                                 Set z = A*p
!
         CALL AMULTP (K, P, Z)
         GO TO 10
      END IF
      TNOPRE = CPSEC() - TNOPRE
!
      WRITE (NOUT,'(A32, I4)') 'Iterations, no preconditioner = ', &
                             INFO(8)
!
!                                 Solve again using the diagonal blocks
!                                 of A as the preconditioning matrix M
      R = 1.0E0
      X = 1.0E0
!                                 Define M
      CALL SSET (N-1, -1.0, B, 1)
      CALL SSET (N-1, -1.0, C, 1)
      CALL SSET (N, 4.0, A, 1)
      INFO(4) = 1
      TOL     = AMACH(4)
      TOL     = 100.0*TOL
      IDO     = 0
      TPRE    = CPSEC()
!                                 Compute the LDU factorization of M
!
      CALL LSLCR (C, A, B, Y, U, IR, IS, IJOB=6)
   20 CONTINUE
      CALL G2RES (IDO, N, X, P, R, Z, TOL, INFO, G8RES, G9RES, WORK)
         IF (IDO .EQ. 1) THEN
!
!                                Set z = A*p
!
         CALL AMULTP (K, P, Z)
         GO TO 20
      ELSE IF (IDO .EQ. 2) THEN
```

```
!
!                                  Set z = inv(M)*p
!
         CALL SCOPY (N, P, 1, Z, 1)
         CALL LSLCR (C, A, B, Z, U, IR, IS, IJOB=5)
         GO TO 20
      ELSE IF (IDO .EQ. 3) THEN
!
!                                  Set z = A*inv(M)*p
!
         CALL LSLCR (C, A, B, P, U, IR, IS, IJOB=5)
         CALL AMULTP (K, P, Z)
         GO TO 20
      END IF
      TPRE = CPSEC() - TPRE
      WRITE (NOUT,'(A35, I4)') 'Iterations, with preconditioning = ',&
                               INFO(8)
      WRITE (NOUT,'(A45, F10.5)') '(Precondition time)/(No '// &
                                  'precondition time) = ', TPRE/TNOPRE
!
      END
!
      SUBROUTINE AMULTP (K, P, Z)
      USE IMSL_LIBRARIES
!                                   Specifications for arguments
      INTEGER    K
      REAL       P(*), Z(*)
!                                   Specifications for local variables
      INTEGER    I, N
!
      N = K*K
!                                   Multiply by diagonal blocks
!
      CALL SVCAL (N, 4.0, P, 1, Z, 1)
      CALL SAXPY (N-1, -1.0, P(2:(N)), 1, Z, 1)
      CALL SAXPY (N-1, -1.0, P, 1, Z(2:(N)), 1)
!
!                                   Correct for terms not properly in
!                                   block diagonal
      DO 10  I=K, N - K, K
         Z(I)   = Z(I) + P(I+1)
         Z(I+1) = Z(I+1) + P(I)
      10 CONTINUE
!                                   Do the super and subdiagonal blocks,
!                                   the -I's
!
      CALL SAXPY (N-K, -1.0, P((K+1):(N)), 1, Z, 1)
      CALL SAXPY (N-K, -1.0, P, 1, Z((K+1):(N)), 1)
!
      RETURN
      END
```

Output

```
Iterations, no preconditioner =  329
Iterations, with preconditioning =  192
(Precondition time)/(No precondition time) =    0.66278
```

ARPACK_SVD

Computes some singular values and left and right singular vectors of a real rectangular matrix $A_{MxN} = USV^T$.

There is no restriction on the relative sizes, M and N. The user supplies matrix-vector products $y = Ax$ and $y = A^Tx$ for the iterative method. This routine calls `ARPACK_SYMMETRIC`. Descriptions for both `ARPACK_SVD` and `ARPACK_SYMMETRIC` are found in *Chapter 2, "Eigensystem Analysis"*.

LSQRR

more... more...

Solves a linear least-squares problem without iterative refinement.

Required Arguments

A — `NRA` by `NCA` matrix containing the coefficient matrix of the least-squares system to be solved. (Input)

B — Vector of length `NRA` containing the right-hand side of the least-squares system. (Input)

X — Vector of length `NCA` containing the solution vector with components corresponding to the columns not used set to zero. (Output)

RES — Vector of length `NRA` containing the residual vector `B – A * X`. (Output)

KBASIS — Scalar containing the number of columns used in the solution.

Optional Arguments

NRA — Number of rows of `A`. (Input)
Default: `NRA` = size (`A`,1).

NCA — Number of columns of `A`. (Input)
Default: `NCA` = size (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = size (`A`,1).

TOL — Scalar containing the nonnegative tolerance used to determine the subset of columns of *A* to be included in the solution. (Input)
If `TOL` is zero, a full complement of min(`NRA`, `NCA`) columns is used. See Comments.
Default: `TOL` = 0.0

FORTRAN 90 Interface

Generic: `CALL LSQRR (A, B, X, RES, KBASIS [, …])`

Specific: The specific interface names are `S_LSQRR` and `D_LSQRR`.

FORTRAN 77 Interface

Single: `CALL LSQRR (NRA, NCA, A, LDA, B, TOL, X, RES, KBASIS)`

Double: The double precision name is `DLSQRR`.

ScaLAPACK Interface

Generic: `CALL LSQRR (A0, B0, X0, RES0, KBASIS [, …])`

Specific: The specific interface names are `S_LSQRR` and `D_LSQRR`.

See the *ScaLAPACK Usage Notes* below for a description of the arguments for distributed computing.

Description

Routine `LSQRR` solves the linear least-squares problem. The underlying code is based on either LINPACK, LAPACK, or ScaLAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see *Using ScaLAPACK, LAPACK, LINPACK, and EISPACK* in the Introduction section of this manual. The routine `LQRRR` is first used to compute the *QR* decomposition of *A*. Pivoting, with all rows free, is used. Column *k* is in the basis if

$$|R_{kk}| \le \tau |R_{11}|$$

with τ = `TOL`. The truncated least-squares problem is then solved using IMSL routine `LQRSL`. Finally, the components in the solution, with the same index as columns that are not in the basis, are set to zero; and then, the permutation determined by the pivoting in IMSL routine `LQRRR` is applied.

Comments

1. Workspace may be explicitly provided, if desired, by use of `L2QRR/DL2QRR`. The reference is:

   `CALL L2QRR (NRA, NCA, A, LDA, B, TOL, X, RES, KBASIS, QR, QRAUX, IPVT, WORK)`

   The additional arguments are as follows:

   QR — Work vector of length `NRA * NCA` representing an `NRA` by `NCA` matrix that contains information from the *QR* factorization of `A`. The upper trapezoidal part of *QR* contains the upper trapezoidal part of *R* with its diagonal elements ordered in decreasing magnitude. The strict lower trapezoidal part of *QR* contains information to recover the orthogonal matrix *Q* of the factorization. If A is not needed, *QR* can share the same storage locations as A.

QRAUX — Work vector of length NCA containing information about the orthogonal factor of the *QR* factorization of A.

IPVT — Integer work vector of length NCA containing the pivoting information for the QR factorization of A.

WORK — Work vector of length 2 * NCA – 1.

2. Routine LSQRR calculates the *QR* decomposition with pivoting of a matrix A and tests the diagonal elements against a user-supplied tolerance TOL. The first integer KBASIS = k is determined for which

$$|r_{k+1,k+1}| \le \mathrm{TOL} * |r_{11}|$$

In effect, this condition implies that a set of columns with a condition number approximately bounded by 1.0/TOL is used. Then, LQRSL performs a truncated fit of the first KBASIS columns of the permuted A to an input vector B. The coefficient of this fit is unscrambled to correspond to the original columns of A, and the coefficients corresponding to unused columns are set to zero. It may be helpful to scale the rows and columns of A so that the error estimates in the elements of the scaled matrix are roughly equal to TOL.

3. *Integer Options* with *Chapter 11* Options Manager

16 This option uses four values to solve memory bank conflict (access inefficiency) problems. In routine L2QRR the leading dimension of QR is increased by IVAL(3) when N is a multiple of IVAL(4). The values IVAL(3) and IVAL(4) are temporarily replaced by IVAL(1) and IVAL(2), respectively, in LSQRR. Additional memory allocation for QR and option value restoration are done automatically in LSQRR. Users directly calling L2QRR can allocate additional space for QR and set IVAL(3) and IVAL(4) so that memory bank conflicts no longer cause inefficiencies. There is no requirement that users change existing applications that use LSQRR or L2QRR. Default values for the option are IVAL(*) = 1, 16, 0, 1.

17 This option has two values that determine if the L_1 condition number is to be computed. Routine LSQRR temporarily replaces IVAL(2) by IVAL(1). The routine L2CRG computes the condition number if IVAL(2) = 2. Otherwise L2CRG skips this computation. LSQRR restores the option. Default values for the option are IVAL(*) = 1, 2.

ScaLAPACK Usage Notes

The arguments which differ from the standard version of this routine are:

A0 — MXLDA by MXCOL local matrix containing the local portions of the distributed matrix A. A contains the coefficient matrix of the least squares system to be solved. (Input)

B0 — Local vector of length MXLDA containing the local portions of the distributed vector B. B contains the right-hand side of the least squares system. (Input)

X0 — Local vector of length MXLDX containing the local portions of the distributed vector X. X contains the solution vector with components corresponding to the columns not used set to zero. (Output)

RES0 — Local vector of length MXLDA containing the local portions of the distributed vector RES. RES contains the residual vector B - A * X. (Output)

All other arguments are global and are the same as described for the standard version of the routine. In the argument descriptions above, MXLDA, MXLDX, and MXCOL can be obtained through a call to SCALAPACK_GETDIM (see *Utilities*) after a call to SCALAPACK_SETUP (see *Utilities*) has been made. See the *ScaLAPACK Example* below.

Examples

Example 1

Consider the problem of finding the coefficients c_i in

$$f(x) = c_0 + c_1 x + c_2 x_2$$

given data at x = 1, 2, 3 and 4, using the method of least squares. The row of the matrix A contains the value of 1, x and x_2 at the data points. The vector b contains the data, chosen such that $c_0 \approx 1$, $c_1 \approx 2$ and $c_2 \approx 0$. The routine LSQRR solves this least-squares problem.

```
      USE LSQRR_INT
      USE UMACH_INT
      USE WRRRN_INT
!                                 Declare variables
      PARAMETER  (NRA=4, NCA=3, LDA=NRA)
      REAL       A(LDA,NCA), B(NRA), X(NCA), RES(NRA), TOL
!
!                                 Set values for A
!
!                                 A = (  1    2     4   )
!                                     (  1    4    16   )
!                                     (  1    6    36   )
!                                     (  1    8    64   )
!
      DATA A/4*1.0, 2.0, 4.0, 6.0, 8.0, 4.0, 16.0, 36.0, 64.0/
!
!                                 Set values for B
!
      DATA B/ 4.999,  9.001,  12.999,  17.001 /
!
!                                 Solve the least squares problem
      TOL = 1.0E-4
      CALL LSQRR (A, B, X, RES, KBASIS, TOL=TOL)
!                                 Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,*) 'KBASIS = ', KBASIS
      CALL WRRRN ('X', X, 1, NCA, 1)
      CALL WRRRN ('RES', RES, 1, NRA, 1)
```

```
!
      END
```

Output

```
 KBASIS =   3

            X
     1       2       3
 0.999   2.000   0.000

                     RES
         1           2           3           4
 -0.000400   0.001200  -0.001200   0.000400
```

ScaLAPACK Example

The previous example is repeated here as a distributed computing example. Consider the problem of finding the coefficients c_i in

$$f(x) = c_0 + c_1 x + c_2 x_2$$

given data at x = 1, 2, 3 and 4, using the method of least squares. The row of the matrix A contains the value of 1, x and x_2 at the data points. The vector b contains the data, chosen such that $c_0 \approx 1$, $c_1 \approx 2$ and $c_2 \approx 0$. The routine `LSQRR` solves this least-squares problem. `SCALAPACK_MAP` and `SCALAPACK_UNMAP` are IMSL utility routines (se e *Chapter 19, "Utilities"* used to map and unmap arrays to and from the processor grid. They are used here for brevity. `DESCINIT` is a ScaLAPACK tools routine which initializes the descriptors for the local arrays.

```
      USE MPI_SETUP_INT
      USE LSQRR_INT
      USE UMACH_INT
      USE WRRRN_INT
      USE SCALAPACK_SUPPORT
      IMPLICIT NONE
      INCLUDE 'mpif.h'
!                                  Declare variables
      INTEGER       LDA, NRA, NCA, DESCA(9), DESCX(9), DESCR(9)
      INTEGER       INFO, KBASIS, MXCOL, MXLDA, MXCOLX, MXLDX, NOUT
      REAL          TOL
      REAL, ALLOCATABLE ::         A(:,:), B(:), X(:), RES(:)
      REAL, ALLOCATABLE ::         A0(:,:), B0(:), X0(:), RES0(:)
      PARAMETER  (NRA=4, NCA=3, LDA=NRA)
!                                  Set up for MPI
      MP_NPROCS = MP_SETUP()
      IF(MP_RANK .EQ. 0) THEN
          ALLOCATE (A(LDA,NCA), B(NRA), X(NCA), RES(NRA))
!                                  Set values for A and B
          A(1,:) = (/ 1.0,   2.0,    4.0/)
          A(2,:) = (/ 1.0,   4.0,   16.0/)
          A(3,:) = (/ 1.0,   6.0,   36.0/)
          A(4,:) = (/ 1.0,   8.0,   64.0/)
!
          B = (/4.999, 9.001,  12.999, 17.001/)
      ENDIF
!                                   Set up a 2D processor grid and define
!                                   its context ID, MP_ICTXT
      CALL SCALAPACK_SETUP(NRA, NCA, .TRUE., .FALSE.)
```

```
!                                   Get the array descriptor entities MXLDA,
!                                   MXCOL, MXLDX, and MXCOLX
      CALL SCALAPACK_GETDIM(NRA, NCA, MP_MB, MP_NB, MXLDA, MXCOL)
      CALL SCALAPACK_GETDIM(NCA, 1, MP_NB, 1, MXLDX, MXCOLX)
!                                   Set up the array descriptors
      CALL DESCINIT(DESCA, NRA, NCA, MP_MB, MP_NB, 0, 0, MP_ICTXT, MXLDA, &
                    INFO)
      CALL DESCINIT(DESCX, NCA, 1, MP_NB, 1, 0, 0, MP_ICTXT, MXLDX, INFO)
      CALL DESCINIT(DESCR, NRA, 1, MP_MB, 1, 0, 0, MP_ICTXT, MXLDA, INFO)
!                                   Allocate space for the local arrays
      ALLOCATE (A0(MXLDA,MXCOL), B0(MXLDA), X0(MXLDX), RES0(MXLDA))
!                                  Map input arrays to the processor grid
      CALL SCALAPACK_MAP(A, DESCA, A0)
      CALL SCALAPACK_MAP(B, DESCR, B0)
!                                  Solve the least squares problem
      TOL = 1.0E-4
      CALL LSQRR (A0, B0, X0, RES0, KBASIS, TOL=TOL)
!                                  Unmap the results from the distributed
!                                  arrays back to a non-distributed array.
!                                  After the unmap, only Rank=0 has the full
!                                  array.
      CALL SCALAPACK_UNMAP(X0, DESCX, X)
      CALL SCALAPACK_UNMAP(RES0, DESCR, RES)
!                                 Print results.
!                                  Only Rank=0 has the solution.
      IF(MP_RANK .EQ. 0)THEN
         CALL UMACH (2, NOUT)
         WRITE (NOUT,*) 'KBASIS = ', KBASIS
         CALL WRRRN ('X', X, 1, NCA, 1)
         CALL WRRRN ('RES', RES, 1, NRA, 1)
      ENDIF
      IF (MP_RANK .EQ. 0) DEALLOCATE(A, B, RES, X)
      DEALLOCATE(A0, B0, RES0, X0)
!                                 Exit ScaLAPACK usage
      CALL SCALAPACK_EXIT(MP_ICTXT)
!                                 Shut down MPI
      MP_NPROCS = MP_SETUP('FINAL')
      END
```

Output

```
KBASIS =   3

            X
    1       2       3
0.999   2.000   0.000

                     RES
        1           2           3           4
-0.000400   0.001200  -0.001200   0.000400
```

LQRRV

more...

more...

Computes the least-squares solution using Householder transformations applied in blocked form.

Required Arguments

A — Real LDA by (NCA + NUMEXC) array containing the matrix and right-hand sides. (Input)
The right-hand sides are input in A(1 : NRA, NCA + j), j = 1, …, NUMEXC. The array A is preserved upon output. The Householder factorization of the matrix is computed and used to solve the systems.

X — Real LDX by NUMEXC array containing the solution. (Output)

Optional Arguments

NRA — Number of rows in the matrix. (Input)
Default: NRA = size (A,1).

NCA — Number of columns in the matrix. (Input)
Default: NCA = size (A,2) – NUMEXC.

NUMEXC — Number of right-hand sides. (Input)
Default: NUMEXC = size (X,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

LDX — Leading dimension of the solution array X exactly as specified in the dimension statement of the calling program. (Input)
Default: LDX = size (X,1).

FORTRAN 90 Interface

Generic: `CALL LQRRV (A, X [, …])`

Specific: The specific interface names are `S_LQRRV` and `D_LQRRV`.

FORTRAN 77 Interface

Single: `CALL LQRRV (NRA, NCA, NUMEXC, A, LDA, X, LDX)`

Double: The double precision name is `DLQRRV`.

ScaLAPACK Interface

Generic: `CALL LQRRV (A0, X0 [, …])`

Specific: The specific interface names are `S_LQRRV` and `D_LQRRV`.

See the *ScaLAPACK Usage Notes* below for a description of the arguments for distributed computing.

Description

The routine `LQRRV` computes the *QR* decomposition of a matrix *A* using blocked Householder transformations. The underlying code is based on either LINPACK , LAPACK, or ScaLAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see *Using ScaLAPACK, LAPACK, LINPACK, and EISPACK* in the Introduction section of this manual. The standard algorithm is based on the storage-efficient *WY* representation for products of Householder transformations. See Schreiber and Van Loan (1989).

The routine `LQRRV` determines an orthogonal matrix *Q* and an upper triangular matrix *R* such that *A* = *QR*. The *QR* factorization of a matrix *A* having `NRA` rows and `NCA` columns is as follows:

Initialize $A_1 \leftarrow A$

For $k = 1$, min(`NRA` – 1, `NCA`)

Determine a Householder transformation for column *k* of A_k having the form

$$H_k = I - \tau_k \mu_k \mu_k^T$$

where u_k has zeros in the first $k - 1$ positions and τ_k is a scalar.

Update

$$A_k \leftarrow H_k A_{k-1} = A_{k-1} - \tau_k \mu_k \left(A_{k-1}^T \mu_k \right)^T$$

End *k*

Thus,

$$A_p = H_p H_{p-1} \cdots H_1 A = Q^T A = R$$

where p = min(NRA − 1, NCA). The matrix Q is not produced directly by LQRRV. The information needed to construct the Householder transformations is saved instead. If the matrix Q is needed explicitly, Q^T can be determined while the matrix is factored. No pivoting among the columns is done. The primary purpose of LQRRV is to give the user a high-performance QR least-squares solver. It is intended for least-squares problems that are well-posed. For background, see Golub and Van Loan (1989, page 225). During the QR factorization, the most time-consuming step is computing the matrix-vector update $A_k \leftarrow H_k A_{k-1}$. The routine LQRRV constructs “block” of NB Householder transformations in which the update is “rich” in matrix multiplication. The product of NB Householder transformations are written in the form

$$H_k H_{k+1} \cdots H_{k+nb-1} = I + YTY^T$$

where $Y_{NRA \times NB}$ is a lower trapezoidal matrix and $T_{NB \times NB}$ is upper triangular. The optimal choice of the block size parameter NB varies among computer systems. Users may want to change it from its default value of 1.

Comments

1. Workspace may be explicitly provided, if desired, by use of L2RRV/DL2RRV. The reference is:

   CALL L2RRV (NRA, NCA, NUMEXC, A, LDA, X, LDX, FACT, LDFACT, WK)

   The additional arguments are as follows:

   FACT — LDFACT × (NCA + NUMEXC) work array containing the Householder factorization of the matrix on output. If the input data is not needed, A and FACT can share the same storage locations.

   LDFACT — Leading dimension of the array FACT exactly as specified in the dimension statement of the calling program. (Input)
   If A and FACT are sharing the same storage, then LDA = LDFACT is required.

   WK — Work vector of length (NCA + NUMEXC + 1) * (NB + 1) . The default value is NB = 1. This value can be reset. See item 3 below.

2. Informational errors

Type	Code	Description
4	1	The input matrix is singular.

3. *Integer Options* with *Chapter 11* Options Manager

   5 This option allows the user to reset the blocking factor used in computing the factorization. On some computers, changing IVAL(*) to a value larger than 1 will result in greater efficiency. The value IVAL(*) is the maximum value to use. (The software is specialized so that IVAL(*)

is reset to an "optimal" used value within routine L2RRV.) The user can control the blocking by resetting IVAL(*) to a smaller value than the default. Default values are IVAL(*) = 1, IMACH(5).

6 This option is the vector dimension where a shift is made from in-line level-2 loops to the use of level-2 BLAS in forming the partial product of Householder transformations. Default value is IVAL(*) = IMACH(5).

10 This option allows the user to control the factorization step. If the value is 1 the Householder factorization will be computed. If the value is 2, the factorization will not be computed. In this latter case the decomposition has already been computed. Default value is IVAL(*) = 1.

11 This option allows the user to control the solving steps. The rules for IVAL(*) are:

1. Compute $b \leftarrow Q^T b$, and $x \leftarrow R^+ b$.
2. Compute $b \leftarrow Q^T b$.
3. Compute $b \leftarrow Qb$.
4. Compute $x \leftarrow R^+ b$.

Default value is IVAL (*) = 1. Note that IVAL (*) = 2 or 3 may only be set when calling L2RRV/DL2RRV.

ScaLAPACK Usage Notes

The arguments which differ from the standard version of this routine are:

A0 — MXLDA by MXCOL local matrix containing the local portions of the distributed matrix A. A contains the matrix and right-hand sides. (Input)
The right-hand sides are input in A(1 : NRA, NCA + j), j = 1, …, NUMEXC. The array A is preserved upon output. The Householder factorization of the matrix is computed and used to solve the systems.. (Input)

X0 — MXLDX by MXCOLX local matrix containing the local portions of the distributed matrix X. X contains the solution. (Output)

All other arguments are global and are the same as described for the standard version of the routine. In the argument descriptions above, MXLDA, MXLDX, MXCOL, and MXCOLX can be obtained through a call to SCALAPACK_GETDIM (see *Utilities*) after a call to SCALAPACK_SETUP (see *Utilities*) has been made. See the *ScaLAPACK Example* below.

Examples

Example

Given a real $m \times k$ matrix B it is often necessary to compute the k least-squares solutions of the linear system $AX = B$, where A is an $m \times n$ real matrix. When $m > n$ the system is considered *overdetermined*. A solution with a zero residual normally does not exist. Instead the minimization problem

$$\min_{x_j \in R^n} \left\| Ax_j - b_j \right\|_2$$

is solved k times where x_j, b_j are the j-th columns of the matrices X, B respectively. When A is of full column rank there exits a unique solution X_{LS} that solves the above minimization problem. By using the routine LQRRV, X_{LS} is computed.

```
      USE LQRRV_INT
      USE WRRRN_INT
      USE SGEMM_INT
!                                 Declare variables
      INTEGER    LDA, LDX, NCA, NRA, NUMEXC
      PARAMETER  (NCA=3, NRA=5, NUMEXC=2, LDA=NRA, LDX=NCA)
!                                 SPECIFICATIONS FOR LOCAL VARIABLES
      REAL       X(LDX,NUMEXC)
!                                 SPECIFICATIONS FOR SAVE VARIABLES
      REAL       A(LDA,NCA+NUMEXC)
      SAVE       A
!                                 SPECIFICATIONS FOR SUBROUTINES
!
!                                 Set values for A and the
!                                 righthand sides.
!
!                                 A = (  1    2     4 |   7  10)
!                                     (  1    4    16 |  21  10)
!                                     (  1    6    36 |  43  9 )
!                                     (  1    8    64 |  73  10)
!                                     (  1   10   100 | 111  10)
!
      DATA A/5*1.0, 2.0, 4.0, 6.0, 8.0, 10.0, 4.0, 16.0, 36.0, 64.0, &
          100.0, 7.0, 21.0, 43.0, 73.0, 111.0, 2*10., 9., 2*10./
!
!
!                                 QR factorization and solution
      CALL LQRRV (A, X)
      CALL WRRRN ('SOLUTIONS 1-2', X)
!                                 Compute residuals and print
      CALL SGEMM ('N', 'N', NRA, NUMEXC, NCA, 1.E0, A, LDA, X, LDX, &
                 -1.E0, A(1:,(NCA+1):),LDA)
      CALL WRRRN ('RESIDUALS 1-2', A(1:,(NCA+1):))
!
      END
```

Output

```
     SOLUTIONS 1-2
          1        2
 1     1.00    10.80
 2     1.00    -0.43
```

```
3    1.00    0.04

   RESIDUALS 1-2
        1         2
1   0.0000   0.0857
2   0.0000  -0.3429
3   0.0000   0.5143
4   0.0000  -0.3429
5   0.0000   0.0857
```

ScaLAPACK Example

The previous example is repeated here as a distributed computing example. Given a real $m \times k$ matrix B it is often necessary to compute the k least-squares solutions of the linear system $AX = B$, where A is an $m \times n$ real matrix. When $m > n$ the system is considered *overdetermined*. A solution with a zero residual normally does not exist. Instead the minimization problem

$$\min_{x_j \in R^n} \| Ax_j - b_j \|_2$$

is solved k times where x_j, b_j are the j-th columns of the matrices X, B respectively. When A is of full column rank there exits a unique solution X_{LS} that solves the above minimization problem. By using the routine LQRRV, X_{LS} is computed. SCALAPACK_MAP and SCALAPACK_UNMAP are IMSL utility routines (see *Utilities*) used to map and unmap arrays to and from the processor grid. They are used here for brevity. DESCINIT is a ScaLAPACK tools routine which initializes the descriptors for the local arrays.

```
      USE MPI_SETUP_INT
      USE LQRRV_INT
      USE SGEMM_INT
      USE WRRRN_INT
      USE SCALAPACK_SUPPORT
      IMPLICIT NONE
      INCLUDE 'mpif.h'
!                                  Declare variables
      INTEGER    LDA, LDX, NCA, NRA, NUMEXC, DESCA(9), DESCX(9)
      INTEGER       INFO, MXCOL, MXLDA, MXLDX, MXCOLX
      INTEGER       K      REAL, ALLOCATABLE ::        A(:,:), X(:)
      REAL, ALLOCATABLE ::         A0(:,:), X0(:)
      PARAMETER  (NRA=5, NCA=3, NUMEXC=2, LDA=NRA, LDX=NCA)
!                                  Set up for MPI
      MP_NPROCS = MP_SETUP()
      IF(MP_RANK .EQ. 0) THEN
          ALLOCATE (A(LDA,NCA+NUMEXC), X(LDX, NUMEXC))
!                                  Set values for A and the righthand sides
          A(1,:) = (/ 1.0,  2.0,   4.0,   7.0, 10.0/)
          A(2,:) = (/ 1.0,  4.0,  16.0,  21.0, 10.0/)
          A(3,:) = (/ 1.0,  6.0,  36.0,  43.0,  9.0/)
          A(4,:) = (/ 1.0,  8.0,  64.0,  73.0, 10.0/)
          A(5,:) = (/ 1.0, 10.0, 100.0, 111.0, 10.0/)
      ENDIF
!                                   Set up a 1D processor grid and define
!                                   its context ID, MP_ICTXT
      CALL SCALAPACK_SETUP(NRA, NCA+NUMEXC, .TRUE., .TRUE.)
!                                   Get the array descriptor entities MXLDA,
!                                   and MXCOL
      CALL SCALAPACK_GETDIM(NRA, NCA+NUMEXC, MP_MB, MP_NB, MXLDA, MXCOL)
!                                   Set up the array descriptors
```

```
      CALL DESCINIT(DESCA, NRA, NCA+NUMEXC, MP_MB, MP_NB, 0, 0, MP_ICTXT, &
              MXLDA, INFO)
      K = MIN0(NRA, NCA)
!                                  Need to get dimensions of local x
!                                  separate since x's leading
!                                  dimension differs from A's
!                                  Get the array descriptor entities
!                                  MXLDX, AND MXCOLX
      CALL SCALAPACK_GETDIM(K, NUMEXC, MP_MB, MP_NB, MXLDX, MXCOLX)
      CALL DESCINIT (DESCX, K, NUMEXC, MP_NB, MP_NB, 0, 0, MP_ICTXT, &
      MXLDX, INFO)
!                                 Allocate space for the local arrays
      ALLOCATE (A0(MXLDA,MXCOL), X0(MXLDX,MXCOLX))
!                                 Map input array to the processor grid
      CALL SCALAPACK_MAP(A, DESCA, A0)
!                                 Solve the least squares problem
      CALL LQRRV (A0, X0)
!                                 Unmap the results from the distributed
!                                 arrays back to a non-distributed array.
!                                 After the unmap, only Rank=0 has the full
!                                 array.
      CALL SCALAPACK_UNMAP(X0, DESCX, X)
!                                Print results.
!                                Only Rank=0 has the solution, X.
      IF(MP_RANK .EQ. 0)THEN
         CALL WRRRN (’SOLUTIONS 1-2’, X)
!                                 Compute residuals and print
      CALL SGEMM (’N’, ’N’, NRA, NUMEXC, NCA, 1.E0, A, LDA, X, LDX, &
                -1.E0, A(1:,(NCA+1):),LDA)
      CALL WRRRN (’RESIDUALS 1-2’, A(1:,(NCA+1):))
      ENDIF
!                                Exit ScaLAPACK usage
      CALL SCALAPACK_EXIT(MP_ICTXT)
!                                Shut down MPI
      MP_NPROCS = MP_SETUP(‘FINAL’)
      END
```

LSBRR

more...

Solves a linear least-squares problem with iterative refinement.

Required Arguments

A — Real NRA by NCA matrix containing the coefficient matrix of the least-squares system to be solved. (Input)

B — Real vector of length NRA containing the right-hand side of the least-squares system. (Input)

X — Real vector of length NCA containing the solution vector with components corresponding to the columns not used set to zero. (Output)

Optional Arguments

NRA — Number of rows of A. (Input)
Default: NRA = size (A,1).

NCA — Number of columns of A. (Input)
Default: NCA = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

TOL — Real scalar containing the nonnegative tolerance used to determine the subset of columns of A to be included in the solution. (Input)
If TOL is zero, a full complement of min(NRA, NCA) columns is used. See Comments.
Default: TOL = 0.0

RES — Real vector of length NRA containing the residual vector $B - AX$. (Output)

KBASIS — Integer scalar containing the number of columns used in the solution. (Output)

FORTRAN 90 Interface

Generic: CALL LSBRR (A, B, X [, …])

Specific: The specific interface names are S_LSBRR and D_LSBRR.

FORTRAN 77 Interface

Single: CALL LSBRR (NRA, NCA, A, LDA, B, TOL, X, RES, KBASIS)

Double: The double precision name is DLSBRR.

Description

Routine LSBRR solves the linear least-squares problem using iterative refinement. The iterative refinement algorithm is due to Björck (1967, 1968). It is also described by Golub and Van Loan (1983, pages 182−183).

Comments

1. Workspace may be explicitly provided, if desired, by use of L2BRR/DL2BRR. The reference is:

   CALL L2BRR (NRA, NCA, A, LDA, B, TOL, X, RES, KBASIS, QR, BRRUX, IPVT, WK)

   The additional arguments are as follows:

   QR — Work vector of length NRA * NCA representing an NRA by NCA matrix that contains information from the *QR* factorization of A. See LQRRR for details.

   BRRUX — Work vector of length NCA containing information about the orthogonal factor of the *QR* factorization of A. See LQRRR for details.

   IPVT — Integer work vector of length NCA containing the pivoting information for the *QR* factorization of A. See LQRRR for details.

   WK — Work vector of length NRA + 2 * NCA − 1.

2. Informational error

Type	Code	Description
4	1	The data matrix is too ill-conditioned for iterative refinement to be effective.

3. Routine LSBRR calculates the *QR* decomposition with pivoting of a matrix *A* and tests the diagonal elements against a user-supplied tolerance TOL. The first integer KBASIS = *k* is determined for which

$$|r_{k+1,k+1}| \le \text{TOL} * |r_{11}|$$

In effect, this condition implies that a set of columns with a condition number approximately bounded by 1.0/TOL is used. Then, LQRSL performs a truncated fit of the first KBASIS columns of the permuted A to an input vector B. The coefficient of this fit is unscrambled to correspond to the original columns of A, and the coefficients corresponding to unused columns are set to zero. It may be helpful to scale the rows and columns of A so that the error estimates in the elements of the scaled matrix are roughly equal to TOL. The iterative refinement method of Björck is then applied to this factorization.

4. *Integer Options* with *Chapter 11* Options Manager

16 This option uses four values to solve memory bank conflict (access inefficiency) problems. In routine L2BRR the leading dimension of QR is increased by IVAL(3) when N is a multiple of IVAL(4). The values IVAL(3) and IVAL(4) are temporarily replaced by IVAL(1) and IVAL(2), respectively, in LSBRR. Additional memory allocation for QR and option value restoration are done automatically in LSBRR. Users directly calling L2BRR can allocate additional space for QR and set IVAL(3) and IVAL(4) so that memory bank conflicts no longer cause inefficiencies. There is no requirement that users change existing applications that use LSBRR or L2BRR. Default values for the option are IVAL(*) = 1, 16, 0, 1.

17 This option has two values that determine if the L_1 condition number is to be computed. Routine LSBRR temporarily replaces IVAL(2) by IVAL(1). The routine L2CRG computes the condition number if IVAL(2) = 2. Otherwise L2CRG skips this computation. LSBRR restores the option. Default values for the option are IVAL(*) = 1, 2.

Example

This example solves the linear least-squares problem with *A*, an 8 × 4 matrix. Note that the second and fourth columns of *A* are identical. Routine LSBRR determines that there are three columns in the basis.

```
      USE LSBRR_INT
      USE UMACH_INT
      USE WRRRN_INT
!                                 Declare variables
      PARAMETER  (NRA=8, NCA=4, LDA=NRA)
      REAL       A(LDA,NCA), B(NRA), X(NCA), RES(NRA), TOL
!
!                                 Set values for A
!
!                                 A = (  1    5    15    5  )
!                                     (  1    4    17    4  )
!                                     (  1    7    14    7  )
!                                     (  1    3    18    3  )
!                                     (  1    1    15    1  )
!                                     (  1    8    11    8  )
!                                     (  1    3     9    3  )
!                                     (  1    4    10    4  )
!
      DATA A/8*1, 5., 4., 7., 3., 1., 8., 3., 4., 15., 17., 14., &
        18., 15., 11., 9., 10., 5., 4., 7., 3., 1., 8., 3., 4. /
!
!                                 Set values for B
```

```
!
      DATA B/ 30., 31., 35., 29., 18., 35., 20., 22. /
!
!                               Solve the least squares problem
      TOL = 1.0E-4
      CALL LSBRR (A, B, X, tol=tol, RES=RES, KBASIS=KBASIS)
!                               Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,*) 'KBASIS = ', KBASIS
      CALL WRRRN ('X', X, 1, NCA, 1)
      CALL WRRRN ('RES', RES, 1, NRA, 1)
!
      END
```

Output

```
KBASIS =   3
                X
      1       2       3       4
  0.636   2.845   1.058   0.000

                              RES
      1       2       3       4       5       6       7       8
 -0.733   0.996  -0.365   0.783  -1.353  -0.036   1.306  -0.597
```

LCLSQ

Solves a linear least-squares problem with linear constraints.

Required Arguments

A — Matrix of dimension NRA by NCA containing the coefficients of the NRA least squares equations. (Input)

B — Vector of length NRA containing the right-hand sides of the least squares equations. (Input)

C — Matrix of dimension NCON by NCA containing the coefficients of the NCON constraints. (Input)
If NCON = 0, C is not referenced.

BL — Vector of length NCON containing the lower limit of the general constraints. (Input)
If there is no lower limit on the I-th constraint, then BL(I) will not be referenced.

BU — Vector of length NCON containing the upper limit of the general constraints. (Input)
If there is no upper limit on the I-th constraint, then BU(I) will not be referenced. If there is no range constraint, BL and BU can share the same storage locations.

IRTYPE — Vector of length NCON indicating the type of constraints exclusive of simple bounds, where IRTYPE(I) = 0, 1, 2, 3 indicates .EQ., .LE., .GE., and range constraints respectively. (Input)

XLB — Vector of length NCA containing the lower bound on the variables. (Input)
If there is no lower bound on the I-th variable, then XLB(I) should be set to 1.0E30.

XUB — Vector of length NCA containing the upper bound on the variables. (Input)
If there is no upper bound on the I-th variable, then XUB(I) should be set to −1.0E30.

X — Vector of length NCA containing the approximate solution. (Output)

Optional Arguments

NRA — Number of least-squares equations. (Input)
Default: NRA = size (A,1).

NCA — Number of variables. (Input)
Default: NCA = size (A,2).

NCON — Number of constraints. (Input)
Default: NCON = size (C,1).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
LDA must be at least NRA.
Default: LDA = size (A,1).

LDC — Leading dimension of C exactly as specified in the dimension statement of the calling program. (Input)
LDC must be at least NCON.
Default: LDC = size (C,1).

RES — Vector of length NRA containing the residuals $B - AX$ of the least-squares equations at the approximate solution. (Output)

FORTRAN 90 Interface

Generic: CALL LCLSQ (A, B, C, BL, BU, IRTYPE, XLB, XUB, X [, …])

Specific: The specific interface names are S_LCLSQ and D_LCLSQ.

FORTRAN 77 Interface

Single: CALL LCLSQ (NRA, NCA, NCON, A, LDA, B, C, LDC, BL, BU, IRTYPE, XLB, XUB, X, RES)

Double: The double precision name is DLCLSQ.

Description

The routine LCLSQ solves linear least-squares problems with linear constraints. These are systems of least-squares equations of the form $Ax \cong b$, subject to

$$b_l \le C_x \le b_u$$
$$x_l \le x \le x_u$$

Here, A is the coefficient matrix of the least-squares equations, b is the right-hand side, and C is the coefficient matrix of the constraints. The vectors b_l, b_u, x_l and x_u are the lower and upper bounds on the constraints and the variables, respectively. The system is solved by defining dependent variables $y \equiv Cx$ and then solving the least squares system with the lower and upper bounds on x and y. The equation $Cx - y = 0$ is a set of equality constraints. These constraints are realized by heavy weighting, i.e. a penalty method, Hanson, (1986, pages 826−834).

Comments

1. Workspace may be explicitly provided, if desired, by use of L2LSQ/DL2LSQ. The reference is:

CALL L2LSQ (NRA, NCA, NCON, A, LDA, B, C, LDC, BL, BU, IRTYPE, XLB, XUB, X, RES, WK, IWK)

The additional arguments are as follows:

WK — Real work vector of length (NCON + MAXDIM) * (NCA + NCON + 1) + 10 * NCA + 9 * NCON + 3.

IWK — Integer work vector of length 3 * (NCON + NCA).

2. Informational errors

Type	Code	Description
3	1	The rank determination tolerance is less than machine precision.
4	2	The bounds on the variables are inconsistent.
4	3	The constraint bounds are inconsistent.
4	4	Maximum number of iterations exceeded.

3. *Integer Options* with *Chapter 11* Options Manager

13 Debug output flag. If more detailed output is desired, set this option to the value 1. Otherwise, set it to 0. Default value is 0.

14 Maximum number of add/drop iterations. If the value of this option is zero, up to 5 * max(nra, nca) iterations will be allowed. Otherwise set this option to the desired iteration limit. Default value is 0.

4. *Floating Point Options* with *Chapter 11* Options Manager

2 The value of this option is the relative rank determination tolerance to be used. Default value is sqrt(AMACH (4)).

5 The value of this option is the absolute rank determination tolerance to be used. Default value is sqrt(AMACH (4)).

Example

A linear least-squares problem with linear constraints is solved.

```
      USE LCLSQ_INT
      USE UMACH_INT
      USE SNRM2_INT
!
!     Solve the following in the least squares sense:
!           3x1 + 2x2 +  x3 = 3.3
!           4x1 + 2x2 +  x3 = 2.3
!           2x1 + 2x2 +  x3 = 1.3
!            x1 +  x2 +  x3 = 1.0
!
!     Subject to:  x1 + x2 + x3 <= 1
!                  0 <= x1 <= .5
!                  0 <= x2 <= .5
!                  0 <= x3 <= .5
!
! ----------------------------------------------------------------------
```

```
!                                  Declaration of variables
!
      INTEGER     NRA, NCA, MCON, LDA, LDC
      PARAMETER   (NRA=4, NCA=3, MCON=1, LDC=MCON, LDA=NRA)
!
      INTEGER     IRTYPE(MCON), NOUT
      REAL        A(LDA,NCA), B(NRA), BC(MCON), C(LDC,NCA), RES(NRA), &
                 RESNRM, XSOL(NCA), XLB(NCA), XUB(NCA)
!                                  Data initialization!
      DATA A/3.0E0, 4.0E0, 2.0E0, 1.0E0, 2.0E0, &
            2.0E0, 2.0E0, 1.0E0, 1.0E0, 1.0E0, 1.0E0, 1.0E0/, &
            B/3.3E0, 2.3E0, 1.3E0, 1.0E0/, &
            C/3*1.0E0/, &
            BC/1.0E0/, IRTYPE/1/, XLB/3*0.0E0/, XUB/3*.5E0/
!
!                                  Solve the bounded, constrained
!                                  least squares problem.
!
      CALL LCLSQ (A, B, C, BC, BC, IRTYPE, XLB, XUB, XSOL, RES=res)
!                                  Compute the 2-norm of the residuals.
      RESNRM = SNRM2 (NRA, RES, 1)
!                                  Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT, 999) XSOL, RES, RESNRM
!
 999  FORMAT ('  The solution is ', 3F9.4, //, '  The residuals ', &
            'evaluated at the solution are ', /, 18X, 4F9.4, //, &
            '  The norm of the residual vector is ', F8.4)
!
      END
```

Output

```
The solution is    0.5000   0.3000   0.2000
The residuals evaluated at the solution are
                   -1.0000   0.5000   0.5000   0.0000

The norm of the residual vector is   1.2247
```

LQRRR

more... more...

Computes the *QR* decomposition, *AP* = *QR*, using Householder transformations.

Required Arguments

A — Real `NRA` by `NCA` matrix containing the matrix whose *QR* factorization is to be computed. (Input)

QR — Real `NRA` by `NCA` matrix containing information required for the *QR* factorization. (Output)
The upper trapezoidal part of *QR* contains the upper trapezoidal part of *R* with its diagonal elements ordered in decreasing magnitude. The strict lower trapezoidal part of *QR* contains information to recover the orthogonal matrix *Q* of the factorization. Arguments `A` and `QR` can occupy the same storage locations. In this case, `A` will not be preserved on output.

QRAUX — Real vector of length `NCA` containing information about the orthogonal part of the decomposition in the first min(`NRA`, `NCA`) position. (Output)

Optional Arguments

NRA — Number of rows of `A`. (Input)
Default: `NRA` = size (`A`,1).

NCA — Number of columns of `A`. (Input)
Default: `NCA` = size (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = size (`A`,1).

PIVOT — Logical variable. (Input)
`PIVOT` = `.TRUE.` means column pivoting is enforced.
`PIVOT` = `.FALSE.` means column pivoting is not done.
Default: `PIVOT` = `.TRUE.`

IPVT — Integer vector of length NCA containing information that controls the final order of the columns of the factored matrix A. (Input/Output)
On input, if IPVT(K) > 0, then the K-th column of A is an initial column. If IPVT(K) = 0, then the K-th column of A is a free column. If IPVT(K) < 0, then the K-th column of A is a final column. See the Comments section below. On output, IPVT(K) contains the index of the column of A that has been interchanged into the K-th column. This defines the permutation matrix *P*. The array IPVT is referenced only if PIVOT is equal to .TRUE.
Default: IPVT = 0.

LDQR — Leading dimension of QR exactly as specified in the dimension statement of the calling program. (Input)
Default: LDQR = size (QR,1).

CONORM — Real vector of length NCA containing the norms of the columns of the input matrix. (Output)
If this information is not needed, CONORM and QRAUX can share the same storage locations.

FORTRAN 90 Interface

Generic: CALL LQRRR (A, QR, QRAUX [, …])

Specific: The specific interface names are S_LQRRR and D_LQRRR.

FORTRAN 77 Interface

Single: CALL LQRRR (NRA, NCA, A, LDA, PIVOT, IPVT, QR, LDQR, QRAUX, CONORM)

Double: The double precision name is DLQRRR.

ScaLAPACK Interface

Generic: CALL LQRRR (A0, QR0, QRAUX0 [, …])

Specific: The specific interface names are S_LQRRR and D_LQRRR.

See the *ScaLAPACK Usage Notes* below for a description of the arguments for distributed computing.

Description

The routine LQRRR computes the *QR* decomposition of a matrix using Householder transformations. The underlying code is based on either LINPACK , LAPACK, or ScaLAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see *Using ScaLAPACK, LAPACK, LINPACK, and EISPACK* in the Introduction section of this manual.

LQRRR determines an orthogonal matrix Q, a permutation matrix P, and an upper trapezoidal matrix R with diagonal elements of nonincreasing magnitude, such that $AP = QR$. The Householder transformation for column k is of the form

$$I - \frac{u_k u_k^T}{p_k}$$

for $k = 1, 2, \ldots, \min(\mathrm{NRA}, \mathrm{NCA})$, where u has zeros in the first $k - 1$ positions. The matrix Q is not produced directly by LQRRR . Instead the information needed to reconstruct the Householder transformations is saved. If the matrix Q is needed explicitly, the subroutine LQERR can be called after LQRRR. This routine accumulates Q from its factored form.

Before the decomposition is computed, initial columns are moved to the beginning of the array A and the final columns to the end. Both initial and final columns are frozen in place during the computation. Only free columns are pivoted. Pivoting, when requested, is done on the free columns of largest reduced norm.

Comments

1. Workspace may be explicitly provided, if desired, by use of L2RRR/DL2RRR. The reference is:

   CALL L2RRR (NRA, NCA, A, LDA, PIVOT, IPVT, QR, LDQR, QRAUX, CONORM, WORK)

   The additional argument is

   WORK — Work vector of length 2NCA − 1. Only NCA − 1 locations of WORK are referenced if PIVOT = .FALSE. .

2. LQRRR determines an orthogonal matrix Q, permutation matrix P, and an upper trapezoidal matrix R with diagonal elements of nonincreasing magnitude, such that $AP = QR$. The Householder transformation for column k, $k = 1, \ldots, \min(\mathrm{NRA}, \mathrm{NCA})$ is of the form

   $$I - u_k^{-1} u u^T$$

   where u has zeros in the first $k - 1$ positions. If the explicit matrix Q is needed, the user can call routine LQERR after calling LQRRR. This routine accumulates Q from its factored form.

3. Before the decomposition is computed, initial columns are moved to the beginning and the final columns to the end of the array A. Both initial and final columns are not moved during the computation. Only free columns are moved. Pivoting, if requested, is done on the free columns of largest reduced norm.

4. When pivoting has been selected by having entries of IPVT initialized to zero, an estimate of the condition number of A can be obtained from the output by computing the magnitude of the number QR(1, 1)/QR(K, K), where K = MIN(NRA, NCA). This estimate can be used to select the number of columns, KBASIS, used in the solution step computed with routine LQRSL.

ScaLAPACK Usage Notes

The arguments which differ from the standard version of this routine are:

A0 — MXLDA by MXCOL local matrix containing the local portions of the distributed matrix A. A contains the matrix whose *QR* factorization is to be computed. (Input)

QR0 — MXLDA by MXCOL local matrix containing the local portions of the distributed matrix QR. QR contains the information required for the *QR* factorization. (Output)
The upper trapezoidal part of *QR* contains the upper trapezoidal part of *R* with its diagonal elements ordered in decreasing magnitude. The strict lower trapezoidal part of *QR* contains information to recover the orthogonal matrix *Q* of the factorization. Arguments A and QR can occupy the same storage locations. In this case, A will not be preserved on output.

QRAUX0 — Real vector of length MXCOL containing the local portions of the distributed matrix QRAUX. QRAUX contains information about the orthogonal part of the decomposition in the first MIN(NRA, NCA) position. (Output)

IPVT0 — Integer vector of length MXLDB containing the local portions of the distributed vector IPVT. IPVT contains the information that controls the final order of the columns of the factored matrix A. (Input/Output)
On input, if IPVT(K) > 0, then the K-th column of A is an initial column. If IPVT(K) = 0, then the K-th column of A is a free column. If IPVT(K) < 0, then the K-th column of A is a final column. See Comments.
On output, IPVT(K) contains the index of the column of A that has been interchanged into the K-th column. This defines the permutation matrix *P*. The array IPVT is referenced only if PIVOT is equal to .TRUE.
Default: IPVT = 0.

All other arguments are global and are the same as described for the standard version of the routine. In the argument descriptions above, MXLDA, MXLDB, and MXCOL can be obtained through a call to SCALAPACK_GETDIM (see *Utilities*) after a call to SCALAPACK_SETUP (see *Utilities*) has been made. See the *ScaLAPACK Example* below.

Examples

Example

In various statistical algorithms it is necessary to compute $q = x^T(A^T A)^{-1}x$, where A is a rectangular matrix of full column rank. By using the *QR* decomposition, q can be computed without forming $A^T A$. Note that

$$A^T A = (QRP^{-1})^T(QRP^{-1}) = P^{-T} R^T (Q^T Q)RP^{-1} = P R^T RP^T$$

since Q is orthogonal ($Q^T Q = I$) and P is a permutation matrix. Let

$$Q^T AP = R = \begin{bmatrix} R_1 \\ 0 \end{bmatrix}$$

where R_1 is an upper triangular nonsingular matrix. Then

$$x^T \left(A^T A \right)^{-1} x = x^T P R_1^{-1} R_1^{-T} P^{-1} x = \left\| R_1^{-T} P^{-1} x \right\|_2^2$$

In the following program, first the vector $t = P^{-1} x$ is computed. Then

$$t := R_1^{-T} t$$

Finally,

$$q = \|t\|^2$$

```
      USE IMSL_LIBRARIES
!                                 Declare variables
      INTEGER    LDA, LDQR, NCA, NRA
      PARAMETER  (NCA=3, NRA=4, LDA=NRA, LDQR=NRA)
!                                 SPECIFICATIONS FOR PARAMETERS
      INTEGER    LDQ
      PARAMETER  (LDQ=NRA)
!                                 SPECIFICATIONS FOR LOCAL VARIABLES
      INTEGER    IPVT(NCA), NOUT
      REAL       CONORM(NCA), Q, QR(LDQR,NCA), QRAUX(NCA), T(NCA)
      LOGICAL    PIVOT
      REAL       A(LDA,NCA), X(NCA)
!
!                                 Set values for A
!
!                                 A = (  1    2     4   )
!                                     (  1    4    16   )
!                                     (  1    6    36   )
!                                     (  1    8    64   )
!
      DATA A/4*1.0, 2.0, 4.0, 6.0, 8.0, 4.0, 16.0, 36.0, 64.0/
!
!                                 Set values for X
!
!                                 X = (  1    2     3  )
      DATA X/1.0, 2.0, 3.0/
!
!                                 QR factorization
      PIVOT = .TRUE.
      IPVT=0
      CALL LQRRR (A, QR, QRAUX, pivot=pivot, IPVT=IPVT)
!                                 Set t = inv(P)*x
      CALL PERMU (X, IPVT, T, IPATH=1)
!                                 Compute t = inv(trans(R))*t
      CALL LSLRT (QR, T, T, IPATH=4)
!                                 Compute 2-norm of t, squared.
      Q = SDOT(NCA,T,1,T,1)
!                                 Print result
      CALL UMACH (2, NOUT)
      WRITE (NOUT,*) 'Q = ', Q
!
      END
```

Output

```
Q =    0.840624
```

ScaLAPACK Example

The previous example is repeated here as a distributed computing example. In various statistical algorithms it is necessary to compute $q = x^T(A^T A)^{-1}x$, where A is a rectangular matrix of full column rank. By using the QR decomposition, q can be computed without forming $A^T A$. Note that

$$A^T A = (QRP^{-1})^T(QRP^{-1}) = P^{-T}R^T(Q^TQ)RP^{-1} = P R^T R P^T$$

since Q is orthogonal ($Q^TQ = I$) and P is a permutation matrix. Let

$$Q^T AP = R = \begin{bmatrix} R_1 \\ 0 \end{bmatrix}$$

where R_1 is an upper triangular nonsingular matrix. Then

$$x^T\left(A^T A\right)^{-1} x = x^T P R_1^{-1} R_1^{-T} P^{-1} x = \left\|R_1^{-T} P^{-1} x\right\|_2^2$$

In the following program, first the vector $t = P^{-1} x$ is computed. Then

$$t := R_1{}^{-T} t$$

Finally,

$$q = \|t\|^2$$

`SCALAPACK_MAP` and `SCALAPACK_UNMAP` are IMSL utility routines (see *Utilities*) used to map and unmap arrays to and from the processor grid. They are used here for brevity. `DESCINIT` is a ScaLAPACK tools routine which initializes the descriptors for the local arrays.

```
      USE MPI_SETUP_INT
      USE LQRRR_INT
      USE PERMU_INT
      USE LSLRT_INT
      USE UMACH_INT
      USE SCALAPACK_SUPPORT
      IMPLICIT NONE
      INCLUDE 'mpif.h'
!                                   Declare variables
      INTEGER    LDA, LDQR, NCA, NRA, DESCA(9), DESCB(9), DESCL(9)
      INTEGER       INFO, MXCOL, MXLDA, MXLDB, MXCOLB, NOUT
      INTEGER, ALLOCATABLE ::      IPVT(:), IPVT0(:)
      LOGICAL       PIVOT
      REAL          Q
      REAL, ALLOCATABLE ::         A(:,:), X(:), T(:)
      REAL, ALLOCATABLE ::         A0(:,:), T0(:), QR0(:,:), QRAUX0(:)
      REAL, (KIND(1E0))SDOT
      PARAMETER  (NRA=4, NCA=3, LDA=NRA, LDQR=NRA)
!                                   Set up for MPI
```

```
      MP_NPROCS = MP_SETUP()
      IF(MP_RANK .EQ. 0) THEN
          ALLOCATE (A(LDA,NCA), X(NCA), T(NCA), IPVT(NCA))
!                                Set values for A and the righthand side
          A(1,:) = (/ 1.0,  2.0,   4.0/)
          A(2,:) = (/ 1.0,  4.0,  16.0/)
          A(3,:) = (/ 1.0,  6.0,  36.0/)
          A(4,:) = (/ 1.0,  8.0,  64.0/)
!
          X      = (/ 1.0,  2.0,   3.0/)
!
          IPVT = 0
      ENDIF
!                                 Set up a 1D processor grid and define
!                                 its context ID, MP_ICTXT
      CALL SCALAPACK_SETUP(NRA, NCA, .TRUE., .TRUE.)
!                                 Get the array descriptor entities MXLDA,
!                                 MXCOL, MXLDB, MXCOLB
      CALL SCALAPACK_GETDIM(NRA, NCA, MP_MB, MP_NB, MXLDA, MXCOL)
      CALL SCALAPACK_GETDIM(NCA, 1, MP_NB, 1, MXLDB, MXCOLB)
!                                 Set up the array descriptors
      CALL DESCINIT(DESCA, NRA, NCA, MP_MB, MP_NB, 0, 0, MP_ICTXT, MXLDA, &
      INFO)
      CALL DESCINIT(DESCL, 1, NCA, 1, MP_NB, 0, 0, MP_ICTXT, 1, INFO)
      CALL DESCINIT(DESCB, NCA, 1, MP_NB, 1, 0, 0, MP_ICTXT, MXLDB, &
      INFO)
!                                 Allocate space for the local arrays
      ALLOCATE (A0(MXLDA,MXCOL), QR0(MXLDA,MXCOL), QRAUX0(MXCOL), &
                IPVT0(MXCOL), T0(MXLDB))
!                                Map input array to the processor grid
      CALL SCALAPACK_MAP(A, DESCA, A0)
      PIVOT = .TRUE.

      CALL SCALAPACK_MAP(IPVT, DESCL, IPVT0)
!                                QR factorization
      CALL LQRRR (A0, QR0, QRAUX0, PIVOT=PIVOT, IPVT=IPVT0)
!                                Unmap the results from the distributed
!                                array back to a non-distributed array.
!                                After the unmap, only Rank=0 has the full
!                                array.
      CALL SCALAPACK_UNMAP(IPVT0, DESCL, IPVT, NCA, .FALSE.)
      IF(MP_RANK .EQ. 0) CALL PERMU (X, IPVT, T, IPATH=1)
      CALL SCALAPACK_MAP(T, DESCB, T0)
      CALL LSLRT (QR0, T0, T0, IPATH=4)
      CALL SCALAPACK_UNMAP(T0, DESCB, T)
!                               Print results.
!                               Only Rank=0 has the solution.
      IF(MP_RANK .EQ. 0)THEN
         Q = SDOT(NCA, T, 1, T, 1)
         CALL UMACH (2, NOUT)
         WRITE (NOUT, *) 'Q = ', Q
      ENDIF
!                               Exit ScaLAPACK usage
      CALL SCALAPACK_EXIT(MP_ICTXT)
!                               Shut down MPI
      MP_NPROCS = MP_SETUP('FINAL')
      END
```

Output

```
Q =    0.840624
```

LQERR

more...

more...

Accumulates the orthogonal matrix *Q* from its factored form given the *QR* factorization of a rectangular matrix *A*.

Required Arguments

QR — Real `NRQR` by `NCQR` matrix containing the factored form of the matrix `Q` in the first min(`NRQR`, `NCQR`) columns of the strict lower trapezoidal part of `QR` as output from subroutine `LQRRR`/`DLQRRR`. (Input)

QRAUX — Real vector of length `NCQR` containing information about the orthogonal part of the decomposition in the first min(`NRQR`, `NCQR`) position as output from routine `LQRRR`/`DLQRRR`. (Input)

Q — Real `NRQR` by `NRQR` matrix containing the accumulated orthogonal matrix `Q`; `Q` and `QR` can share the same storage locations if `QR` is not needed. (Output)

Optional Arguments

NRQR — Number of rows in `QR`. (Input)
Default: `NRQR` = size (`QR`,1).

NCQR — Number of columns in `QR`. (Input)
Default: `NCQR` = size (`QR`,2).

LDQR — Leading dimension of `QR` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDQR` = size (`QR`,1).

LDQ — Leading dimension of `Q` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDQ` = size (`Q`,1).

FORTRAN 90 Interface

Generic: `CALL LQERR (QR, QRAUX, Q [, …])`

Specific: The specific interface names are `S_LQERR` and `D_LQERR`.

FORTRAN 77 Interface

Single: `CALL LQERR (NRQR, NCQR, QR, LDQR, QRAUX, Q, LDQ)`

Double: The double precision name is `DLQERR`.

ScaLAPACK Interface

Generic: `CALL LQERR (QR0, QRAUX0, Q0 [, …])`

Specific: The specific interface names are `S_LQERR` and `D_LQERR`.

See the *ScaLAPACK Usage Notes* below for a description of the arguments for distributed computing.

Description

The routine `LQERR` accumulates the Householder transformations computed by IMSL routine `LQRRR` to produce the orthogonal matrix *Q*.

The underlying code is based on either LINPACK , LAPACK, or ScaLAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see *Using ScaLAPACK, LAPACK, LINPACK, and EISPACK* in the Introduction section of this manual.

Comments

1. Workspace may be explicitly provided, if desired, by use of `L2ERR/DL2ERR`. The reference is:

   `CALL L2ERR (NRQR, NCQR, QR, LDQR, QRAUX, Q, LDQ, WK)`

   The additional argument is

   WK — Work vector of length 2 * `NRQR`.

ScaLAPACK Usage Notes

The arguments which differ from the standard version of this routine are:

QR0 — MXLDA by MXCOL local matrix containing the local portions of the distributed matrix QR. QR contains the factored form of the matrix Q in the first min(NRQR, NCQR) columns of the strict lower trapezoidal part of QR as output from subroutine LQRRR/DLQRRR. (Input)

QRAUX0 — Real vector of length MXCOL containing the local portions of the distributed matrix QRAUX. QRAUX contains the information about the orthogonal part of the decomposition in the first min(NRA, NCA) positions as output from subroutine LQRRR/DLQRRR. (Input)

Q0 — MXLDA by MXLDA local matrix containing the local portions of the distributed matrix Q. Q contains the accumulated orthogonal matrix ; Q and QR can share the same storage locations if QR is not needed. (Output)

All other arguments are global and are the same as described for the standard version of the routine. In the argument descriptions above, MXLDA and MXCOL can be obtained through a call to SCALAPACK_GETDIM (see *Utilities*) after a call to SCALAPACK_SETUP (see *Utilities*) has been made. See the *ScaLAPACK Example* below.

Examples

Example 1

In this example, the orthogonal matrix *Q* in the *QR* decomposition of a matrix *A* is computed. The product *X* = *QR* is also computed. Note that *X* can be obtained from *A* by reordering the columns of *A* according to IPVT.

```
      USE IMSL_LIBRARIES
!                                 Declare variables
      INTEGER    LDA, LDQ, LDQR, NCA, NRA
      PARAMETER  (NCA=3, NRA=4, LDA=NRA, LDQ=NRA, LDQR=NRA)
!
      INTEGER    IPVT(NCA), J
      REAL       A(LDA,NCA), CONORM(NCA), Q(LDQ,NRA), QR(LDQR,NCA), &
                 QRAUX(NCA), R(NRA,NCA), X(NRA,NCA)
      LOGICAL    PIVOT
!
!                                 Set values for A
!
!                                 A = (  1    2     4   )
!                                     (  1    4    16   )
!                                     (  1    6    36   )
!                                     (  1    8    64   )
!
      DATA A/4*1.0, 2.0, 4.0, 6.0, 8.0, 4.0, 16.0, 36.0, 64.0/
!
!                                 QR factorization
!                                 Set IPVT = 0 (all columns free)
      IPVT = 0
      PIVOT = .TRUE.
      CALL LQRRR (A, QR, QRAUX, IPVT=IPVT, PIVOT=PIVOT)
!                                 Accumulate Q
      CALL LQERR (QR, QRAUX, Q)
!                                 R is the upper trapezoidal part of QR
      R = 0.0E0
      DO 10  J=1, NCA
         CALL SCOPY (J, QR(:,J), 1, R(:,J), 1)
```

```
   10 CONTINUE
!                                 Compute X = Q*R
      CALL MRRRR (Q, R, X)
!                                 Print results
      CALL WRIRN ('IPVT', IPVT, 1, NCA, 1)
      CALL WRRRN ('Q', Q)
      CALL WRRRN ('R', R)
      CALL WRRRN ('X = Q*R', X)
!
      END
```

Output

```
   IPVT
 1   2   3
 3   2   1
                 Q
         1         2         3         4
1  -0.0531  -0.5422   0.8082  -0.2236
2  -0.2126  -0.6574  -0.2694   0.6708
3  -0.4783  -0.3458  -0.4490  -0.6708
4  -0.8504   0.3928   0.2694   0.2236

            R
        1        2        3
1  -75.26  -10.63   -1.59
2    0.00   -2.65   -1.15
3    0.00    0.00    0.36
4    0.00    0.00    0.00

          X = Q*R
        1        2        3
1    4.00     2.00     1.00
2   16.00     4.00     1.00
3   36.00     6.00     1.00
4   64.00     8.00     1.00
```

ScaLAPACK Example

In this example, the orthogonal matrix *Q* in the *QR* decomposition of a matrix *A* is computed. `SCALAPACK_MAP` and `SCALAPACK_UNMAP` are IMSL utility routines (see *Utilities*) used to map and unmap arrays to and from the processor grid. They are used here for brevity. `DESCINIT` is a ScaLAPACK tools routine which initializes the descriptors for the local arrays.

```
      USE MPI_SETUP_INT
      USE LQRRR_INT
      USE LQERR_INT
      USE WRRRN_INT
      USE SCALAPACK_SUPPORT
      IMPLICIT NONE
      INCLUDE 'mpif.h'
!                                 Declare variables
      INTEGER    LDA, LDQR, NCA, NRA, DESCA(9), DESCL(9), DESCQ(9)
      INTEGER       INFO, MXCOL, MXLDA, LDQ
      INTEGER, ALLOCATABLE ::     IPVT(:), IPVT0(:)
      LOGICAL       PIVOT
      REAL, ALLOCATABLE ::        A(:,:), QR(:,:), Q(:,:), QRAUX(:)
      REAL, ALLOCATABLE ::        A0(:,:), QR0(:,:), Q0(:,:), QRAUX0(:)
      PARAMETER  (NRA=4, NCA=3, LDA=NRA, LDQR=NRA, LDQ=NRA)
!                                 Set up for MPI
      MP_NPROCS = MP_SETUP()
```

```
      IF(MP_RANK .EQ. 0) THEN
          ALLOCATE (A(NRA,NCA), Q(NRA,NRA), QR(NRA,NCA), &
          QRAUX(NCA), IPVT(NCA))
!                                 Set values for A and the righthand sides
          A(1,:) = (/ 1.0,  2.0,   4.0/)
          A(2,:) = (/ 1.0,  4.0,  16.0/)
          A(3,:) = (/ 1.0,  6.0,  36.0/)
          A(4,:) = (/ 1.0,  8.0,  64.0/)
!
          IPVT = 0
      ENDIF
!                                  Set up a 1D processor grid and define
!                                  its context ID, MP_ICTXT
      CALL SCALAPACK_SETUP(NRA, NCA, .FALSE., .TRUE.)
!                                  Get the array descriptor entities MXLDA,
!                                  and MXCOL
      CALL SCALAPACK_GETDIM(NRA, NCA, MP_MB, MP_NB, MXLDA, MXCOL)
!                                  Set up the array descriptors
      CALL DESCINIT(DESCA, NRA, NCA, MP_MB, MP_NB, 0, 0, MP_ICTXT, MXLDA, &
      INFO)
      CALL DESCINIT(DESCL, 1, NCA, 1, MP_NB, 0, 0, MP_ICTXT, 1, INFO)
      CALL DESCINIT(DESCQ, NRA, NRA, MP_MB, MP_NB, 0, 0, MP_ICTXT, MXLDA, &
      INFO)
!                                  Allocate space for the local arrays
      ALLOCATE (A0(MXLDA,MXCOL), QR0(MXLDA,MXCOL), QRAUX0(MXCOL), &
                IPVT0(MXCOL), Q0(MXLDA,MXLDA))
!                                 Map input array to the processor grid
      CALL SCALAPACK_MAP(A, DESCA, A0)
      PIVOT = .TRUE.

      CALL SCALAPACK_MAP(IPVT, DESCL, IPVT0)
!                                 QR factorization
      CALL LQRRR (A0, QR0, QRAUX0, PIVOT=PIVOT, IPVT=IPVT0)
      CALL LQERR (QR0, QRAUX0, Q0)
!                                 Unmap the results from the distributed
!                                 array back to a non-distributed array.
!                                 After the unmap, only Rank=0 has the full
!                                 array.
      CALL SCALAPACK_UNMAP(Q0, DESCQ, Q)
!                                 Print results.
!                                 Only Rank=0 has the solution, Q.
      IF(MP_RANK .EQ. 0) CALL WRRRN ('Q', Q)
!                                Exit Scalapack usage
      CALL SCALAPACK_EXIT(MP_ICTXT)
!                                Shut down MPI
      MP_NPROCS = MP_SETUP('FINAL')
      END
```

LQRSL

more...

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Computes the coordinate transformation, projection, and complete the solution of the least-squares problem $Ax = b$.

Required Arguments

KBASIS — Number of columns of the submatrix A_k of *A*. (Input)
The value KBASIS must not exceed min(NRA, NCA), where NCA is the number of columns in matrix *A*. The value NCA is an argument to routine LQRRR. The value of KBASIS is normally NCA unless the matrix is rank-deficient. The user must analyze the problem data and determine the value of KBASIS. See Comments.

QR — NRA by NCA array containing information about the *QR* factorization of *A* as output from routine LQRRR/DLQRRR. (Input)

QRAUX — Vector of length NCA containing information about the *QR* factorization of *A* as output from routine LQRRR/DLQRRR. (Input)

B — Vector *b* of length NRA to be manipulated. (Input)

IPATH — Option parameter specifying what is to be computed. (Input)
The value IPATH has the decimal expansion IJKLM, such that:
I ≠ 0 means compute Qb;
J ≠ 0 means compute $Q^T b$;
K ≠ 0 means compute Q^Tb and x;
L ≠ 0 means compute Q^Tb and $b - Ax$;
M ≠ 0 means compute $Q^T b$ and Ax.

For example, if the decimal number IPATH = 01101, then I = 0, J = 1, K = 1, L = 0, and M = 1.

Optional Arguments

NRA — Number of rows of matrix *A*. (Input)
Default: NRA = size (QR,1).

LDQR — Leading dimension of *QR* exactly as specified in the dimension statement of the calling program. (Input)
Default: LDQR = size (QR,1).

QB — Vector of length NRA containing *Qb* if requested in the option IPATH. (Output)

QTB — Vector of length NRA containing $Q^T b$ if requested in the option IPATH. (Output)

X — Vector of length KBASIS containing the solution of the least-squares problem $A_k x = b$, if this is requested in the option IPATH. (Output)
If pivoting was requested in routine LQRRR/DLQRRR, then the J-th entry of X will be associated with column IPVT(J) of the original matrix *A*. See Comments.

RES — Vector of length NRA containing the residuals $(b - Ax)$ of the least-squares problem if requested in the option IPATH. (Output)
This vector is the orthogonal projection of *b* onto the orthogonal complement of the column space of *A*.

AX — Vector of length NRA containing the least-squares approximation *Ax* if requested in the option IPATH. (Output)
This vector is the orthogonal projection of *b* onto the column space of *A*.

FORTRAN 90 Interface

Generic: CALL LQRSL (KBASIS, QR, QRAUX, B, IPATH [, …])

Specific: The specific interface names are S_LQRSL and D_LQRSL.

FORTRAN 77 Interface

Single: CALL LQRSL (NRA, KBASIS, QR, LDQR, QRAUX, B, IPATH, QB, QTB, X, RES, AX)

Double: The double precision name is DLQRSL.

ScaLAPACK Interface

Generic: CALL LQRSL (KBASIS, QR0, QRAUX0, B0, IPATH [, …])

Specific: The specific interface names are S_LQRSL and D_LQRSL.

See the *ScaLAPACK Usage Notes* below for a description of the arguments for distributed computing.

Description

The underlying code of routine LQRSL is based on either LINPACK , LAPACK, or ScaLAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see *Using ScaLAPACK, LAPACK, LINPACK, and EISPACK* in the Introduction section of this manual.

The most important use of LQRSL is for solving the least-squares problem $Ax = b$, with coefficient matrix A and data vector b. This problem can be formulated, using the *normal equations* method, as $A^T Ax = A^Tb$. Using LQRRR the QR decomposition of A, $AP = QR$, is computed. Here P is a permutation matrix ($P = P$), Q is an orthogonal matrix ($Q = Q^T$) and R is an upper trapezoidal matrix. The normal equations can then be written as

$$(PR^T)(Q^TQ)R(P^Tx) = (PR^T)Q^T b$$

If A^TA is nonsingular, then R is also nonsingular and the normal equations can be written as $R(P^Tx) = Q^Tb$. LQRSL can be used to compute $Q^T b$ and then solve for $P^T x$. Note that the *permuted* solution is returned.

The routine LQRSL can also be used to compute the least-squares residual, $b - Ax$. This is the projection of b onto the orthogonal complement of the column space of A. It can also compute Qb, Q^Tb and Ax, the orthogonal projection of x onto the column space of A.

Comments

1. Informational error

Type	Code	Description
4	1	Computation of the least-squares solution of AK * X = B is requested, but the upper triangular matrix R from the *QR* factorization is singular.

2. This routine is designed to be used together with LQRRR. It assumes that LQRRR/DLQRR has been called to get QR, QRAUX and IPVT. The submatrix A_k mentioned above is actually equal to A_k = (A(IPVT(1)), A(IPVT(2)), …, A(IPVT (KBASIS))), where A(IPVT(I)) is the IPVT(I)-th column of the original matrix.

ScaLAPACK Usage Notes

The arguments which differ from the standard version of this routine are:

QR0 — MXLDA by MXCOL local matrix containing the local portions of the distributed matrix QR. QR contains the factored form of the matrix Q in the first min(NRQR, NCQR) columns of the strict lower trapezoidal part of QR as output from subroutine LQRRR/DLQRRR. (Input)

QRAUX0 — Real vector of length MXCOL containing the local portions of the distributed matrix QRAUX. QRAUX contains the information about the orthogonal part of the decomposition in the first min(NRA, NCA) positions as output from subroutine LQRRR/DLQRRR. (Input)

B0 — Real vector of length MXLDA containing the local portions of the distributed vector B. B contains the vector to be manipulated. (Input)

QB0 — Real vector of length MXLDA containing the local portions of the distributed vector Qb if requested in the option IPATH. (Output)

QTB0 — Real vector of length MXLDA containing the local portions of the distributed vector $Q^T b$ if requested in the option IPATH. (Output)

X0 — Real vector of length MXLDX containing the local portions of the distributed vector X. X contains the solution of the least-squares problem $A_k x = b$, if this is requested in the option IPATH. (Output)
If pivoting was requested in routine LQRRR/DLQRRR, then the J-th entry of X will be associated with column IPVT(J) of the original matrix A. See Comments.

RES0 — Real vector of length MXLDA containing the local portions of the distributed vector RES. RES contains the residuals ($b - Ax$) of the least-squares problem if requested in the option IPATH. (Output)
This vector is the orthogonal projection of b onto the orthogonal complement of the column space of A.

AX0 — Real vector of length MXLDA containing the local portions of the distributed vector AX. AX contains the least-squares approximation Ax if requested in the option IPATH. (Output)
This vector is the orthogonal projection of b onto the column space of A.

All other arguments are global and are the same as described for the standard version of the routine. In the argument descriptions above, MXLDA, MXLDX and MXCOL can be obtained through a call to SCALAPACK_GETDIM (see *Utilities*) after a call to SCALAPACK_SETUP (see *Utilities*) has been made. See the *ScaLAPACK Example* below.

Examples

Example 1

Consider the problem of finding the coefficients c_i in

$$f(x) = c_0 + c_1 x + c_2 x_2$$

given data at $x_i = 2_i$, i = 1, 2, 3, 4, using the method of least squares. The row of the matrix A contains the value of 1, x_i and x_i^2 at the data points. The vector b contains the data. The routine LQRRR is used to compute the QR decomposition of A. Then LQRSL is then used to solve the least-squares problem and compute the residual vector.

```
      USE IMSL_LIBRARIES
!                                 Declare variables
      PARAMETER  (NRA=4, NCA=3, KBASIS=3, LDA=NRA, LDQR=NRA)
      INTEGER    IPVT(NCA)
      REAL       A(LDA,NCA), QR(LDQR,NCA), QRAUX(NCA), CONORM(NCA), &
                 X(KBASIS), QB(1), QTB(NRA), RES(NRA), &
                 AX(1), B(NRA)
      LOGICAL    PIVOT
!
!                                 Set values for A
!
!                                 A = (  1    2     4   )
!                                     (  1    4    16   )
!                                     (  1    6    36   )
!                                     (  1    8    64   )
!
      DATA A/4*1.0, 2.0, 4.0, 6.0, 8.0, 4.0, 16.0, 36.0, 64.0/
!
!                                 Set values for B
!
!                                 B = ( 16.99  57.01  120.99  209.01 )
      DATA B/ 16.99,  57.01,  120.99,  209.01 /
!
!                                 QR factorization
      PIVOT = .TRUE.
      IPVT = 0
      CALL LQRRR (A, QR, QRAUX, PIVOT=PIVOT, IPVT=IPVT)
!                                 Solve the least squares problem
      IPATH = 00110
      CALL LQRSL (KBASIS, QR, QRAUX, B, IPATH, X=X, RES=RES)
!                                 Print results
      CALL WRIRN ('IPVT', IPVT, 1, NCA, 1)
      CALL WRRRN ('X', X, 1, KBASIS, 1)
      CALL WRRRN ('RES', RES, 1, NRA, 1)
!
      END
```

Output

```
   IPVT
 1   2   3
 3   2   1

          X
    1        2        3
3.000    2.002    0.990

                    RES
      1          2          3          4
-0.00400    0.01200   -0.01200    0.00400
```

Note that since IPVT is (3, 2, 1) the array X contains the solution coefficients c_i in reverse order.

ScaLAPACK Example

The previous example is repeated here as a distributed example. Consider the problem of finding the coefficients c_i in

$$f(x) = c_0 + c_1x + c_2x_2$$

given data at $x_i = 2_i$, $i = 1, 2, 3, 4$, using the method of least squares. The row of the matrix A contains the value of 1, x_i and x_i^2 at the data points. The vector b contains the data. The routine `LQRRR` is used to compute the QR decomposition of A. Then `LQRSL` is then used to solve the least-squares problem and compute the residual vector. `SCALAPACK_MAP` and `SCALAPACK_UNMAP` are IMSL utility routines (see *Utilities*) used to map and unmap arrays to and from the processor grid. They are used here for brevity. `DESCINIT` is a ScaLAPACK tools routine which initializes the descriptors for the local arrays.

```
      USE MPI_SETUP_INT
      USE LQRRR_INT
      USE LQRSL_INT
      USE WRIRN_INT
      USE WRRRN_INT
      USE SCALAPACK_SUPPORT
      IMPLICIT NONE
      INCLUDE 'mpif.h'
!                                  Declare variables
      INTEGER       KBASIS, LDA, LDQR, NCA, NRA, DESCA(9), DESCL(9), &
                    DESCX(9), DESCB(9)
      INTEGER       INFO, MXCOL, MXCOLX, MXLDA, MXLDX, LDQ, IPATH
      INTEGER, ALLOCATABLE ::      IPVT(:), IPVT0(:)
      REAL, ALLOCATABLE ::         A(:,:), B(:), QR(:,:), QRAUX(:), X(:), &
                                   RES(:)
      REAL, ALLOCATABLE ::         A0(:,:), QR0(:,:), QRAUX0(:), X0(:), &
                                   RES0(:), B0(:), QTB0(:)
      LOGICAL        PIVOT
      PARAMETER  (NRA=4, NCA=3, LDA=NRA, LDQR=NRA, KBASIS=3)
!                                  Set up for MPI
      MP_NPROCS = MP_SETUP()
      IF(MP_RANK .EQ. 0) THEN
          ALLOCATE (A(LDA,NCA), B(NRA), QR(LDQR,NCA), &
          QRAUX(NCA), IPVT(NCA), X(NCA), RES(NRA))
!                                  Set values for A and the righthand sides
          A(1,:) = (/ 1.0,  2.0,   4.0/)
          A(2,:) = (/ 1.0,  4.0,  16.0/)
          A(3,:) = (/ 1.0,  6.0,  36.0/)
          A(4,:) = (/ 1.0,  8.0,  64.0/)
!
          B      = (/ 16.99, 57.01, 120.99, 209.01 /)
!
          IPVT = 0
      ENDIF
!                                   Set up a 1D processor grid and define
!                                   its context ID, MP_ICTXT
      CALL SCALAPACK_SETUP(NRA, NCA, .TRUE., .TRUE.)
!                                   Get the array descriptor entities MXLDA,
!                                   and MXCOL
      CALL SCALAPACK_GETDIM(NRA, NCA, MP_MB, MP_NB, MXLDA, MXCOL)
      CALL SCALAPACK_GETDIM(KBASIS, 1, MP_NB, 1, MXLDX, MXCOLX)
!                                   Set up the array descriptors
      CALL DESCINIT(DESCA, NRA, NCA, MP_MB, MP_NB, 0, 0, MP_ICTXT, &
                    MXLDA,INFO)
      CALL DESCINIT(DESCL, 1, NCA, 1, MP_NB, 0, 0, MP_ICTXT, 1, INFO)
```

```
      CALL DESCINIT(DESCX, KBASIS, 1, MP_NB, 1, 0, 0, MP_ICTXT, MXLDX, INFO)
      CALL DESCINIT(DESCB, NRA, 1, MP_MB, 1, 0, 0, MP_ICTXT, MXLDA, INFO)
!                               Allocate space for the local arrays
      ALLOCATE (A0(MXLDA,MXCOL), QR0(MXLDA,MXCOL), QRAUX0(MXCOL), &
      IPVT0(MXCOL), B0(MXLDA), X0(MXLDX), RES0(MXLDA), QTB0(MXLDA))
!                              Map input array to the processor grid
      CALL SCALAPACK_MAP(A, DESCA, A0)
      CALL SCALAPACK_MAP(B, DESCB, B0)
      PIVOT = .TRUE.
      CALL SCALAPACK_MAP(IPVT, DESCL, IPVT0)
!                              QR factorization
      CALL LQRRR (A0, QR0, QRAUX0, PIVOT=PIVOT, IPVT=IPVT0)
      IPATH = 00110
      CALL LQRSL (KBASIS, QR0, QRAUX0, B0, IPATH, QTB=QTB0, X=X0, RES=RES0)
!                              Unmap the results from the distributed
!                              array back to a non-distributed array.
!                              After the unmap, only Rank=0 has the full
!                              array.
      CALL SCALAPACK_UNMAP(IPVT0, DESCL, IPVT, NCA, .FALSE.)
      CALL SCALAPACK_UNMAP(X0, DESCX, X)
      CALL SCALAPACK_UNMAP(RES0, DESCB, RES)
!                              Print results.
!                              Only Rank=0 has the solution, X.
      IF(MP_RANK .EQ. 0) THEN
         CALL WRIRN ('IPVT', IPVT, 1, NCA, 1)
         CALL WRRRN ('X', X, 1, KBASIS, 1)
         CALL WRRRN ('RES', RES, 1, NRA, 1)
      ENDIF

!                             Exit ScaLAPACK usage
      CALL SCALAPACK_EXIT(MP_ICTXT)
!                             Shut down MPI
      MP_NPROCS = MP_SETUP('FINAL')
      END
```

Output

```
   IPVT
 1   2   3
 3   2   1

          X
    1       2       3
3.000   2.002   0.990

                     RES
      1         2         3         4
-0.00400   0.01200  -0.01200   0.00400
```

Note that since `IPVT` is (3, 2, 1) the array X contains the solution coefficients c_i in reverse order.

LUPQR

Computes an updated QR factorization after the rank-one matrix αxy^T is added.

Required Arguments

ALPHA — Scalar determining the rank-one update to be added. (Input)

W — Vector of length `NROW` determining the rank-one matrix to be added. (Input)
The updated matrix is $A + \alpha xy^T$. If `I` = 0 then W contains the vector x. If `I` = 1 then W contains the vector $Q^T x$.

Y — Vector of length `NCOL` determining the rank-one matrix to be added. (Input)

R — Matrix of order `NROW` by `NCOL` containing the R matrix from the QR factorization. (Input)
Only the upper trapezoidal part of `R` is referenced.

IPATH — Flag used to control the computation of the QR update. (Input)
`IPATH` has the decimal expansion `IJ` such that: `I` = 0 means W contains the vector x.
`I`= 1 means `W` contains the vector $Q^T x$.
`J` = 0 means do not update the matrix `Q`. `J` = 1 means update the matrix Q. For example, if `IPATH` = 10 then, `I` = 1 and `J` = 0.

RNEW — Matrix of order `NROW` by `NCOL` containing the updated `R` matrix in the QR factorization. (Output)
Only the upper trapezoidal part of `RNEW` is updated. `R` and `RNEW` may be the same.

Optional Arguments

NROW — Number of rows in the matrix $A = Q * R$. (Input)
Default: `NROW` = size (`W`,1).

NCOL — Number of columns in the matrix $A = Q * R$. (Input)
Default: `NCOL` = size (`Y`,1).

Q — Matrix of order `NROW` containing the Q matrix from the QR factorization. (Input)
Ignored if `IPATH` = 0.
Default: `Q` is 1x1 and un-initialized.

LDQ — Leading dimension of Q exactly as specified in the dimension statement of the calling program. (Input)
Ignored if IPATH = 0.
Default: LDQ = size (Q,1).

LDR — Leading dimension of R exactly as specified in the dimension statement of the calling program. (Input)
Default: LDR = size (R,1).

QNEW — Matrix of order NROW containing the updated Q matrix in the *QR* factorization. (Output)
Ignored if J = 0. See IPATH for a definition of J.

LDQNEW — Leading dimension of QNEW exactly as specified in the dimension statement of the calling program. (Input)
Ignored if J = 0. See IPATH for a definition of J.
Default: LDQNEW = size (QNEW,1).

LDRNEW — Leading dimension of RNEW exactly as specified in the dimension statement of the calling program. (Input)
Default: LDRNEW = size (RNEW,1).

FORTRAN 90 Interface

Generic: CALL LUPQR (ALPHA, W, Y, R, IPATH, RNEW [, …])

Specific: The specific interface names are S_LUPQR and D_LUPQR.

FORTRAN 77 Interface

Single: CALL LUPQR (NROW, NCOL, ALPHA, W, Y, Q, LDQ, R, LDR, IPATH, QNEW, LDQNEW, RNEW, LDRNEW)

Double: The double precision name is DLUPQR.

Description

Let A be an $m \times n$ matrix and let $A = QR$ be its QR decomposition. (In the program, m is called NROW and n is called NCOL) Then

$$A + \alpha x y^T = QR + \alpha x y^T = Q(R + \alpha Q^T x y^T) = Q(R + \alpha w y^T)$$

where $w = Q^T x$. An orthogonal transformation J can be constructed, using a sequence of $m - 1$ Givens rotations, such that $Jw = \omega e_1$, where $\omega = \pm\|w\|_2$ and $e_1 = (1, 0, \ldots, 0)^T$. Then

$$A + \alpha xy^T = (QJ^T)(JR + \alpha\omega e_1 y^T)$$

Since JR is an upper Hessenberg matrix, $H = JR + \alpha\omega e_1 y^T$ is also an upper Hessenberg matrix. Again using $m - 1$ Givens rotations, an orthogonal transformation G can be constructed such that GH is an upper triangular matrix. Then

$$A + \alpha xy^T = \tilde{Q}\tilde{R}, \text{ where } \tilde{Q} = QJ^T G^T$$

is orthogonal and

$$\tilde{R} = GH$$

is upper triangular.

If the last k components of w are zero, then the number of Givens rotations needed to construct J or G is $m - k - 1$ instead of $m - 1$.

For further information, see Dennis and Schnabel (1983, pages 55–58 and 311–313), or Golub and Van Loan (1983, pages 437– 439).

Comments

1. Workspace may be explicitly provided, if desired, by use of L2PQR/DL2PQR. The reference is:

   CALL L2PQR (NROW, NCOL, ALPHA, W, Y, Q, LDQ, R, LDR, IPATH, QNEW, LDQNEW, RNEW, LDRNEW, Z, WORK)

   The additional arguments are as follows:

   Z — Work vector of length NROW.

   WORK — Work vector of length MIN(NROW − 1, NCOL).

Example

The QR factorization of A is found. It is then used to find the QR factorization of $A + xy^T$. Since pivoting is used, the QR factorization routine finds $AP = QR$, where P is a permutation matrix determined by IPVT. We compute

$$AP + \alpha xy^T = \left(A + \alpha x\left(Py\right)^T\right)P = \tilde{Q}\tilde{R}$$

The IMSL routine PERMU (see *Utilities*) is used to compute Py. As a check

$$\tilde{Q}\tilde{R}$$

is computed and printed. It can also be obtained from $A + xy^T$ by permuting its columns using the order given by IPVT.

```
      USE IMSL_LIBRARIES
!                                 Declare variables
      INTEGER    LDA, LDAQR, LDQ, LDQNEW, LDQR, LDR, LDRNEW, NCOL, NROW
      PARAMETER  (NCOL=3, NROW=4, LDA=NROW, LDAQR=NROW, LDQ=NROW, &
                 LDQNEW=NROW, LDQR=NROW, LDR=NROW, LDRNEW=NROW)
!
      INTEGER    IPATH, IPVT(NCOL), J, MIN0
      REAL       A(LDA,NCOL), ALPHA, AQR(LDAQR,NCOL), CONORM(NCOL), &
                 Q(LDQ,NROW), QNEW(LDQNEW,NROW), QR(LDQR,NCOL), &
                 QRAUX(NCOL), R(LDR,NCOL), RNEW(LDRNEW,NCOL), W(NROW), &
                 Y(NCOL)
      LOGICAL    PIVOT
      INTRINSIC  MIN0
!
!                                 Set values for A
!
!                                 A = (  1    2     4   )
!                                     (  1    4    16   )
!                                     (  1    6    36   )
!                                     (  1    8    64   )
!
      DATA A/4*1.0, 2.0, 4.0, 6.0, 8.0, 4.0, 16.0, 36.0, 64.0/
!                                 Set values for W and Y
      DATA W/1., 2., 3., 4./
      DATA Y/3., 2., 1./
!
!                                 QR factorization
!                                 Set IPVT = 0 (all columns free)
      IPVT = 0
      PIVOT = .TRUE.
      CALL LQRRR (A, QR, QRAUX, IPVT=IPVT, PIVOT=PIVOT)
!                                 Accumulate Q
      CALL LQERR (QR, QRAUX, Q)
!                                 Permute Y
      CALL PERMU (Y, IPVT, Y)
!                                 R is the upper trapezoidal part of QR
      R = 0.0E0
      DO 10  J=1, NCOL
         CALL SCOPY (MIN0(J,NROW), QR(:,J), 1, R(:,J), 1)
   10 CONTINUE
!                                 Update Q and R
      ALPHA = 1.0
      IPATH = 01
      CALL LUPQR (ALPHA, W, Y, R, IPATH, RNEW, Q=Q, QNEW=QNEW)
!                                 Compute AQR = Q*R
      CALL MRRRR (QNEW, RNEW, AQR)
!                                 Print results
      CALL WRIRN ('IPVT', IPVT, 1, NCOL,1)
      CALL WRRRN ('QNEW', QNEW)
      CALL WRRRN ('RNEW', RNEW)
      CALL WRRRN ('QNEW*RNEW', AQR)
      END
```

Output

```
   IPVT
 1   2   3
 3   2   1

             QNEW
         1         2         3         4
1  -0.0620  -0.5412   0.8082  -0.2236
2  -0.2234  -0.6539  -0.2694   0.6708
3  -0.4840  -0.3379  -0.4490  -0.6708
```

```
  4  -0.8438   0.4067   0.2694   0.2236

             RNEW
           1        2        3
  1  -80.59  -21.34  -17.62
  2    0.00   -4.94   -4.83
  3    0.00    0.00    0.36
  4    0.00    0.00    0.00

           QNEW*RNEW
           1        2        3
  1    5.00    4.00    4.00
  2   18.00    8.00    7.00
  3   39.00   12.00   10.00
  4   68.00   16.00   13.00
```

LCHRG

Computes the Cholesky decomposition of a symmetric positive definite matrix with optional column pivoting.

Required Arguments

A — N by N symmetric positive definite matrix to be decomposed. (Input)
Only the upper triangle of A is referenced.

FACT — N by N matrix containing the Cholesky factor of the permuted matrix in its upper triangle. (Output)
If A is not needed, A and FACT can share the same storage locations.

Optional Arguments

N — Order of the matrix A. (Input)
Default: N = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

PIVOT — Logical variable. (Input)
PIVOT = .TRUE. means column pivoting is done. PIVOT = .FALSE. means no pivoting is done.
Default: PIVOT = .TRUE.

IPVT — Integer vector of length N containing information that controls the selection of the pivot columns. (Input/Output)
On input, if IPVT(*K*) > 0, then the *K*-th column of A is an initial column; if IPVT(*K*) = 0, then the *K*-th column of A is a free column; if IPVT(*K*) < 0, then the *K*-th column of A is a final column. See Comments. On output, IPVT(*K*) contains the index of the diagonal element of A that was moved into the *K*-th position. IPVT is only referenced when PIVOT is equal to .TRUE..

LDFACT — Leading dimension of FACT exactly as specified in the dimension statement of the calling program. (Input)
Default: LDFACT = size (FACT,1).

FORTRAN 90 Interface

Generic: `CALL LCHRG (A, FACT [, …])`

Specific: The specific interface names are `S_LCHRG` and `D_LCHRG`.

FORTRAN 77 Interface

Single: `CALL LCHRG (N, A, LDA, PIVOT, IPVT, FACT, LDFACT)`

Double: The double precision name is `DLCHRG`.

Description

Routine `LCHRG` is based on the LINPACK routine `SCHDC`; see Dongarra et al. (1979).

Before the decomposition is computed, initial elements are moved to the leading part of *A* and final elements to the trailing part of *A*. During the decomposition only rows and columns corresponding to the free elements are moved. The result of the decomposition is an upper triangular matrix *R* and a permutation matrix *P* that satisfy $P^T AP = R^T R$, where *P* is represented by `IPVT`.

Comments

1. Informational error

Type	Code	Description
4	1	The input matrix is not positive definite.

2. Before the decomposition is computed, initial elements are moved to the leading part of `A` and final elements to the trailing part of `A`. During the decomposition only rows and columns corresponding to the free elements are moved. The result of the decomposition is an upper triangular matrix `R` and a permutation matrix `P` that satisfy $P^T AP = R^T R$, where `P` is represented by `IPVT`.

3. `LCHRG` can be used together with subroutines `PERMU` and `LSLDS` to solve the positive definite linear system `AX` = `B` with the solution *X* overwriting the right-hand side *B* as follows:

```
CALL ISET  (N, 0, IPVT, 1)
CALL LCHRG (A, FACT, N, LDA,.TRUE, IPVT, LDFACT)
CALL PERMU (B, IPVT, B, N, 1)
CALL LSLDS (FACT, B, B, N, LDFACT)
CALL PERMU (B, IPVT, B, N, 2)
```

Example

Routine LCHRG can be used together with the IMSL routines PERMU (see *Chapter 11*) and LFSDS to solve a positive definite linear system $Ax = b$. Since $A = PR^T RP$, the system $Ax = b$ is equivalent to $R^T R(Px) = Pb$. LFSDS is used to solve $R^T Ry = Pb$ for y. The routine PERMU is used to compute both Pb and $x = Py$.

```
      USE IMSL_LIBRARIES
!                                 Declare variables
      PARAMETER  (N=3, LDA=N, LDFACT=N)
      INTEGER    IPVT(N)
      REAL       A(LDA,N), FACT(LDFACT,N), B(N), X(N)
      LOGICAL    PIVOT
!
!                                 Set values for A and B
!
!                                 A = (   1   -3   2  )
!                                     (  -3   10  -5  )
!                                     (   2   -5   6  )
!
!                                 B = (  27  -78  64  )
!
      DATA A/1.,-3.,2.,-3.,10.,-5.,2.,-5.,6./
      DATA B/27.,-78.,64./
!                                 Pivot using all columns
      PIVOT = .TRUE.
      IPVT = 0
!                                 Compute Cholesky factorization
      CALL LCHRG (A, FACT, PIVOT=PIVOT, IPVT=IPVT)
!                                 Permute B and store in X
      CALL PERMU (B, IPVT, X, IPATH=1)
!                                 Solve for X
      CALL LFSDS (FACT, X, X)
!                                 Inverse permutation
      CALL PERMU (X, IPVT, X, IPATH=2)
!                                 Print X
      CALL WRRRN ('X', X, 1, N, 1)
!
      END
```

Output

```
           X
    1        2        3
1.000   -4.000    7.000
```

LUPCH

Updates the $R^T R$ Cholesky factorization of a real symmetric positive definite matrix after a rank-one matrix is added.

Required Arguments

R — N by N upper triangular matrix containing the upper triangular factor to be updated. (Input)
Only the upper triangle of R is referenced.

X — Vector of length N determining the rank-one matrix to be added to the factorization $R^T R$. (Input)

RNEW — N by N upper triangular matrix containing the updated triangular factor of $R^T R + XX^T$. (Output)
Only the upper triangle of RNEW is referenced. If R is not needed, R and RNEW can share the same storage locations.

Optional Arguments

N — Order of the matrix. (Input)
Default: N = size (R,2).

LDR — Leading dimension of R exactly as specified in the dimension statement of the calling program. (Input)
Default: LDR = size (R,1).

LDRNEW — Leading dimension of RNEW exactly as specified in the dimension statement of the calling program. (Input)
Default: LDRNEW = size (RNEW,1).

CS — Vector of length N containing the cosines of the rotations. (Output)

SN — Vector of length N containing the sines of the rotations. (Output)

FORTRAN 90 Interface

Generic: CALL LUPCH (R, X, RNEW [, …])

Specific: The specific interface names are S_LUPCH and D_LUPCH.

FORTRAN 77 Interface

Single: `CALL LUPCH (N, R, LDR, X, RNEW, LDRNEW, CS, SN)`

Double: The double precision name is `DLUPCH`.

Description

The routine `LUPCH` is based on the LINPACK routine `SCHUD`; see Dongarra et al. (1979).

The Cholesky factorization of a matrix is $A = R^T R$, where R is an upper triangular matrix. Given this factorization, `LUPCH` computes the factorization

$$A + xx^T = \tilde{R}^T \tilde{R}$$

In the program

$$\tilde{R}$$

is called `RNEW`.

`LUPCH` determines an orthogonal matrix U as the product $G_N \ldots G_1$ of Givens rotations, such that

$$U \begin{bmatrix} R \\ x^T \end{bmatrix} = \begin{bmatrix} \tilde{R} \\ 0 \end{bmatrix}$$

By multiplying this equation by its transpose, and noting that $U^T U = I$, the desired result

$$R^T R + xx^T = \tilde{R}^T \tilde{R}$$

is obtained.

Each Givens rotation, G_i, is chosen to zero out an element in x^T. The matrix G_i is $(N + 1) \times (N + 1)$ and has the form

$$G_i = \begin{bmatrix} I_{i-1} & 0 & 0 & 0 \\ 0 & c_i & 0 & s_i \\ 0 & 0 & I_{N-i} & 0 \\ 0 & -s_i & 0 & c_i \end{bmatrix}$$

Where I_k is the identity matrix of order k and $c_i = \cos\theta_i =$ `CS(I)`, $s_i = \sin\theta_i =$ `SN(I)` for some θ_i.

Example

A linear system $Az = b$ is solved using the Cholesky factorization of A. This factorization is then updated and the system $(A + xx^T)\, z = b$ is solved using this updated factorization.

```
      USE IMSL_LIBRARIES
!                                 Declare variables
      INTEGER    LDA, LDFACT, N
      PARAMETER  (LDA=3, LDFACT=3, N=3)
      REAL       A(LDA,LDA), FACT(LDFACT,LDFACT), FACNEW(LDFACT,LDFACT), &
                X(N), B(N), CS(N), SN(N), Z(N)
!
!                                 Set values for A
!                                 A = (  1.0  -3.0   2.0)
!                                     ( -3.0  10.0  -5.0)
!                                     (  2.0  -5.0   6.0)
!
      DATA A/1.0, -3.0, 2.0, -3.0, 10.0, -5.0, 2.0, -5.0, 6.0/
!
!                                 Set values for X and B
      DATA X/3.0, 2.0, 1.0/
      DATA B/53.0, 20.0, 31.0/
!                                 Factor the matrix A
      CALL LFTDS (A, FACT)
!                                 Solve the original system
      CALL LFSDS (FACT, B, Z)
!                                 Print the results
      CALL WRRRN ('FACT', FACT, ITRING=1)
      CALL WRRRN ('Z', Z, 1, N, 1)
!                                 Update the factorization
      CALL LUPCH (FACT, X, FACNEW)
!                                 Solve the updated system
      CALL LFSDS (FACNEW, B, Z)
!                                 Print the results
      CALL WRRRN ('FACNEW', FACNEW, ITRING=1)
      CALL WRRRN ('Z', Z, 1, N, 1)
!
      END
```

Output

```
          FACT
         1        2        3
1    1.000   -3.000    2.000
2             1.000    1.000
3                      1.000
           Z
      1          2          3
1860.0     433.0     -254.0

       FACNEW
         1        2        3
1    3.162    0.949    1.581
2             3.619   -1.243
3                     -1.719

        Z
     1        2        3
4.000    1.000    2.000
```

LDNCH

more...

Downdates the $R^T R$ Cholesky factorization of a real symmetric positive definite matrix after a rank-one matrix is removed.

Required Arguments

R — N by N upper triangular matrix containing the upper triangular factor to be downdated. (Input)
Only the upper triangle of R is referenced.

X — Vector of length N determining the rank-one matrix to be subtracted from the factorization $R^T R$. (Input)

RNEW — N by N upper triangular matrix containing the downdated triangular factor of $R^T R - X X^T$. (Output)
Only the upper triangle of RNEW is referenced. If R is not needed, R and RNEW can share the same storage locations.

Optional Arguments

N — Order of the matrix. (Input)
Default: N = size (R,2).

LDR — Leading dimension of R exactly as specified in the dimension statement of the calling program. (Input)
Default: LDR = size (R,1).

LDRNEW — Leading dimension of RNEW exactly as specified in the dimension statement of the calling program. (Input)
Default: LDRNEW = size (RNEW,1).

CS — Vector of length N containing the cosines of the rotations. (Output)

SN — Vector of length N containing the sines of the rotations. (Output)

FORTRAN 90 Interface

Generic: `CALL LDNCH (R, X, RNEW [, …])`

Specific: The specific interface names are `S_LDNCH` and `D_LDNCH`.

FORTRAN 77 Interface

Single: `CALL LDNCH (N, R, LDR, X, RNEW, LDRNEW, CS, SN)`

Double: The double precision name is `DLDNCH`.

Description

The routine `LDNCH` is based on the LINPACK routine `SCHDD`; see Dongarra et al. (1979).

The Cholesky factorization of a matrix is $A = R^T R$, where R is an upper triangular matrix. Given this factorization, `LDNCH` computes the factorization

$$A - xx^T = \tilde{R}^T \tilde{R}$$

In the program

$$\tilde{R}$$

is called `RNEW`. This is not always possible, since $A - xx^T$ may not be positive definite.

`LDNCH` determines an orthogonal matrix U as the product $G_N \ldots G_1$ of Givens rotations, such that

$$U \begin{bmatrix} R \\ 0 \end{bmatrix} = \begin{bmatrix} \tilde{R} \\ x^T \end{bmatrix}$$

By multiplying this equation by its transpose and noting that $U^T U = I$, the desired result

$$R^T R - xx^T = \tilde{R}^T \tilde{R}$$

is obtained.

Let a be the solution of the linear system $R^T a = x$ and let

$$\alpha = \sqrt{1 - \|a\|_2^2}$$

The Givens rotations, G_i, are chosen such that

$$G_1 \cdots G_N \begin{bmatrix} a \\ \alpha \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

The G_i are $(N + 1) \times (N + 1)$ matrices of the form

$$G_{\mathrm{i}} = \begin{bmatrix} I_{i-1} & 0 & 0 & 0 \\ 0 & c_i & 0 & -s_i \\ 0 & 0 & I_{N-i} & 0 \\ 0 & s_i & 0 & c_i \end{bmatrix}$$

where I_k is the identity matrix of order k; and $c_i = \cos\theta_i$ = `CS(I)`, $s_i = \sin\theta_i$ = `SN(I)` for some θ_i.

The Givens rotations are then used to form

$$\tilde{R}, G_1 \cdots G_N \begin{bmatrix} R \\ 0 \end{bmatrix} = \begin{bmatrix} \tilde{R} \\ \tilde{x}^T \end{bmatrix}$$

The matrix

$$\tilde{R}$$

is upper triangular and

$$\tilde{x} = x$$

because

$$x = \left(R^{\mathrm{T}} 0\right) \begin{bmatrix} a \\ \alpha \end{bmatrix} = \left(R^{\mathrm{T}} 0\right) U^{\mathrm{T}} U \begin{bmatrix} a \\ \alpha \end{bmatrix} = \left(\tilde{R}^{\mathrm{T}} \tilde{x}\right) \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \tilde{x}$$

Comments

Informational error

Type	Code	Description
4	1	$R^T R - X X^T$ is not positive definite. `R` cannot be downdated.

Example

A linear system $Az = b$ is solved using the Cholesky factorization of A. This factorization is then downdated, and the system $(A - xx^T)z = b$ is solved using this downdated factorization.

```
      USE LDNCH_INT
      USE LFTDS_INT
      USE LFSDS_INT
      USE WRRRN_INT
!                                 Declare variables
      INTEGER    LDA, LDFACT, N
      PARAMETER  (LDA=3, LDFACT=3, N=3)
      REAL       A(LDA,LDA), FACT(LDFACT,LDFACT), FACNEW(LDFACT,LDFACT), &
                X(N), B(N), CS(N), SN(N), Z(N)
!
!                                 Set values for A
!                                 A = ( 10.0   3.0   5.0)
!                                     (  3.0  14.0  -3.0)
!                                     (  5.0  -3.0   7.0)
!
      DATA A/10.0, 3.0, 5.0, 3.0, 14.0, -3.0, 5.0, -3.0, 7.0/
!
!                                 Set values for X and B
      DATA X/3.0, 2.0, 1.0/
      DATA B/53.0, 20.0, 31.0/
!                                 Factor the matrix A
      CALL LFTDS (A, FACT)
!                                 Solve the original system
      CALL LFSDS (FACT, B, Z)
!                                 Print the results
      CALL WRRRN ('FACT', FACT, ITRING=1)
      CALL WRRRN ('Z', Z, 1, N, 1)
!                                 Downdate the factorization
      CALL LDNCH (FACT, X, FACNEW)
!                                 Solve the updated system
      CALL LFSDS (FACNEW, B, Z)
!                                 Print the results
      CALL WRRRN ('FACNEW', FACNEW, ITRING=1)
      CALL WRRRN ('Z', Z, 1, N, 1)
!
      END
```

Output

```
          FACT
        1       2       3
1   3.162   0.949   1.581
2           3.619  -1.243
3                   1.719
            Z
      1       2       3
  4.000   1.000   2.000

          FACNEW
        1       2       3
1   1.000  -3.000   2.000
2           1.000   1.000
3                   1.000

             Z
     1        2        3
1859.9    433.0   -254.0
```

LSVRR

more... more...

Computes the singular value decomposition of a real matrix.

Required Arguments

A — NRA by NCA matrix whose singular value decomposition is to be computed. (Input)

IPATH — Flag used to control the computation of the singular vectors. (Input)
IPATH has the decimal expansion IJ such that:
I = 0 means do not compute the left singular vectors.
I = 1 means return the NRA left singular vectors in U.

NOTE: This option is not available for the ScaLAPACK interface. If this option is chosen for ScaLAPACK usage, the min(NRA, NCA) left singular vectors will be returned.

I = 2 means return only the min(NRA, NCA) left singular vectors in U.
J = 0 means do not compute the right singular vectors.
J = 1 means return the right singular vectors in V.

NOTE: If this option is chosen for ScaLAPACK usage, the min(NRA, NCA) right singular vectors will be returned.

For example, IPATH = 20 means I = 2 and J = 0.

S — Vector of length min(NRA + 1, NCA) containing the singular values of A in descending order of magnitude in the first min(NRA, NCA) positions. (Output)

Optional Arguments

NRA — Number of rows in the matrix A. (Input)
Default: NRA = size (A,1).

NCA — Number of columns in the matrix A. (Input)
Default: NCA = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

TOL — Scalar containing the tolerance used to determine when a singular value is negligible. (Input)
If TOL is positive, then a singular value σ_i considered negligible if $\sigma_i \leq$ TOL . If TOL is negative, then a singular value σ_i considered negligible if $\sigma_i \leq$ |TOL| * $\|A\|_\infty$. In this case, |TOL| generally contains an estimate of the level of the relative error in the data.
Default: TOL = 1.0e-5 for single precision and 1.0d-10 for double precision.

IRANK — Scalar containing an estimate of the rank of A. (Output)

U — NRA by NCU matrix containing the left singular vectors of A. (Output)
NCU must be equal to NRA if I is equal to 1. NCU must be equal to min(NRA, NCA) if I is equal to 2. U will not be referenced if I is equal to zero. If NRA is less than or equal to NCU, then U can share the same storage locations as A. See Comments.

LDU — Leading dimension of U exactly as specified in the dimension statement of the calling program. (Input)
Default: LDU = size (U,1).

V — NCA by NCA matrix containing the right singular vectors of A. (Output)
V will not be referenced if J is equal to zero. V can share the same storage location as A, however, U and V cannot both coincide with A simultaneously.

LDV — Leading dimension of V exactly as specified in the dimension statement of the calling program. (Input)
Default: LDV = size (V,1).

FORTRAN 90 Interface

Generic: CALL LSVRR (A, IPATH, S [, …])

Specific: The specific interface names are S_LSVRR and D_LSVRR.

FORTRAN 77 Interface

Single: CALL LSVRR (NRA, NCA, A, LDA, IPATH, TOL, IRANK, S, U, LDU, V, LDV)

Double: The double precision name is DLSVRR.

ScaLAPACK Interface

Generic: CALL LSVRR (A0, IPATH, S [, …])

Specific: The specific interface names are S_LSVRR and D_LSVRR.

See the *ScaLAPACK Usage Notes* below for a description of the arguments for distributed computing.

Description

The underlying code of routine LSVRR is based on either LINPACK, LAPACK, or ScaLAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see *Using ScaLAPACK, LAPACK, LINPACK, and EISPACK* in the Introduction section of this manual.

Let n = NRA (the number of rows in A) and let p = NCA (the number of columns in A). For any $n \times p$ matrix A, there exists an $n \times n$ orthogonal matrix U and a $p \times p$ orthogonal matrix V such that

$$U^T AV = \begin{cases} \begin{bmatrix} \Sigma \\ 0 \end{bmatrix} & \text{if } n \ge p \\ \begin{bmatrix} \Sigma & 0 \end{bmatrix} & \text{if } n \le p \end{cases}$$

where $\Sigma = \mathrm{diag}(\sigma_1, \ldots, \sigma_m)$, and $m = \min(n, p)$. The scalars $\sigma_1 \ge \sigma_2 \ge \ldots \ge \sigma_m \ge 0$ are called the *singular values* of A. The columns of U are called the *left singular vectors* of A. The columns of V are called the *right singular vectors* of A.

The estimated rank of A is the number of σ_k that is larger than a tolerance η. If τ is the parameter TOL in the program, then

$$\eta = \begin{cases} \tau & \text{if } \tau > 0 \\ |\tau| \, \|A\|_\infty & \text{if } \tau < 0 \end{cases}$$

Comments

1. Workspace may be explicitly provided, if desired, by use of L2VRR/DL2VRR. The reference is:

   CALL L2VRR (NRA, NCA, A, LDA, IPATH, TOL, IRANK, S, U, LDU, V, LDV, ACOPY, WK)

   The additional arguments are as follows:

   ACOPY — NRA × NCA work array for the matrix A. If A is not needed, then A and ACOPY may share the same storage locations.

   WK — Work vector of length NRA + NCA + max(NRA, NCA) − 1.

2. Informational error

Type	Code	Description
4	1	Convergence cannot be achieved for all the singular values and their corresponding singular vectors.

3. When NRA is much greater than NCA, it might not be reasonable to store the whole matrix U. In this case, IPATH with I = 2 allows a singular value factorization of A to be computed in which only the first NCA columns of U are computed, and in many applications those are all that are needed.

4. *Integer Options* with *Chapter 11* Options Manager

   16This option uses four values to solve memory bank conflict (access inefficiency) problems. In routine L2VRR the leading dimension of ACOPY is increased by IVAL(3) when N is a multiple of IVAL(4). The values IVAL(3) and IVAL(4) are temporarily replaced by IVAL(1) and IVAL(2), respectively, in LSVRR. Additional memory allocation for ACOPY and option value restoration are done automatically in LSVRR. Users directly calling L2VRR can allocate additional space for ACOPY and set IVAL(3) and IVAL(4) so that memory bank conflicts no longer cause inefficiencies. There is no requirement that users change existing applications that use LSVRR or L2VRR. Default values for the option are IVAL(*) = 1, 16, 0, 1.

   17 This option has two values that determine if the L_1 condition number is to be computed. Routine LSVRR temporarily replaces IVAL(2) by IVAL(1). The routine L2CRG computes the condition number if IVAL(2) = 2. Otherwise L2CRG skips this computation. LSVRR restores the option. Default values for the option are IVAL(*) = 1, 2.

ScaLAPACK Usage Notes

The arguments which differ from the standard version of this routine are:

A0 — MXLDA by MXCOL local matrix containing the local portions of the distributed matrix A. A contains the matrix whose singular value decomposition is to be computed. (Input)

U0 — MXLDU by MXCOLU local matrix containing the local portions of the left singular vectors of the distributed matrix A. (Output)
U0 will not be referenced if I is equal to zero. In contrast to the LINPACK and LAPACK based versions of LSVRR, U0 and A0 cannot share the same storage locations.

V0 — MXLDV by MXCOLV local matrix containing the local portions of the right singular vectors of the distributed matrix A. (Output)
V0 will not be referenced if J is equal to zero. In contrast to the LINPACK and LAPACK based versions of LSVRR, V0 and A0 cannot share the same storage locations.

Furthermore, the optional arguments NRA, NCA, LDA, LDU and LDV describe properties of the local arrays A0, U0, and V0, respectively. For example, NRA is the number of rows in matrix A0 which defaults to NRA = size (A0,1). The remaining arguments IPATH, S, TOL and IRANK are global and are the same as described for the standard version of the routine.

In the argument descriptions above, MXLDA, MXCOL, MXLDU, MXCOLU, MXLDV and MXCOLV can be obtained through a call to ScaLAPACK_GETDIM (*Chapter 11, "Utilities"*) after a call to ScaLAPACK_SETUP (*Chapter 11, "Utilities"*) has been made. If MXLDA or MXCOL is equal to 0, then A0 should be defined as an array of nonzero size, e.g., a 1 by 1 array. The same applies to the MXLDU/MXCOLU and MXLDV/MXCOLV pairs, respectively. See the *ScaLAPACK Example* below.

Examples

Example 1

This example computes the singular value decomposition of a 6×4 matrix *A*. The matrices *U* and *V* containing the left and right singular vectors, respectively, and the diagonal of Σ, containing singular values, are printed. On some systems, the signs of some of the columns of *U* and *V* may be reversed.

```
      USE IMSL_LIBRARIES
!                                 Declare variables
      PARAMETER  (NRA=6, NCA=4, LDA=NRA, LDU=NRA, LDV=NCA)
      REAL       A(LDA,NCA), U(LDU,NRA), V(LDV,NCA), S(NCA)
!
!                                 Set values for A
!
!                                 A = (  1    2    1    4  )
!                                     (  3    2    1    3  )
!                                     (  4    3    1    4  )
!                                     (  2    1    3    1  )
!                                     (  1    5    2    2  )
!                                     (  1    2    2    3  )
!
      DATA A/1., 3., 4., 2., 1., 1., 2., 2., 3., 1., 5., 2., 3*1., &
            3., 2., 2., 4., 3., 4., 1., 2., 3./
!
!                                 Compute all singular vectors
      IPATH = 11
      TOL   = AMACH(4)
      TOL   = 10.*TOL
      CALL LSVRR(A, IPATH, S, TOL=TOL, IRANK=IRANK, U=U, V=V)
!                                 Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT, *) 'IRANK = ', IRANK
      CALL WRRRN ('U', U, NRA, NCA)
      CALL WRRRN ('S', S, 1, NCA, 1)
      CALL WRRRN ('V', V)
!
      END
```

Output

```
    IRANK =            4

                        U
            1         2         3         4
  1   -0.3805   -0.1197   -0.4391    0.5654
  2   -0.4038   -0.3451    0.0566   -0.2148
  3   -0.5451   -0.4293   -0.0514   -0.4321
  4   -0.2648    0.0683    0.8839    0.2153
  5   -0.4463    0.8168   -0.1419   -0.3213
```

```
  6  -0.3546   0.1021   0.0043   0.5458

                  S
       1        2        3        4
   11.49     3.27     2.65     2.09

                     V
             1        2         3         4
  1  -0.4443  -0.5555   0.4354  -0.5518
  2  -0.5581   0.6543  -0.2775  -0.4283
  3  -0.3244   0.3514   0.7321   0.4851
  4  -0.6212  -0.3739  -0.4444   0.5261
```

ScaLAPACK Example

The previous example is repeated here as a distributed example. This example computes the singular value decomposition of a 6 × 4 matrix *A*. The matrices *U* and *V* containing the left and right singular vectors, respectively, and the diagonal of S, containing singular values, are printed. On some systems, the signs of some of the columns of *U* and *V* may be reversed..

```
      USE LSVRR_INT
      USE WRRRN_INT
      USE AMACH_INT
      USE UMACH_INT
      USE MPI_SETUP_INT
      USE SCALAPACK_SUPPORT
      IMPLICIT NONE
      INCLUDE 'mpif.h'
!                                 Declare variables
      INTEGER :: DESCA(9), DESCU(9), DESCV(9), MXLDV, &
                 MXCOLV, NSZ, NSZP1, MXLDU, MXCOLU
      INTEGER :: INFO, MXCOL, MXLDA, IPATH, IRANK, NOUT
      REAL :: TOL
      REAL, ALLOCATABLE :: A(:,:),U(:,:), V(:,:), S(:)
      REAL, ALLOCATABLE :: A0(:,:), U0(:,:), V0(:,:)
      INTEGER, PARAMETER :: NRA=6, NCA=4
!
      NSZ = MIN(NRA,NCA)
      NSZP1 = MIN(NRA+1,NCA)
!                                 Set up for MPI
      MP_NPROCS = MP_SETUP()
      IF(MP_RANK .EQ. 0) THEN
          ALLOCATE (A(NRA,NCA), U(NRA,NSZ), V(NCA,NSZ))
!                                 Set values for A
          A(1,:) = (/ 1.0,  2.0,  1.0,  4.0/)
          A(2,:) = (/ 3.0,  2.0,  1.0,  3.0/)
          A(3,:) = (/ 4.0,  3.0,  1.0,  4.0/)
          A(4,:) = (/ 2.0,  1.0,  3.0,  1.0/)
          A(5,:) = (/ 1.0,  5.0,  2.0,  2.0/)
          A(6,:) = (/ 1.0,  2.0,  2.0,  3.0/)
      ENDIF
!                                  Set up a 1D processor grid and define
!                                  its context ID, MP_ICTXT
      CALL SCALAPACK_SETUP(NRA, NCA, .TRUE., .TRUE.)
!                                  Get the array descriptor entities MXLDA,
!                                  MXCOL, MXLDU, MXCOLU, MXLDV, AND MXCOLV
      CALL SCALAPACK_GETDIM(NRA, NCA, MP_MB, MP_NB, MXLDA, MXCOL)
      CALL SCALAPACK_GETDIM(NRA, NSZ, MP_MB, MP_NB, MXLDU, MXCOLU)
      CALL SCALAPACK_GETDIM(NCA, NSZ, MP_MB, MP_NB, MXLDV, MXCOLV)
!                                  Set up the array descriptors
      CALL DESCINIT(DESCA, NRA, NCA, MP_MB, MP_NB, 0, 0, MP_ICTXT, &
                    MAX(1,MXLDA), INFO)
```

```
      CALL DESCINIT(DESCU, NRA, NSZ, MP_MB, MP_NB, 0, 0, MP_ICTXT, &
                    MAX(1,MXLDU), INFO)
      CALL DESCINIT(DESCV, NCA, NSZ, MP_MB, MP_NB, 0, 0, MP_ICTXT, &
                    MAX(1,MXLDV), INFO)
!                                  Allocate space for the local arrays and
!                                  array S
      IF (MXLDA .EQ. 0 .OR. MXCOL .EQ. 0) THEN
         ALLOCATE (A0(1,1))
      ELSE
         ALLOCATE (A0(MXLDA,MXCOL))
      END IF

      IF (MXLDU .EQ. 0 .OR. MXCOLU .EQ. 0) THEN
         ALLOCATE (U0(1,1))
      ELSE
         ALLOCATE (U0(MXLDU,MXCOLU))
      END IF

      IF (MXLDV .EQ. 0 .OR. MXCOLV .EQ. 0) THEN
         ALLOCATE (V0(1,1))
      ELSE
         ALLOCATE (V0(MXLDV,MXCOLV))
      END IF

      ALLOCATE(S(NSZP1))
!                                  Map input array to the processor grid
      CALL SCALAPACK_MAP(A, DESCA, A0)
!                                  Compute all singular vectors
      IPATH = 11
      TOL = AMACH(4)
      TOL = 10.0 * TOL
      CALL LSVRR (A0, IPATH, S, TOL=TOL, IRANK=IRANK, U=U0, V=V0)
!                                  Unmap the results from the distributed
!                                  array back to a non-distributed array.
!                                  After the unmap, only Rank=0 has the full
!                                  array.
      CALL SCALAPACK_UNMAP(U0, DESCU, U)
      CALL SCALAPACK_UNMAP(V0, DESCV, V)
!                                  Print results.
!                                  Only Rank=0 has the singular vectors.
      IF(MP_RANK .EQ. 0) THEN
         CALL UMACH (2, NOUT)
         WRITE (NOUT, *) 'IRANK = ', IRANK
         CALL WRRRN ('U', U)
         CALL WRRRN ('S', S, 1, NSZ, 1)
         CALL WRRRN ('V', V)
      ENDIF
!                                 Exit ScaLAPACK usage
      CALL SCALAPACK_EXIT(MP_ICTXT)
!                                 Shut down MPI
      MP_NPROCS = MP_SETUP('FINAL')
      END
```

Output

```
 IRANK =            4

                  U
          1         2         3         4
 1  -0.3805   -0.1197   -0.4391    0.5654
 2  -0.4038   -0.3451    0.0566   -0.2148
 3  -0.5451   -0.4293   -0.0514   -0.4321
 4  -0.2648    0.0683    0.8839    0.2153
 5  -0.4463    0.8168   -0.1419   -0.3213
 6  -0.3546    0.1021    0.0043    0.5458
```

```
                 S
      1       2       3       4
  11.49    3.27    2.65    2.09

                    V
          1         2         3         4
 1  -0.4443  -0.5555   0.4354  -0.5518
 2  -0.5581   0.6543  -0.2775  -0.4283
 3  -0.3244   0.3514   0.7321   0.4851
 4  -0.6212  -0.3739  -0.4444   0.5261
```

LSVCR

more...

Computes the singular value decomposition of a complex matrix.

Required Arguments

A — Complex NRA by NCA matrix whose singular value decomposition is to be computed. (Input)

IPATH — Integer flag used to control the computation of the singular vectors. (Input)
IPATH has the decimal expansion IJ such that:
I=0 means do not compute the left singular vectors.
I=1 means return the NCA left singular vectors in U.
I=2 means return only the min(NRA, NCA) left singular vectors in U.
J=0 means do not compute the right singular vectors.
J=1 means return the right singular vectors in V.

For example, IPATH = 20 means I = 2 and J = 0.

S — Complex vector of length min(NRA + 1, NCA) containing the singular values of A in descending order of magnitude in the first min(NRA, NCA) positions. (Output)

Optional Arguments

NRA — Number of rows in the matrix A. (Input)
Default: NRA = size (A,1).

NCA — Number of columns in the matrix A. (Input)
Default: NCA = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

TOL — Real scalar containing the tolerance used to determine when a singular value is negligible. (Input)
If TOL is positive, then a singular value SI is considered negligible if SI ≤ TOL. If TOL is negative, then a singular value SI is considered negligible if SI ≤ |TOL|*(Infinity norm of A). In this case |TOL| should generally contain an estimate of the level of relative error in the data.
Default: TOL = 1.0e-5 for single precision and 1.0d-10 for double precision.

IRANK — Integer scalar containing an estimate of the rank of A. (Output)

U — Complex matrix, NRA by NRA if I = 1, or NRA by min(NRA, NCA) if I = 2, containing the left singular vectors of A. (Output)
U will not be referenced if I is equal to zero. If NRA ≤ NCA or IPATH = 2, then U can share the same storage locations as A.

LDU — Leading dimension of U exactly as specified in the dimension statement of the calling program. (Input)
Default: LDU = size (U,1).

V — Complex NCA by NCA matrix containing the right singular vectors of A. (Output)
V will not be referenced if J is equal to zero. If NCA is less than or equal to NRA, then V can share the same storage locations as A; however U and V cannot both coincide with A simultaneously.

LDV — Leading dimension of V exactly as specified in the dimension statement of the calling program. (Input)
Default: LDV = size (V,1).

FORTRAN 90 Interface

Generic: CALL LSVCR (A, IPATH, S [, …])

Specific: The specific interface names are S_LSVCR and D_LSVCR.

FORTRAN 77 Interface

Single: CALL LSVCR (NRA, NCA, A, LDA, IPATH, TOL, IRANK, S, U, LDU, V, LDV)

Double: The double precision name is DLSVCR.

Description

The underlying code of routine LSVCR is based on either LINPACK or LAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see *Using ScaLAPACK, LAPACK, LINPACK, and EISPACK* in the Introduction section of this manual.

Let n = NRA (the number of rows in A) and let p = NCA (the number of columns in A).For any $n \times p$ matrix A there exists an $n \times n$ orthogonal matrix U, and a $p \times p$ orthogonal matrix V such that

$$U^T AV = \begin{cases} \begin{bmatrix} \Sigma \\ 0 \end{bmatrix} & \text{if } n \geq p \\ \begin{bmatrix} \Sigma \; 0 \end{bmatrix} & \text{if } n \leq p \end{cases}$$

where $\Sigma = \text{diag}(\sigma_1, \ldots, \sigma_m)$, and $m = \min(n, p)$. The scalars $\sigma_1 \geq \sigma_2 \geq \ldots \geq 0$ are called the *singular values* of A. The columns of U are called the *left singular vectors* of A. The columns of V are called the *right singular vectors* of A.

The estimated rank of A is the number of σ_k which are larger than a tolerance η. If τ is the parameter TOL in the program, then

$$\eta = \begin{cases} \tau & \text{if } \tau > 0 \\ |\,\tau\,|\,\|A\|_\infty & \text{if } \tau < 0 \end{cases}$$

Comments

1. Workspace may be explicitly provided, if desired, by use of L2VCR/DL2VCR. The reference is

   CALL L2VCR (NRA, NCA, A, LDA, IPATH, TOL, IRANK, S, U, LDU, V, LDV, ACOPY, WK)

   The additional arguments are as follows:

   ACOPY — NRA * NCA complex work array of length for the matrix A. If A is not needed, then A and ACOPY can share the same storage locations.

   WK — Complex work vector of length NRA + NCA + max(NRA, NCA) − 1.

2. Informational error

Type	Code	Description
4	1	Convergence cannot be achieved for all the singular values and their corresponding singular vectors.

3. When NRA is much greater than NCA, it might not be reasonable to store the whole matrix U. In this case IPATH with I = 2 allows a singular value factorization of A to be computed in which only the first NCA columns of U are computed, and in many applications those are all that are needed.

4. *Integer Options* with *Chapter 11* Options Manager

   16This option uses four values to solve memory bank conflict (access inefficiency) problems. In routine L2VCR the leading dimension of ACOPY is increased by IVAL(3) when N is a multiple of IVAL(4). The values IVAL(3) and IVAL(4) are temporarily replaced by IVAL(1) and IVAL(2), respectively, in LSVCR. Additional memory allocation for ACOPY and option value restoration are done automatically in LSVCR. Users directly calling L2VCR can allocate additional space for ACOPY and set IVAL(3) and IVAL(4) so that memory bank conflicts no longer cause inefficiencies. There is no requirement that users change existing applications that use LSVCR or L2VCR. Default values for the option are IVAL(*) = 1, 16, 0, 1.

17 This option has two values that determine if the L_1 condition number is to be computed. Routine LSVCR temporarily replaces IVAL(2) by IVAL(1). The routine L2CCG computes the condition number if IVAL(2) = 2. Otherwise L2CCG skips this computation. LSVCR restores the option. Default values for the option are IVAL(*) = 1, 2.

Example

This example computes the singular value decomposition of a 6 × 3 matrix *A*. The matrices *U* and *V* containing the left and right singular vectors, respectively, and the diagonal of Σ, containing singular values, are printed. On some systems, the signs of some of the columns of *U* and *V* may be reversed.

```
      USE IMSL_LIBRARIES
!                                 Declare variables
      PARAMETER  (NRA=6, NCA=3, LDA=NRA, LDU=NRA, LDV=NCA)
      COMPLEX    A(LDA,NCA), U(LDU,NRA), V(LDV,NCA), S(NCA)
!
!                                 Set values for A
!
!                                 A = (  1+2i    3+2i    1-4i  )
!                                     (  3-2i    2-4i    1+3i  )
!                                     (  4+3i   -2+1i    1+4i  )
!                                     (  2-1i    3+0i    3-1i  )
!                                     (  1-5i    2-5i    2+2i  )
!                                     (  1+2i    4-2i    2-3i  )
!
      DATA A/(1.0,2.0), (3.0,-2.0), (4.0,3.0), (2.0,-1.0), (1.0,-5.0), &
            (1.0,2.0), (3.0,2.0), (2.0,-4.0), (-2.0,1.0), (3.0,0.0), &
            (2.0,-5.0), (4.0,-2.0), (1.0,-4.0), (1.0,3.0), (1.0,4.0), &
            (3.0,-1.0), (2.0,2.0), (2.0,-3.0)/
!
!                                 Compute all singular vectors
      IPATH = 11
      TOL   = AMACH(4)
      TOL   = 10. * TOL
      CALL LSVCR(A, IPATH, S, TOL = TOL, IRANK=IRANK, U=U, V=V)
!                                 Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT, *) 'IRANK = ', IRANK
      CALL WRCRN ('U', U, NRA, NCA)
      CALL WRCRN ('S', S, 1, NCA, 1)
      CALL WRCRN ('V', V)
!
      END
```

Output

```
 IRANK =             3

                             U
                   1                    2                    3
 1  (-0.1968,-0.2186)  ( 0.5011, 0.0217)  ( 0.2007, 0.1003)
 2  (-0.3443, 0.3542)  (-0.2933, 0.0248)  (-0.1155, 0.2338)
 3  (-0.1457,-0.2307)  (-0.5424, 0.1381)  ( 0.4361, 0.4407)
```

```
   4  (-0.3016, 0.0844)  ( 0.2157, 0.2659)  ( 0.0523, 0.0894)
   5  (-0.2283, 0.6008)  (-0.1325, 0.1433)  (-0.3152, 0.0090)
   6  (-0.2876, 0.0350)  ( 0.4377,-0.0400)  (-0.0458, 0.6205)

                               S
                 1                   2                   3
  ( 11.77,  0.00)  (  9.30,  0.00)  (  4.99,  0.00)

                                     V
                       1                      2                      3
   1  (-0.6616, 0.0000)  (-0.2651, 0.0000)  ( 0.7014, 0.0000)
   2  (-0.7355,-0.0379)  ( 0.3850,-0.0707)  (-0.5482,-0.0624)
   3  (-0.0507, 0.1317)  ( 0.1724, 0.8642)  ( 0.0173, 0.4509)
```

LSGRR

more...

more...

Computes the generalized inverse of a real matrix.

Required Arguments

A — `NRA` by `NCA` matrix whose generalized inverse is to be computed. (Input)

GINVA — `NCA` by `NRA` matrix containing the generalized inverse of `A`. (Output)

Optional Arguments

NRA — Number of rows in the matrix `A`. (Input)
Default: `NRA` = size (`A`,1).

NCA — Number of columns in the matrix `A`. (Input)
Default: `NCA` = size (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = size (`A`,1).

TOL — Scalar containing the tolerance used to determine when a singular value (from the singular value decomposition of `A`) is negligible. (Input)
If `TOL` is positive, then a singular value σ_i considered negligible if $\sigma_i \le$ `TOL` . If `TOL` is negative, then a singular value σ_i considered negligible if $\sigma_i \le$ |`TOL`| * $\|A\|_\infty$. In this case, |`TOL`| generally contains an estimate of the level of the relative error in the data.
Default: `TOL` = 1.0e-5 for single precision and 1.0d-10 for double precision.

IRANK — Scalar containing an estimate of the rank of `A`. (Output)

LDGINV — Leading dimension of `GINVA` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDGINV` = size (`GINV`,1).

FORTRAN 90 Interface

Generic: CALL LSGRR (A, GINVA [, …])

Specific: The specific interface names are S_LSGRR and D_LSGRR.

FORTRAN 77 Interface

Single: CALL LSGRR (NRA, NCA, A, LDA, TOL, IRANK, GINVA, LDGINV)

Double: The double precision name is DLSGRR.

ScaLAPACK Interface

Generic: CALL LSGRR (A0, GINVA0 [, …])

Specific: The specific interface names are S_LSGRR and D_LSGRR.

See the *ScaLAPACK Usage Notes* below for a description of the arguments for distributed computing.

Description

Let k = IRANK, the rank of A; let n = NRA, the number of rows in A; let p = NCA, the number of columns in A; and let

$$A^{\dagger} = GINV$$

be the generalized inverse of A.

To compute the *Moore-Penrose generalized inverse*, the routine LSVRR is first used to compute the singular value decomposition of A. A singular value decomposition of A consists of an $n \times n$ orthogonal matrix U, a $p \times p$ orthogonal matrix V and a diagonal matrix $\Sigma = \text{diag}(\sigma_1, \ldots, \sigma_m)$, $m = \min(n, p)$, such that $U^T AV = [\Sigma, 0]$ if $n \le p$ and $U^T AV = [\Sigma, 0]^T$ if $n \ge p$. Only the first p columns of U are computed. The rank k is estimated by counting the number of nonnegligible σ_i.

The matrices U and V can be partitioned as $U = (U_1, U_2)$ and $V = (V_1, V_2)$ where both U_1 and V_1 are $k \times k$ matrices. Let $\Sigma_1 = \text{diag}(\sigma_1, \ldots, \sigma_k)$. The Moore-Penrose generalized inverse of A is

$$A^{\dagger} = V_1 \Sigma_1^{-1} U_1^T$$

The underlying code of routine LSGRR is based on either LINPACK, LAPACK, or ScaLAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation see *Using ScaLAPACK, LAPACK, LINPACK, and EISPACK* in the Introduction section of this manual.

Comments

1. Workspace may be explicitly provided, if desired, by use of L2GRR/DL2GRR. The reference is:

   CALL L2GRR (NRA, NCA, A, LDA, TOL, IRANK, GINVA, LDGINV, WKA, WK)

   The additional arguments are as follows:

   WKA — Work vector of length NRA * NCA used as workspace for the matrix A. If A is not needed, WKA and A can share the same storage locations.

   WK — Work vector of length LWK where LWK is equal to $\mathrm{NRA}^2 + \mathrm{NCA}^2 + \min(\mathrm{NRA} + 1, \mathrm{NCA}) + \mathrm{NRA} + \mathrm{NCA} + \max(\mathrm{NRA}, \mathrm{NCA}) - 2$.

2. Informational error

Type	Code	Description
4	1	Convergence cannot be achieved for all the singular values and their corresponding singular vectors.

ScaLAPACK Usage Notes

The arguments which differ from the standard version of this routine are:

A0 — MXLDA by MXCOL local matrix containing the local portions of the distributed matrix A. A contains the matrix for which the generalized inverse is to be computed. (Input)

GINVA0 — MXLDG by MXCOLG local matrix containing the local portions of the distributed matrix GINVA. GINVA contains the generalized inverse of matrix A. (Output)

All other arguments are global and are the same as described for the standard version of the routine. In the argument descriptions above, MXLDA, MXCOL, MXLDG, and MXCOLG can be obtained through a call to SCALAPACK_GETDIM (see *Utilities*) after a call to SCALAPACK_SETUP (see *Chapter 11, "Utilities"*) has been made. See the *ScaLAPACK Example* below.

Examples

Example

This example computes the generalized inverse of a 3 × 2 matrix *A*. The rank *k* = IRANK and the inverse

$$A^{\dagger} = GINV$$

are printed.

```
USE IMSL_LIBRARIES
```

```
!                                 Declare variables
      PARAMETER  (NRA=3, NCA=2, LDA=NRA, LDGINV=NCA)
      REAL       A(LDA,NCA), GINV(LDGINV,NRA)
!
!                                 Set values for A
!
!                                 A = (   1    0   )
!                                     (   1    1   )
!                                     ( 100  -50   )
      DATA A/1., 1., 100., 0., 1., -50./

!
!                                 Compute generalized inverse
      TOL = AMACH(4)
      TOL = 10.*TOL
      CALL LSGRR (A, GINV,TOL=TOL, IRANK=IRANK)
!                                 Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT, *) 'IRANK = ', IRANK
      CALL WRRRN ('GINV', GINV)
!
      END
```

Output

```
IRANK =   2
             GINV
         1         2         3
1   0.1000    0.3000    0.0060
2   0.2000    0.6000   -0.0080
```

ScaLAPACK Example

This example computes the generalized inverse of a 6 × 4 matrix A as a distributed example. The rank k = `IRANK` and the inverse

$$A^{\dagger} = \mathrm{GINV}$$

are printed.

```
      USE MPI_SETUP_INT
      USE IMSL_LIBRARIES
      USE SCALAPACK_SUPPORT
      IMPLICIT NONE
      INCLUDE 'mpif.h'
!                                 Declare variables
      INTEGER       IRANK, LDA, NCA, NRA, DESCA(9), DESCG(9), &
                    LDGINV, MXLDG, MXCOLG, NOUT
      INTEGER       INFO, MXCOL, MXLDA
      REAL          TOL, AMACH
      REAL, ALLOCATABLE ::        A(:,:),GINVA(:,:)
      REAL, ALLOCATABLE ::        A0(:,:), GINVA0(:,:)
      PARAMETER  (NRA=6, NCA=4, LDA=NRA, LDGINV=NCA)
!                                 Set up for MPI
      MP_NPROCS = MP_SETUP()
      IF(MP_RANK .EQ. 0) THEN
          ALLOCATE (A(LDA,NCA), GINVA(NCA,NRA))
!                                 Set values for A
          A(1,:) = (/ 1.0,  2.0,  1.0,  4.0/)
          A(2,:) = (/ 3.0,  2.0,  1.0,  3.0/)
          A(3,:) = (/ 4.0,  3.0,  1.0,  4.0/)
```

```
        A(4,:) = (/ 2.0,  1.0,  3.0,  1.0/)
        A(5,:) = (/ 1.0,  5.0,  2.0,  2.0/)
        A(6,:) = (/ 1.0,  2.0,  2.0,  3.0/)
    ENDIF
!                                Set up a 1D processor grid and define
!                                its context ID, MP_ICTXT
    CALL SCALAPACK_SETUP(NRA, NCA, .TRUE., .TRUE.)
!                                Get the array descriptor entities MXLDA,
!                                MXCOL, MXLDG, and MXCOLG
    CALL SCALAPACK_GETDIM(NRA, NCA, MP_MB, MP_NB, MXLDA, MXCOL)

    CALL SCALAPACK_GETDIM(NCA, NRA, MP_NB, MP_MB, MXLDG, MXCOLG)
!                                Set up the array descriptors
    CALL DESCINIT(DESCA, NRA, NCA, MP_MB, MP_NB, 0, 0, MP_ICTXT, MXLDA, &
    INFO)
    CALL DESCINIT(DESCG, NCA, NRA, MP_NB, MP_MB, 0, 0, MP_ICTXT, MXLDG, &
    INFO)
!                               Allocate space for the local arrays
    ALLOCATE (A0(MXLDA,MXCOL), GINVA0(MXLDG,MXCOLG))
!                               Map input array to the processor grid
    CALL SCALAPACK_MAP(A, DESCA, A0)
!                               Compute the generalized inverse
    TOL = AMACH(4)
    TOL = 10. * TOL
    CALL LSGRR (A0, GINVA0, TOL=TOL, IRANK=IRANK)
!                               Unmap the results from the distributed
!                               array back to a non-distributed array.
!                               After the unmap, only Rank=0 has the full
!                               array.
    CALL SCALAPACK_UNMAP(GINVA0, DESCG, GINVA)
!                               Print results.
!                               Only Rank=0 has the solution, GINVA
    IF(MP_RANK .EQ. 0) THEN
       CALL UMACH (2, NOUT)
       WRITE (NOUT, *) 'IRANK = ',IRANK
       CALL WRRRN ('GINVA', GINVA)
    ENDIF
!                               Exit ScaLAPACK usage
    CALL SCALAPACK_EXIT(MP_ICTXT)
!                              Shut down MPI
    MP_NPROCS = MP_SETUP('FINAL')
    END
```

Eigensystem Analysis

Routines

Usage Notes

This chapter includes routines for linear eigensystem analysis. Many of these are for matrices with special properties. Some routines compute just a portion of the eigensystem. Use of the appropriate routine can substantially reduce computing time and storage requirements compared to computing a full eigensystem for a general complex matrix.

An ordinary linear eigensystem problem is represented by the equation $Ax = \lambda x$ where A denotes an $n \times n$ matrix. The value λ is an *eigenvalue* and $x \neq 0$ is the corresponding *eigenvector*. The eigenvector is determined up to a scalar factor. In all routines, we have chosen this factor so that x has Euclidean length with value one, and the component of x of smallest index and largest magnitude is positive. In case x is a complex vector, this largest component is real and positive.

Similar comments hold for the use of the remaining Level 1 routines in the following tables in those cases where the second character of the Level 2 routine name is no longer the character "2".

A generalized linear eigensystem problem is represented by $Ax = \lambda Bx$ where A and B are $n \times n$ matrices. The value λ is an eigenvalue, and x is the corresponding eigenvector. The eigenvectors are normalized in the same manner as for the ordinary eigensystem problem. The linear eigensystem routines have names that begin with the letter "E". The generalized linear eigensystem routines have names that begin with the letter "G". This prefix is followed by a two-letter code for the type of analysis that is performed. That is followed by another two-letter suffix for the form of the coefficient matrix. The following tables summarize the names of the eigensystem routines.

Symmetric and Hermitian Eigensystems			
	Symmetric Full	**Symmetric Band**	**Hermitian Full**
All eigenvalues	EVLSF	EVLSB	EVLHF
All eigenvalues and eigenvectors	EVCSF	EVCSB	EVCHF
Extreme eigenvalues	EVASF	EVASB	EVAHF
Extreme eigenvalues and eigenvectors	EVESF	EVESB	EVEHF
Eigenvalues in an interval	EVBSF	EVBSB	EVBHF
Eigenvalues and eigevectors in an interval	EVFSF	EVFSB	EVFHF
Performance index	EPISF	EPISB	EPIHF

General Eigensystems				
	Real General	**Complex General**	**Real Hessenberg**	**Complex Hessenberg**
All eigenvalues	EVLRG	EVLCG	EVLRH	EVLCH
All eigenvalues and eigenvectors	EVCRG	EVCCG	EVCRH	EVCCH
Performance index	EPIRG	EPICG	EPIRG	EPICG

Generalized Eigensystems $Ax = \lambda Bx$			
	Real General	**Complex General**	**A Symmetric B Positive Definite**
All eigenvalues	GVLRG	GVLCG	GVLSP
All eigenvalues and eigenvectors	GVCRG	GVCCG	GVCSP
Performance index	GPIRG	GPICG	GPISP

Error Analysis and Accuracy

The remarks in this section are for the ordinary eigenvalue problem. Except in special cases, routines will not return the exact eigenvalue-eigenvector pair for the ordinary eigenvalue problem $Ax = \lambda x$. The computed pair

$$\tilde{x}, \tilde{\lambda}$$

is an exact eigenvector-eigenvalue pair for a "nearby" matrix $A + E$. Information about E is known only in terms of bounds of the form $\|E\|_2 \le f(n)\|A\|_2 \varepsilon$. The value of $f(n)$ depends on the algorithm but is typically a small fractional power of n. The parameter ε is the machine precision. By a theorem due to Bauer and Fike (see Golub and Van Loan [1989, page 342]),

$$\min|\tilde{\lambda} - \lambda| \le \kappa(X)\|E\|_2 \qquad \text{for all } \lambda \text{ in } \sigma(A)$$

where $\sigma(A)$ is the set of all eigenvalues of A (called the *spectrum* of A), X is the matrix of eigenvectors, $\|\cdot\|_2$ is the 2-norm, and $\kappa(X)$ is the condition number of X defined as $\kappa(X) = \|X\|_2 \|X^{-1}\|_2$. If A is a real symmetric or complex Hermitian matrix, then its eigenvector matrix X is respectively orthogonal or unitary. For these matrices, $\kappa(X) = 1$.

The eigenvalues

$$\tilde{\lambda}_j$$

and eigenvectors

$$\tilde{x}_j$$

computed by `EVC**` can be checked by computing their performance index τ using `EPI**`. The performance index is defined by Smith et al. (1976, pages 124 – 126) to be

$$\tau = \max_{1 \le j \le n} \frac{\left\| A\tilde{x}_j - \tilde{\lambda}_j \tilde{x}_j \right\|_1}{10 n \varepsilon \left\| A \right\|_1 \left\| \tilde{x}_j \right\|_1}$$

No significance should be attached to the factor of 10 used in the denominator. For a real vector *x*, the symbol $\|x\|_1$ represents the usual 1-norm of *x*. For a complex vector *x*, the symbol $\|x\|_1$ is defined by

$$\|x\|_1 = \sum_{k=1}^{N} \left(| \Re\, x_k | + | \Im\, x_k | \right)$$

The performance index τ is related to the error analysis because

$$\|E\tilde{x}_j\|_2 \doteq \|A\tilde{x}_j - \tilde{\lambda}_j \tilde{x}_j\|_2$$

where *E* is the “nearby” matrix discussed above.

While the exact value of τ is machine and precision dependent, the performance of an eigensystem analysis routine is defined as excellent if $\tau < 1$, good if $1 \le \tau \le 100$, and poor if $\tau > 100$. This is an arbitrary definition, but large values of τ can serve as a warning that there is a blunder in the calculation. There are also similar routines `GPI**` to compute the performance index for generalized eigenvalue problems.

If the condition number $\kappa(X)$ of the eigenvector matrix *X* is large, there can be large errors in the eigenvalues even if τ is small. In particular, it is often difficult to recognize near multiple eigenvalues or unstable mathematical problems from numerical results. This facet of the eigenvalue problem is difficult to understand: A user often asks for the accuracy of an individual eigenvalue. This can be answered approximately by computing the *condition number of an individual eigenvalue.* See Golub and Van Loan (1989, pages 344-345). For matrices *A* such that the computed array of normalized eigenvectors *X* is invertible, the condition number of λ_j is $\kappa_j \equiv$ the Euclidean length of row *j* of the inverse matrix X^{-1}. Users can choose to compute this matrix with routine `LINCG`, see *Chapter 1, “Linear Systems”*. An approximate bound for the accuracy of a computed eigenvalue is then given by $\kappa_j \varepsilon \|A\|$. To compute an approximate bound for the relative accuracy of an eigenvalue, divide this bound by $|\lambda_j|$.

Generalized Eigenvalue Problems

The generalized eigenvalue problem $Ax = \lambda Bx$ is often difficult for users to analyze because it is frequently ill-conditioned. There are occasionally changes of variables that can be performed on the given problem to ease this ill-conditioning. Suppose that B is singular but A is nonsingular. Define the reciprocal $\mu = \lambda^{-1}$. Then, the roles of A and B are interchanged so that the reformulated problem $Bx = \mu Ax$ is solved. Those generalized eigenvalues $\mu_j = 0$ correspond to eigenvalues $\lambda_j = \infty$. The remaining

$$\lambda_j = \mu_j^{-1}$$

The generalized eigenvectors for λ_j correspond to those for μ_j. Other reformulations can be made: If B is nonsingular, the user can solve the ordinary eigenvalue problem $Cx \equiv B^{-1} Ax = \lambda x$. This is not recommended as a computational algorithm for two reasons. First, it is generally less efficient than solving the generalized problem directly. Second, the matrix C will be subject to perturbations due to ill-conditioning and rounding errors when computing $B^{-1} A$. Computing the condition numbers of the eigenvalues for C may, however, be helpful for analyzing the accuracy of results for the generalized problem.

There is another method that users can consider to reduce the generalized problem to an alternate ordinary problem. This technique is based on first computing a matrix decomposition $B = PQ$, where both P and Q are matrices that are “simple” to invert. Then, the given generalized problem is equivalent to the ordinary eigenvalue problem $Fy = \lambda y$. The matrix $F \equiv P^{-1} AQ^{-1}$. The unnormalized eigenvectors of the generalized problem are given by $x = Q^{-1} y$. An example of this reformulation is used in the case where A and B are real and symmetric with B positive definite. The IMSL routines `GVLSP` and `GVCSP` use $P = R^T$ and $Q = R$ where R is an upper triangular matrix obtained from a Cholesky decomposition, $B = R^TR$. The matrix $F = R^{-T} AR^{-1}$ is symmetric and real. Computation of the eigenvalue-eigenvector expansion for F is based on routine `EVCSF`.

Using ARPACK for Ordinary and Generalized Eigenvalue Problems

ARPACK consists of a set of Fortran 77 subroutines which use the Arnoldi method (Sorensen, 1992) to solve eigenvalue problems. ARPACK is well suited for large structured eigenvalue problems where structured means that a matrix-vector product $w \leftarrow Av$ requires O(n) rather than the usual O(n^2) floating point operations.

The suite of features that we have implemented from ARPACK are described in the work of Lehoucq, Sorensen and Yang, *ARPACK Users' Guide*, SIAM Publications, (1998). Users will find access to this *Guide* helpful. Due to the size of the package, we provide for the use of double precision real and complex arithmetic only.

The ARPACK computational algorithm computes a partial set of approximate eigenvalues or singular values for various classes of problems. This includes the ordinary problem, $Ax = \lambda x$, the generalized problem, $Ax = \lambda Bx$, and the singular value decomposition, $A = USV^T$.

The original API for ARPACK is a Reverse Communication Interface. This interface can be used as illustrated in the *Guide*. However, we provide a Fortran 2003 interface to ARPACK that will be preferred by some users. This is a forward communication interface based on user-written functions for matrix-vector products or linear equation solving steps required by the algorithms in ARPACK. It is not necessary that the linear operators be expressed as dense or sparse matrices. That is permitted, but for some problems the best approach is the ability to form a product of the operator with a vector.

The forward communication interface includes an argument of a user-extended derived type or class object. The intent of producing this argument is that an extended type provides access to threaded user data or other required information, including procedure pointers, for use in the user-written product functions. It also hides information that can often be ignored with a first use.

LIN_EIG_SELF

Computes the eigenvalues of a self-adjoint (i.e. real symmetric or complex Hermitian) matrix, A. Optionally, the eigenvectors can be computed. This gives the decomposition $A = VDV^T$, where V is an $n \times n$ orthogonal matrix and D is a real diagonal matrix.

Required Arguments

A — Array of size $n \times n$ containing the matrix. (Input [/Output])

D — Array of size n containing the eigenvalues. The values are in order of decreasing absolute value. (Output)

Optional Arguments

NROWS = `n` (Input)
Uses array `A`(1:`n`, 1:`n`) for the input matrix.
Default: `n` = size(`A`, 1)

v = `v(:,:)` (Output)
Array of the same type and kind as `A`(1:`n`, 1:`n`). It contains the $n \times n$ orthogonal matrix V.

iopt = `iopt(:)` (Input)
Derived type array with the same precision as the input matrix; used for passing optional data to the routine. The options are as follows:

Packaged Options for `LIN_EIG_SELF`		
Option Prefix = ?	**Option Name**	**Option Value**
`s_, d_, c_, z_`	`Lin_eig_self_set_small`	1
`s_, d_, c_, z_`	`Lin_eig_self_overwrite_input`	2
`s_, d_, c_, z_`	`Lin_eig_self_scan_for_NaN`	3
`s_, d_, c_, z_`	`Lin_eig_self_use_QR`	4
`s_, d_, c_, z_`	`Lin_eig_self_skip_Orth`	5
`s_, d_, c_, z_`	`Lin_eig_self_use_Gauss_elim`	6
`s_, d_, c_, z_`	`Lin_eig_self_set_perf_ratio`	7

iopt(IO) = `?_options(?_lin_eig_self_set_small`, *Small*)

If a denominator term is smaller in magnitude than the value *Small*, it is replaced by *Small*.

Default: the smallest number that can be reciprocated safely

iopt(IO) = `?_options(?_lin_eig_self_overwrite_input, ?_dummy)`

Do not save the input array `A(:, :)`.

iopt(IO) = `?_options(?_lin_eig_self_scan_for_NaN, ?_dummy)`

Examines each input array entry to find the first value such that

`isNaN(a(i,j)) == .true.`

See the `isNaN`() function, *Chapter 10*.

Default: The array is not scanned for NaNs.

iopt(IO) = `?_options(?_lin_eig_use_QR, ?_dummy)`

Uses a rational *QR* algorithm to compute eigenvalues. Accumulate the eigenvectors using this algorithm.

Default: the eigenvectors computed using inverse iteration

iopt(IO) = `?_options(?_lin_eig_skip_Orth, ?_dummy)`

If the eigenvalues are computed using inverse iteration, skips the final orthogonalization of the vectors. This will result in a more efficient computation but the eigenvectors, while a complete set, may be far from orthogonal.

Default: the eigenvectors are normally orthogonalized if obtained using inverse iteration.

iopt(IO) = `?_options(?_lin_eig_use_Gauss_elim, ?_dummy)`

If the eigenvalues are computed using inverse iteration, uses standard elimination with partial pivoting to solve the inverse iteration problems.

Default: the eigenvectors computed using cyclic reduction

iopt(IO) = `?_options(?_lin_eig_self_set_perf_ratio`, *perf_ratio*)

Uses residuals for approximate normalized eigenvectors if they have a performance index no larger than *perf_ratio*. Otherwise an alternate approach is taken and the eigenvectors are computed again: Standard elimination is used instead of cyclic reduction, or the standard *QR* algorithm is used as a backup procedure to inverse iteration. Larger values of *perf_ratio* are less likely to cause these exceptions.

Default: *perf_ratio* = 4

FORTRAN 90 Interface

Generic: `CALL LIN_EIG_SELF (A, D [,…])`

Specific: The specific interface names are `S_LIN_EIG_SELF`, `D_LIN_EIG_SELF`, `C_LIN_EIG_SELF`, and `Z_LIN_EIG_SELF`.

Description

Routine LIN_EIG_SELF is an implementation of the *QR algorithm for* self-adjoint matrices. An orthogonal similarity reduction of the input matrix to self-adjoint tridiagonal form is performed. Then, the eigenvalue-eigenvector decomposition of a real tridiagonal matrix is calculated. The expansion of the matrix as $AV = VD$ results from a product of these matrix factors. See Golub and Van Loan (1989, Chapter 8) for details.

Fatal, Terminal, and Warning Error Messages

See the *messages.gls* file for error messages for LIN_EIG_SELF. These error messages are numbered 81–90; 101–110; 121–129; 141–149.

Examples

Example 1: Computing Eigenvalues

The eigenvalues of a self-adjoint matrix are computed. The matrix $A = C + C^T$ is used, where C is random. The magnitudes of eigenvalues of A agree with the singular values of A. Also, see operator_ex25, supplied with the product examples.

```
      use lin_eig_self_int
      use lin_sol_svd_int
      use rand_gen_int

      implicit none

! This is Example 1 for LIN_EIG_SELF.
      integer, parameter :: n=64
      real(kind(1e0)), parameter :: one=1e0
      real(kind(1e0)) :: A(n,n), b(n,0), D(n), S(n), x(n,0), y(n*n)

! Generate a random matrix and from it
! a self-adjoint matrix.
      call rand_gen(y)
      A = reshape(y,(/n,n/))
      A = A + transpose(A)

! Compute the eigenvalues of the matrix.
      call lin_eig_self(A, D)

! For comparison, compute the singular values.
      call lin_sol_svd(A, b, x, nrhs=0, s=S)

! Check the results:  Magnitude of eigenvalues should equal
! the singular values.

      if (sum(abs(abs(D) - S)) <= &
          sqrt(epsilon(one))*S(1)) then
         write (*,*) 'Example 1 for LIN_EIG_SELF is correct.'
      end if
      end
```

Output

```
Example 1 for LIN_EIG_SELF is correct.
```

Example 2: Eigenvalue-Eigenvector Expansion of a Square Matrix

A self-adjoint matrix is generated and the eigenvalues and eigenvectors are computed. Thus, $A = VDV^T$, where V is orthogonal and D is a real diagonal matrix. The matrix V is obtained using an optional argument. Also, see `operator_ex26`, *Chapter 10*.

```
      use lin_eig_self_int
      use rand_gen_int

      implicit none
! This is Example 2 for LIN_EIG_SELF.

      integer, parameter :: n=8
      real(kind(1e0)), parameter :: one=1e0
      real(kind(1e0)) :: a(n,n), d(n), v_s(n,n), y(n*n)

! Generate a random self-adjoint matrix.
      call rand_gen(y)
      a = reshape(y,(/n,n/))
      a = a + transpose(a)
! Compute the eigenvalues and eigenvectors.
      call lin_eig_self(a, d, v=v_s)
! Check the results for small residuals.
      if (sum(abs(matmul(a,v_s)-v_s*spread(d,1,n)))/d(1) <= &
              sqrt(epsilon(one))) then
         write (*,*) 'Example 2 for LIN_EIG_SELF is correct.'
      end if
      end
```

Output

```
Example 2 for LIN_EIG_SELF is correct.
```

Example 3: Computing a few Eigenvectors with Inverse Iteration

A self-adjoint $n \times n$ matrix is generated and the eigenvalues, $\{d_i\}$, are computed. The eigenvectors associated with the first k of these are computed using the self-adjoint solver, `lin_sol_self`, and inverse iteration. With random right-hand sides, these systems are as follows:

$$(A - d_i I)v_i = b_i$$

The solutions are then orthogonalized as in Hanson et al. (1991) to comprise a partial decomposition $AV = VD$ where V is an $n \times k$ matrix resulting from the orthogonalized $\{v_i\}$ and D is the $k \times k$ diagonal matrix of the distinguished eigenvalues. It is necessary to suppress the error message when the matrix is singular. Since these singularities are desirable, it is appropriate to ignore the exceptions and not print the message text. Also, see `operator_ex27`, supplied with the product examples.

```
      use lin_eig_self_int
```

```
      use lin_sol_self_int
      use rand_gen_int
      use error_option_packet

      implicit none

! This is Example 3 for LIN_EIG_SELF.

      integer i, j
      integer, parameter :: n=64, k=8
      real(kind(1d0)), parameter :: one=1d0, zero=0d0
      real(kind(1d0)) big, err
      real(kind(1d0)) :: a(n,n), b(n,1), d(n), res(n,k), temp(n,n), &
              v(n,k), y(n*n)
      type(d_options) :: iopti(2)=d_options(0,zero)

! Generate a random self-adjoint matrix.
      call rand_gen(y)
      a = reshape(y,(/n,n/))
      a = a + transpose(a)

! Compute just the eigenvalues.
      call lin_eig_self(a, d)

      do i=1, k

! Define a temporary array to hold the matrices A - eigenvalue*I.
         temp = a
         do j=1, n
            temp(j,j) = temp(j,j) - d(i)
         end do

! Use packaged option to reset the value of a small diagonal.
         iopti(1) = d_options(d_lin_sol_self_set_small,&
                    epsilon(one)*abs(d(i)))

! Use packaged option to skip singularity messages.
         iopti(2) = d_options(d_lin_sol_self_no_sing_mess,&
                    zero)
         call rand_gen(b(1:n,1))
         call lin_sol_self(temp, b, v(1:,i:i),&
              iopt=iopti)
      end do

! Orthogonalize the eigenvectors.
      do i=1, k
         big = maxval(abs(v(1:,i)))
         v(1:,i) = v(1:,i)/big
         v(1:,i) = v(1:,i)/sqrt(sum(v(1:,i)**2))
         if (i == k) cycle
         v(1:,i+1:k) = v(1:,i+1:k) + &
               spread(-matmul(v(1:,i),v(1:,i+1:k)),1,n)* &
               spread(v(1:,i),2,k-i)
      end do
      do i=k-1, 1, -1
         v(1:,i+1:k) = v(1:,i+1:k) + &
               spread(-matmul(v(1:,i),v(1:,i+1:k)),1,n)* &
               spread(v(1:,i),2,k-i)
      end do

! Check the results for both orthogonality of vectors and small
! residuals.
      res(1:k,1:k) = matmul(transpose(v),v)
      do i=1,k
         res(i,i)=res(i,i)-one
      end do
```

```
       err = sum(abs(res))/k**2
       res = matmul(a,v) - v*spread(d(1:k),1,n)
       if (err <= sqrt(epsilon(one))) then
          if (sum(abs(res))/abs(d(1)) <= sqrt(epsilon(one))) then
             write (*,*) 'Example 3 for LIN_EIG_SELF is correct.'
          end if
       end if
       end
```

Output

```
Example 3 for LIN_EIG_SELF is correct.
```

Example 4: Analysis and Reduction of a Generalized Eigensystem

A generalized eigenvalue problem is $Ax = \lambda Bx$, where A and B are $n \times n$ self-adjoint matrices. The matrix B is positive definite. This problem is reduced to an ordinary self-adjoint eigenvalue problem $Cy = \lambda y$ by changing the variables of the generalized problem to an equivalent form. The eigenvalue-eigenvector decomposition $B = VSV^T$ is first computed, labeling an eigenvalue *too small* if it is less than `epsilon(1.d0)`. The ordinary self-adjoint eigenvalue problem is $Cy = \lambda y$ provided that the rank of B, based on this definition of *Small*, has the value n. In that case,

$$C = DV^T AVD$$

where

$$D = S^{-1/2}$$

The relationship between x and y is summarized as $X = VDY$, computed after the ordinary eigenvalue problem is solved for the eigenvectors Y of C. The matrix X is normalized so that each column has Euclidean length of value one. This solution method is nonstandard for any but the most ill-conditioned matrices B. The standard approach is to compute an ordinary self-adjoint problem following computation of the Cholesky decomposition

$$B = R^T R$$

where R is upper triangular. The computation of C can also be completed efficiently by exploiting its self-adjoint property. See Golub and Van Loan (1989, Chapter 8) for more information. Also, see `operator_ex28`, *Chapter 10*.

```
       use lin_eig_self_int
       use rand_gen_int
       implicit none

 ! This is Example 4 for LIN_EIG_SELF.

       integer i
       integer, parameter :: n=64
       real(kind(1e0)), parameter :: one=1d0
       real(kind(1e0)) b_sum
       real(kind(1e0)), dimension(n,n) :: A, B, C, D(n), lambda(n), &
                 S(n), vb_d, X, ytemp(n*n), res
```

```
! Generate random self-adjoint matrices.
      call rand_gen(ytemp)
      A = reshape(ytemp,(/n,n/))
      A = A + transpose(A)

      call rand_gen(ytemp)
      B = reshape(ytemp,(/n,n/))
      B = B + transpose(B)
       b_sum = sqrt(sum(abs(B**2))/n)

! Add a scalar matrix so B is positive definite.
      do i=1, n
         B(i,i) = B(i,i) + b_sum
      end do

! Get the eigenvalues and eigenvectors for B.

      call lin_eig_self(B, S, v=vb_d)

! For full rank problems, convert to an ordinary self-adjoint
! problem.  (All of these examples are full rank.)
      if (S(n) > epsilon(one)) then

         D = one/sqrt(S)

         C = spread(D,2,n)*matmul(transpose(vb_d), &
                matmul(A,vb_d))*spread(D,1,n)

! Get the eigenvalues and eigenvectors for C.
         call lin_eig_self(C, lambda, v=X)

! Compute the generalized eigenvectors.
         X = matmul(vb_d,spread(D,2,n)*X)

! Normalize the eigenvectors for the generalized problem.
         X = X * spread(one/sqrt(sum(X**2,dim=2)),1,n)

         res =  matmul(A,X) - &
               matmul(B,X)*spread(lambda,1,n)

! Check the results.

         if (sum(abs(res))/(sum(abs(A))+sum(abs(B))) <= &
            sqrt(epsilon(one))) then
            write (*,*) 'Example 4 for LIN_EIG_SELF is correct.'
         end if
end if
end
```

Output

```
Example 4 for LIN_EIG_SELF is correct.
```

LIN_EIG_GEN

more...

Computes the eigenvalues of an $n \times n$ matrix, A. Optionally, the eigenvectors of A or A^T are computed. Using the eigenvectors of A gives the decomposition $AV = VE$, where V is an $n \times n$ complex matrix of eigenvectors, and E is the complex diagonal matrix of eigenvalues. Other options include the reduction of A to upper triangular or Schur form, reduction to block upper triangular form with 2×2 or unit sized diagonal block matrices, and reduction to upper Hessenberg form.

Required Arguments

A — Array of size $n \times n$ containing the matrix. (Input [/Output])

E — Array of size n containing the eigenvalues. These complex values are in order of decreasing absolute value. The signs of imaginary parts of the eigenvalues are in no predictable order. (Output)

Optional Arguments

NROWS = `n` (Input)
Uses array `A(1:n, 1:n)` for the input matrix.
Default: `n = SIZE(A, 1)`

v = `V(:,:)` (Output)
Returns the complex array of eigenvectors for the matrix A.

v_adj = `U(:,:)` (Output)
Returns the complex array of eigenvectors for the matrix A^T. Thus the residuals

$$S = A^T U - U\overline{E}$$

are small.

tri = `T(:,:)` (Output)

Returns the complex upper-triangular matrix *T* associated with the reduction of the matrix *A* to Schur form. Optionally a unitary matrix *W* is returned in array `V(:,:)` such that the residuals *Z* = *AW* – *WT* are small.

iopt = `iopt(:)` (Input)

Derived type array with the same precision as the input matrix. Used for passing optional data to the routine. The options are as follows:

Packaged Options for **LIN_EIG_GEN**		
Option Prefix = ?	**Option Name**	**Option Value**
`s_, d_, c_, z_`	`lin_eig_gen_set_small`	1
`s_, d_, c_, z_`	`lin_eig_gen_overwrite_input`	2
`s_, d_, c_, z_`	`lin_eig_gen_scan_for_NaN`	3
`s_, d_, c_, z_`	`lin_eig_gen_no_balance`	4
`s_, d_, c_, z_`	`lin_eig_gen_set_iterations`	5
`s_, d_, c_, z_`	`lin_eig_gen_in_Hess_form`	6
`s_, d_, c_, z_`	`lin_eig_gen_out_Hess_form`	7
`s_, d_, c_, z_`	`lin_eig_gen_out_block_form`	8
`s_, d_, c_, z_`	`lin_eig_gen_out_tri_form`	9
`s_, d_, c_, z_`	`lin_eig_gen_continue_with_V`	10
`s_, d_, c_, z_`	`lin_eig_gen_no_sorting`	11

iopt(IO) = `?_options(?_lin_eig_gen_set_small`, *Small*)

This is the tolerance used to declare off-diagonal values effectively zero compared with the size of the numbers involved in the computation of a shift.

Default: *Small* = epsilon(), the relative accuracy of arithmetic

iopt(IO) = `?_options(?_lin_eig_gen_overwrite_input, ?_dummy)`

Does not save the input array `A(:, :)`.

Default: The array is saved.

iopt(IO) = `?_options(?_lin_eig_gen_scan_for_NaN, ?_dummy)`

Examines each input array entry to find the first value such that

isNaN(a(i,j)) == `.true.`.

See the isNaN() function, *Chapter 10*.

Default: The array is not scanned for NaNs.

iopt(IO) = `?_options(?_lin_eig_no_balance, ?_dummy)`

The input matrix is not preprocessed searching for isolated eigenvalues followed by rescaling. See Golub and Van Loan (1989, Chapter 7) for references. With some optional uses of the routine, this option flag is required.

Default: The matrix is first balanced.

iopt(IO) = `?_options(?_lin_eig_gen_set_iterations, ?_dummy)`

Resets the maximum number of iterations permitted to isolate each diagonal block matrix.

Default: The maximum number of iterations is 52.

iopt(IO) = `?_options(?_lin_eig_gen_in_Hess_form, ?_dummy)`

The input matrix is in upper Hessenberg form. This flag is used to avoid the initial reduction phase which may not be needed for some problem classes.

Default: The matrix is first reduced to Hessenberg form.

iopt(IO) = `?_options(?_lin_eig_gen_out_Hess_form, ?_dummy)`

The output matrix is transformed to upper Hessenberg form, H_1. If the optional argument "`v=V(:,:)`" is passed by the calling program unit, then the array `V(:,:)` contains an orthogonal matrix $\boldsymbol{Q}_1$ such that

$$AQ_1 - Q_1H_1 \cong 0$$

Requires the simultaneous use of option `?_lin_eig_no_balance`.

Default: The matrix is reduced to diagonal form.

iopt(IO) = `?_options(?_lin_eig_gen_out_block_form, ?_dummy)`

The output matrix is transformed to upper Hessenberg form, $\boldsymbol{H}_2$, which is block upper triangular. The dimensions of the blocks are either 2 × 2 or unit sized. Nonzero subdiagonal values of $\boldsymbol{H}_2$ determine the size of the blocks. If the optional argument "`v=V(:,:)`" is passed by the calling program unit, then the array `V(:,:)` contains an orthogonal matrix $\boldsymbol{Q}_2$, such that

$$AQ_2 - Q_2H_2 \cong 0$$

Requires the simultaneous use of option `?_lin_eig_no_balance`.

Default: The matrix is reduced to diagonal form.

iopt(IO) = `?_options(?_lin_eig_gen_out_tri_form, ?_dummy)`

The output matrix is transformed to upper-triangular form, *T*. If the optional argument "`v=V(:,:)`" is passed by the calling program unit, then the array `V(:,:)` contains a unitary matrix *W* such that $AW - WT \cong 0$. The upper triangular matrix *T* is returned in the optional argument "`tri=T(:,:)`". The eigenvalues of *A* are the diagonal entries of the matrix *T*. They are in no particular order. The output array `E(:)` is blocked with NaNs using this option. This option requires the simultaneous use of option `?_lin_eig_no_balance`.

Default: The matrix is reduced to diagonal form.

iopt(IO) = `?_options(?_lin_eig_gen_continue_with_V, ?_dummy)`

As a convenience or for maintaining efficiency, the calling program unit sets the optional argument "`v=V(:,:)`" to a matrix that has transformed a problem to the similar matrix, $\dot{A}$. The contents of `V(:,:)` are updated by the transformations used in the algorithm. Requires the simultaneous use of option `?_lin_eig_no_balance`.

Default: The array `V(:,:)` is initialized to the identity matrix.

iopt(IO) = `?_options(?_lin_eig_gen_no_sorting, ?_dummy)`

Does not sort the eigenvalues as they are isolated by solving the 2×2 or unit sized blocks. This will have the effect of guaranteeing that complex conjugate pairs of eigenvalues are adjacent in the array `E(:)`.

Default: The entries of `E(:)` are sorted so they are non-increasing in absolute value.

FORTRAN 90 Interface

Generic:`CALL LIN_EIG_GEN (A, E [,…])`

Specific:The specific interface names are `S_LIN_EIG_GEN`, `D_LIN_EIG_GEN`, `C_LIN_EIG_GEN`, `and Z_LIN_EIG_GEN`.

Description

The input matrix *A* is first balanced. The resulting similar matrix is transformed to upper Hessenberg form using orthogonal transformations. The double-shifted *QR* algorithm transforms the Hessenberg matrix so that 2×2 or unit sized blocks remain along the main diagonal. Any off-diagonal that is classified as "small" in order to achieve this block form is set to the value zero. Next the block upper triangular matrix is transformed to upper triangular form with unitary rotations. The eigenvectors of the upper triangular matrix are computed using back substitution. Care is taken to avoid overflows during this process. At the end, eigenvectors are normalized to have Euclidean length one, with the largest component real and positive. This algorithm follows that given in Golub and Van Loan, (1989, Chapter 7), with some novel organizational details for additional options, efficiency and robustness.

Fatal, Terminal, and Warning Error Messages

See the *messages.gls* file for error messages for `LIN_EIG_GEN`. These error messages are numbered 841–858; 861–878; 881–898; 901–918.

Examples

Example 1: Computing Eigenvalues

The eigenvalues of a random real matrix are computed. These values define a complex diagonal matrix *E*. Their correctness is checked by obtaining the eigenvector matrix *V* and verifying that the residuals $R = AV - VE$ are small. Also, see `operator_ex29`, supplied with the product examples.

```
      use lin_eig_gen_int
      use rand_gen_int

      implicit none

! This is Example 1 for LIN_EIG_GEN.

      integer, parameter :: n=32
      real(kind(1d0)), parameter :: one=1d0
      real(kind(1d0)) A(n,n), y(n*n), err
      complex(kind(1d0)) E(n), V(n,n), E_T(n)
      type(d_error) :: d_epack(16) = d_error(0,0d0)

! Generate a random matrix.
      call rand_gen(y)
      A = reshape(y,(/n,n/))

! Compute only the eigenvalues.
      call lin_eig_gen(A, E)

! Compute the decomposition, A*V = V*values,
! obtaining eigenvectors.
      call lin_eig_gen(A, E_T, v=V)

! Use values from the first decomposition, vectors from the
! second decomposition, and check for small residuals.
      err = sum(abs(matmul(A,V) - V*spread(E,DIM=1,NCOPIES=n))) &
                / sum(abs(E))
      if (err  <= sqrt(epsilon(one))) then
         write (*,*) 'Example 1 for LIN_EIG_GEN is correct.'
      end if

      end
```

Output

```
Example 1 for LIN_EIG_GEN is correct.
```

Example 2: Complex Polynomial Equation Roots

The roots of a complex polynomial equation,

$$f(z) \equiv \sum_{k=1}^{n} b_k z^{n-k} + z^n = 0$$

are required. This algebraic equation is formulated as a matrix eigenvalue problem. The equivalent matrix eigenvalue problem is solved using the upper Hessenberg matrix which has the value zero except in row number 1 and along the first subdiagonal. The entries in the first row are given by
$a_{1,j} = -b_j$, $i = 1, \ldots, n$, while those on the first subdiagonal have the value one. This is a *companion matrix* for the polynomial. The results are checked by testing for small values of $|f(e_i)|$, $i = 1, \ldots, n$, at the eigenvalues of the matrix, which are the roots of $f(z)$. Also, see `operator_ex30`, supplied with the product examples.

```
      use lin_eig_gen_int
      use rand_gen_int

      implicit none
! This is Example 2 for LIN_EIG_GEN.

      integer i
      integer, parameter :: n=12
      real(kind(1d0)), parameter :: one=1.0d0, zero=0.0d0
      real(kind(1d0)) err, t(2*n)
      type(d_options) :: iopti(1)=d_options(0,zero)
      complex(kind(1d0)) a(n,n), b(n), e(n), f(n), fg(n)

      call rand_gen(t)
      b = cmplx(t(1:n),t(n+1:),kind(one))

! Define the companion matrix with polynomial coefficients
! in the first row.

      a = zero

      do i=2, n
         a(i,i-1) = one
      end do

      a(1,1:n) = -b

! Note that the input companion matrix is upper Hessenberg.
      iopti(1) = d_options(z_lin_eig_gen_in_Hess_form,zero)

! Compute complex eigenvalues of the companion matrix.

      call lin_eig_gen(a, e, iopt=iopti)

      f=one; fg=one

! Use Horner's method for evaluation of the complex polynomial
! and size gauge at all roots.

      do i=1, n
         f = f*e + b(i)
         fg = fg*abs(e) + abs(b(i))
      end do

! Check for small errors at all roots.

      err = sum(abs(f/fg))/n
      if (err <= sqrt(epsilon(one))) then
         write (*,*) 'Example 2 for LIN_EIG_GEN is correct.'
```

```
      end if
      end
```

Output

```
Example 2 for LIN_EIG_GEN is correct.
```

Example 3: Solving Parametric Linear Systems with a Scalar Change

The efficient solution of a family of linear algebraic equations is required. These systems are $(A + hI)x = b$. Here A is an $n \times n$ real matrix, I is the identity matrix, and b is the right-hand side matrix. The scalar h is such that the coefficient matrix is nonsingular. The method is based on the Schur form for matrix A: $AW = WT$, where W is unitary and T is upper triangular. This provides an efficient solution method for several values of h, once the Schur form is computed. The solution steps solve, for y, the upper triangular linear system

$$\left(T + hI\right)y = \overline{W}^T b$$

Then, $x = x(h) = Wy$. This is an efficient and accurate method for such parametric systems provided the expense of computing the Schur form has a pay-off in later efficiency. Using the Schur form in this way, it is not required to compute an LU factorization of $A + hI$ with each new value of h. Note that even if the data A, h, and b are real, subexpressions for the solution may involve complex intermediate values, with $x(h)$ finally a real quantity. Also, see `operator_ex31`, supplied with the product examples.

```
      use lin_eig_gen_int
      use lin_sol_gen_int
      use rand_gen_int

      implicit none

! This is Example 3 for LIN_EIG_GEN.

      integer i
      integer, parameter :: n=32, k=2
      real(kind(1e0)), parameter :: one=1.0e0, zero=0.0e0
      real(kind(1e0)) a(n,n), b(n,k), x(n,k), temp(n*max(n,k)), h, err
      type(s_options) :: iopti(2)
      complex(kind(1e0)) w(n,n), t(n,n), e(n), z(n,k)

      call rand_gen(temp)
      a = reshape(temp,(/n,n/))

      call rand_gen(temp)
      b = reshape(temp,(/n,k/))

      iopti(1) = s_options(s_lin_eig_gen_out_tri_form,zero)
      iopti(2) = s_options(s_lin_eig_gen_no_balance,zero)

! Compute the Schur decomposition of the matrix.

      call lin_eig_gen(a, e, v=w, tri=t, &
            iopt=iopti)

! Choose a value so that A+h*I is non-singular.
      h = one

! Solve for (A+h*I)x=b using the Schur decomposition.
```

```
      z = matmul(conjg(transpose(w)),b)

! Solve intermediate upper-triangular system with implicit
! additive diagonal, h*I.  This is the only dependence on
! h in the solution process.

       do i=n,1,-1
         z(i,1:k) = z(i,1:k)/(t(i,i)+h)
         z(1:i-1,1:k) = z(1:i-1,1:k) + &
                        spread(-t(1:i-1,i),dim=2,ncopies=k)* &
                        spread(z(i,1:k),dim=1,ncopies=i-1)
      end do

! Compute the solution.  It should be the same as x, but will not be
! exact due to rounding errors.  (The quantity real(z,kind(one)) is
! the real-valued answer when the Schur decomposition method is used.)

      z = matmul(w,z)

! Compute the solution by solving for x directly.

       do i=1, n
         a(i,i) = a(i,i) + h
      end do

      call lin_sol_gen(a, b, x)

! Check that x and z agree approximately.
      err = sum(abs(x-z))/sum(abs(x))
      if (err <= sqrt(epsilon(one))) then
         write (*,*) 'Example 3 for LIN_EIG_GEN is correct.'
      end if

      end
```

Output

```
Example 3 for LIN_EIG_GEN is correct.
```

Example 4: Accuracy Estimates of Eigenvalues Using Adjoint and Ordinary Eigenvectors

A matrix A has entries that are subject to uncertainty. This is expressed as the realization that A can be replaced by the matrix $A + \eta B$, where the value η is "small" but still significantly larger than machine precision. The matrix B satisfies $\|B\| \le \|A\|$. A variation in eigenvalues is estimated using analysis found in Golub and Van Loan, (1989, Chapter 7, p. 344). Each eigenvalue and eigenvector is expanded in a power series in η. With

$$e_i(\eta) \approx e_i + \eta \dot{e}_i \eta$$

and normalized eigenvectors, the bound

$$|\dot{e}_i| \le \frac{\|A\|}{|u_i^* v_i|}$$

is satisfied. The vectors u_i and v_i are the ordinary and adjoint eigenvectors associated respectively with e_i and its complex conjugate. This gives an upper bound on the size of the change to each $|e_i|$ due to changing the matrix data. The reciprocal

$$|u_i^* v_i|^{-1}$$

is defined as the *condition number* of e_i. Also, see `operator_ex32`, *Chapter 10*.

```
      use lin_eig_gen_int
      use rand_gen_int

      implicit none

! This is Example 4 for LIN_EIG_GEN.

      integer i
      integer, parameter :: n=17
      real(kind(1d0)), parameter :: one=1d0
      real(kind(1d0)) a(n,n), c(n,n), variation(n), y(n*n), temp(n), &
              norm_of_a, eta
      complex(kind(1d0)), dimension(n,n) :: e(n), d(n), u, v

! Generate a random matrix.
      call rand_gen(y)
      a = reshape(y,(/n,n/))

! Compute the eigenvalues, left- and right- eigenvectors.
      call lin_eig_gen(a, e, v=v, v_adj=u)

! Compute condition numbers and variations of eigenvalues.
      norm_of_a = sqrt(sum(a**2)/n)
      do i=1, n
         variation(i) = norm_of_a/abs(dot_product(u(1:n,i), &
                                             v(1:n,i)))
      end do

! Now perturb the data in the matrix by the relative factors
! eta=sqrt(epsilon) and solve for values again.  Check the
! differences compared to the estimates.  They should not exceed
! the bounds.

      eta = sqrt(epsilon(one))
      do i=1, n
         call rand_gen(temp)
         c(1:n,i) = a(1:n,i) + (2*temp - 1)*eta*a(1:n,i)
      end do

      call lin_eig_gen(c,d)


! Looking at the differences of absolute values accounts for
! switching signs on the imaginary parts.
      if (count(abs(d)-abs(e) > eta*variation) == 0) then
         write (*,*) 'Example 4 for LIN_EIG_GEN is correct.'
      end if

      end
```

Output

```
Example 4 for LIN_EIG_GEN is correct.
```

LIN_GEIG_GEN

more...

Computes the generalized eigenvalues of an $n \times n$ matrix pencil, $Av = \lambda Bv$. Optionally, the generalized eigenvectors are computed. If either of A or B is nonsingular, there are diagonal matrices α and β, and a complex matrix V, all computed such that $AV\beta = BV\alpha$.

Required Arguments

A — Array of size $n \times n$ containing the matrix A. (Input [/Output])

B — Array of size $n \times n$ containing the matrix B. (Input [/Output])

ALPHA — Array of size n containing diagonal matrix factors of the generalized eigenvalues. These complex values are in order of decreasing absolute value. (Output)

BETAV — Array of size n containing diagonal matrix factors of the generalized eigenvalues. These real values are in order of decreasing value. (Output)

Optional Arguments

NROWS = `n` (Input)
Uses arrays `A`(1:`n`, 1:`n`) and `B`(1:`n`, 1:`n`) for the input matrix pencil.
Default: `n` = `SIZE`(`A`, 1)

v = `V(:,:)` (Output)
Returns the complex array of generalized eigenvectors for the matrix pencil.

iopt = `iopt(:)` (Input)
Derived type array with the same precision as the input matrix. Used for passing optional data to the routine. The options are as follows:

Packaged Options for LIN_GEIG_GEN		
Option Prefix = ?	**Option Name**	**Option Value**
s_, d_, c_, z_	lin_geig_gen_set_small	1
s_, d_, c_, z_	lin_geig_gen_overwrite_input	2
s_, d_, c_, z_	lin_geig_gen_scan_for_NaN	3
s_, d_, c_, z_	lin_geig_gen_self_adj_pos	4
s_, d_, c_, z_	lin_geig_gen_for_lin_sol_self	5
s_, d_, c_, z_	lin_geig_gen_for_lin_eig_self	6
s_, d_, c_, z_	lin_geig_gen_for_lin_sol_lsq	7
s_, d_, c_, z_	lin_geig_gen_for_lin_eig_gen	8

iopt(IO) = ?_options(?_lin_geig_gen_set_small, *Small*)

This tolerance, multiplied by the sum of absolute value of the matrix *B*, is used to define a small diagonal term in the routines lin_sol_lsq and lin_sol_self. That value can be replaced using the option flags lin_geig_gen_for_lin_sol_lsq, and lin_geig_gen_for_lin_sol_self.

Default: *Small* = epsilon(.), the relative accuracy of arithmetic.

iopt(IO) = ?_options(?_lin_geig_gen_overwrite_input, ?_dummy)

Does not save the input arrays A(:, :) and B(:, :).

Default: The array is saved.

iopt(IO) = ?_options(?_lin_geig_gen_scan_for_NaN, ?_dummy)

Examines each input array entry to find the first value such that

isNaN(a(i,j)) .or. isNaN(b(i,j)) == .true.

See the isNaN() function, *Chapter 10*.

Default: The arrays are not scanned for NaNs.

iopt(IO) = ?_options(?_lin_geig_gen_self_adj_pos, ?_dummy)

If both matrices *A* and *B* are self-adjoint and additionally *B* is positive-definite, then the Cholesky algorithm is used to reduce the matrix pencil to an ordinary self-adjoint eigenvalue problem.

iopt(IO) = ?_options(?_lin_geig_gen_for_lin_sol_self, ?_dummy)

iopt(IO+1) = ?_options((k=size of options for lin_sol_self), ?_dummy)

The options for lin_sol_self follow as data in iopt().

iopt(IO) = `?_options(?_lin_geig_gen_for_lin_eig_self, ?_dummy)`

iopt(IO+1) = ?_options((k=size of options for lin_eig_self), ?_dummy)
The options for `lin_eig_self` follow as data in `iopt()`.

iopt(IO) = `?_options(?_lin_geig_gen_for_lin_sol_lsq, ?_dummy)`

iopt(IO+1) = `?_options((k=size of options for lin_sol_lsq), ?_dummy)`
The options for `lin_sol_lsq` follow as data in `iopt()`.

iopt(IO) = `?_options(?_lin_geig_gen_for_lin_eig_gen, ?_dummy)`

iopt(IO+1) = `?_options((k=size of options for lin_eig_gen), ?_dummy)`
The options for `lin_eig_gen` follow as data in `iopt()`.

FORTRAN 90 Interface

Generic:`CALL LIN_GEIG_GEN` (A, B, `ALPHA`, `BETAV` [,…])

Specific:The specific interface names are `S_LIN_GEIG_GEN`, `D_LIN_GEIG_GEN`, `C_LIN_GEIG_GEN`, and `Z_LIN_GEIG_GEN`.

Description

Routine `LIN_GEIG_GEN` implements a standard algorithm that reduces a generalized eigenvalue or matrix pencil problem to an ordinary eigenvalue problem. An orthogonal decomposition is computed

$$BP^T = HR$$

The orthogonal matrix H is the product of $n-1$ row permutations, each followed by a Householder transformation. Column permutations, P, are chosen at each step to maximize the Euclidian length of the pivot column. The matrix R is upper triangular. Using the default tolerance $\tau = \varepsilon\|B\|$, where ε is machine relative precision, each diagonal entry of R exceeds τ in value. Otherwise, R is singular. In that case A and B are interchanged and the orthogonal decomposition is computed one more time. If both matrices are singular the problem is declared *singular* and is not solved. The interchange of A and B is accounted for in the output diagonal matrices α and β. The ordinary eigenvalue problem is $Cx = \lambda x$, where

$$C = H^T A P^T R^{-1}$$

and

$$RPv = x$$

If the matrices A and B are self-adjoint and if, in addition, B is positive-definite, then a more efficient reduction than the default algorithm can be optionally used to solve the problem: A Cholesky decomposition is obtained, $R^T R = PBP^T$. The matrix R is upper triangular and P is a permutation matrix. This is equivalent to the ordinary self-adjoint eigenvalue problem $Cx = \lambda x$, where $RPv = x$ and

$$C = R^{-T} PAP^T R^{-1}$$

The self-adjoint eigenvalue problem is then solved.

Fatal, Terminal, and Warning Error Messages

See the *messages.gls* file for error messages for `LIN_GEIG_GEN`. These error messages are numbered 921–936; 941–956; 961–976; 981–996.

Examples

Example 1: Computing Generalized Eigenvalues

The generalized eigenvalues of a random real matrix pencil are computed. These values are checked by obtaining the generalized eigenvectors and then showing that the residuals

$$AV - BV \alpha \beta^{-1}$$

are *small*. Note that when the matrix B is nonsingular $\beta = I$, the identity matrix. When B is singular and A is nonsingular, some diagonal entries of β are essentially zero. This corresponds to "infinite eigenvalues" of the matrix pencil. This random matrix pencil example has all finite eigenvalues. Also, see `operator_ex33`, *Chapter 10*.

```
      use lin_geig_gen_int
      use rand_gen_int

      implicit none

! This is Example 1 for LIN_GEIG_GEN.

      integer, parameter :: n=32
      real(kind(1d0)), parameter :: one=1d0
      real(kind(1d0)) A(n,n), B(n,n), betav(n), beta_t(n), err, y(n*n)
      complex(kind(1d0)) alpha(n), alpha_t(n), V(n,n)

! Generate random matrices for both A and B.
      call rand_gen(y)
      A = reshape(y,(/n,n/))
      call rand_gen(y)
      B = reshape(y,(/n,n/))

! Compute the generalized eigenvalues.
      call lin_geig_gen(A, B, alpha, betav)
```

```
! Compute the full decomposition once again, A*V = B*V*values.
      call lin_geig_gen(A, B, alpha_t, beta_t, &
                  v=V)

! Use values from the first decomposition, vectors from the
! second decomposition, and check for small residuals.

      err = sum(abs(matmul(A,V) - &
                     matmul(B,V)*spread(alpha/betav,DIM=1,NCOPIES=n))) / &
                  sum(abs(a)+abs(b))
      if (err  <= sqrt(epsilon(one))) then
         write (*,*) 'Example 1 for LIN_GEIG_GEN is correct.'
      end if

      end
```

Output

```
Example 1 for LIN_GEIG_GEN is correct.
```

Example 2: Self-Adjoint, Positive-Definite Generalized Eigenvalue Problem

This example illustrates the use of optional flags for the special case where *A* and B are complex self-adjoint matrices, and *B* is positive-definite. For purposes of maximum efficiency an option is passed to routine `LIN_SOL_SELF` so that pivoting is not used in the computation of the Cholesky decomposition of matrix *B*. This example does not require that secondary option. Also, see `operator_ex34`, supplied with the product examples.

```
      use lin_geig_gen_int
      use lin_sol_self_int
      use rand_gen_int

      implicit none

! This is Example 2 for LIN_GEIG_GEN.

      integer i
      integer, parameter :: n=32
      real(kind(1d0)), parameter :: one=1.0d0, zero=0.0d0
      real(kind(1d0)) betav(n), temp_c(n,n), temp_d(n,n), err
      type(d_options) :: iopti(4)=d_options(0,zero)
      complex(kind(1d0)), dimension(n,n) :: A, B, C, D, V, alpha(n)

! Generate random matrices for both A and B.
      do i=1, n
         call rand_gen(temp_c(1:n,i))
         call rand_gen(temp_d(1:n,i))
      end do
      c = temp_c; d = temp_c
      do i=1, n
         call rand_gen(temp_c(1:n,i))
         call rand_gen(temp_d(1:n,i))
      end do
      c = cmplx(real(c),temp_c,kind(one))
      d = cmplx(real(d),temp_d,kind(one))

      a = conjg(transpose(c)) + c
      b = matmul(conjg(transpose(d)),d)

! Set option so that the generalized eigenvalue solver uses an
```

```
! efficient method for well-posed, self-adjoint problems.
      iopti(1) = d_options(z_lin_geig_gen_self_adj_pos,zero)
      iopti(2) = d_options(z_lin_geig_gen_for_lin_sol_self,zero)

! Number of secondary optional data items and the options:
      iopti(3) =   d_options(1,zero)
      iopti(4) =   d_options(z_lin_sol_self_no_pivoting,zero)

      call lin_geig_gen(a, b, alpha, betav, v=v, &
        iopt=iopti)

! Check that residuals are small.  Use the real part of alpha
! since the values are known to be real.

      err = sum(abs(matmul(a,v) - matmul(b,v)* &
            spread(real(alpha,kind(one))/betav,dim=1,ncopies=n))) / &
            sum(abs(a)+abs(b))
      if (err <= sqrt(epsilon(one))) then
         write (*,*) 'Example 2 for LIN_GEIG_GEN is correct.'
      end if

      end
```

Output

```
Example 2 for LIN_GEIG_GEN is correct.
```

Example 3: A Test for a Regular Matrix Pencil

In the classification of Differential Algebraic Equations (DAE), a system with linear constant coefficients is given by $A\dot{x} + Bx = f$. Here A and B are $n \times n$ matrices, and f is an n-vector that is not part of this example. The DAE system is defined as *solvable* if and only if the quantity *det* ($\mu A + B$) does not vanish identically as a function of the dummy parameter μ. A sufficient condition for solvability is that the generalized eigenvalue problem $Av = \lambda Bv$ is nonsingular. By constructing A and B so that both are singular, the routine flags nonsolvability in the DAE by returning NaN for the generalized eigenvalues. Also, see `operator_ex35`, supplied with the product examples.

```
      use lin_geig_gen_int
      use rand_gen_int
      use error_option_packet
      use isnan_int

      implicit none

! This is Example 3 for LIN_GEIG_GEN.
       integer, parameter :: n=6
      real(kind(1d0)), parameter :: one=1.0d0, zero=0.0d0
      real(kind(1d0)) a(n,n), b(n,n), betav(n), y(n*n)
      type(d_options) iopti(1)
      type(d_error) epack(1)
      complex(kind(1d0)) alpha(n)

! Generate random matrices for both A and B.
      call rand_gen(y)
      a = reshape(y,(/n,n/))

      call rand_gen(y)
      b = reshape(y,(/n,n/))

! Make columns of A and B zero, so both are singular.
      a(1:n,n) = 0; b(1:n,n) = 0
```

```
! Set internal tolerance for a small diagonal term.
      iopti(1) = d_options(d_lin_geig_gen_set_small,sqrt(epsilon(one)))

! Compute the generalized eigenvalues.
      call lin_geig_gen(a, b, alpha, betav, &
        iopt=iopti,epack=epack)

! See if singular DAE system is detected.
! (The size of epack() is too small for the message, so
! output is blocked with NaNs.)
      if (isnan(alpha)) then
         write (*,*) 'Example 3 for LIN_GEIG_GEN is correct.'
      end if

      end
```

Output

```
Example 3 for LIN_GEIG_GEN is correct.
```

Example 4: Larger Data Uncertainty than Working Precision

Data values in both matrices *A* and *B* are assumed to have relative errors that can be as large as $\varepsilon^{1/2}$ where ε is the relative machine precision. This example illustrates the use of an optional flag that resets the tolerance used in routine `lin_sol_lsq` for determining a singularity of either matrix. The tolerance is reset to the new value $\varepsilon^{1/2}\|B\|$ and the generalized eigenvalue problem is solved. We anticipate that *B* might be singular and detect this fact. Also, see `---operator_ex36`, *Chapter 10*.

```
      use lin_geig_gen_int
      use lin_sol_lsq_int
      use rand_gen_int
      use isNaN_int

      implicit none

! This is Example 4 for LIN_GEIG_GEN.

      integer, parameter :: n=32
      real(kind(1d0)), parameter :: one=1d0, zero=0d0
      real(kind(1d0)) a(n,n), b(n,n), betav(n), y(n*n), err
      type(d_options) iopti(4)
      type(d_error) epack(1)
      complex(kind(1d0)) alpha(n), v(n,n)

! Generate random matrices for both A and B.

      call rand_gen(y)
      a = reshape(y,(/n,n/))

      call rand_gen(y)
      b = reshape(y,(/n,n/))

! Set the option, a larger tolerance than default for lin_sol_lsq.
      iopti(1) = d_options(d_lin_geig_gen_for_lin_sol_lsq,zero)

! Number of secondary optional data items
      iopti(2) =   d_options(2,zero)
      iopti(3) =   d_options(d_lin_sol_lsq_set_small,sqrt(epsilon(one))*&
```

```
                      sqrt(sum(b**2)/n))
      iopti(4) =   d_options(d_lin_sol_lsq_no_sing_mess,zero)

! Compute the generalized eigenvalues.
      call lin_geig_gen(A, B, alpha, betav, v=v, &
                  iopt=iopti, epack=epack)

      if(.not. isNaN(alpha)) then

! Check the residuals.
        err = sum(abs(matmul(A,V)*spread(betav,dim=1,ncopies=n) - &
                     matmul(B,V)*spread(alpha,dim=1,ncopies=n))) / &
                sum(abs(a)+abs(b))
        if (err  <= sqrt(epsilon(one))) then
           write (*,*) 'Example 4 for LIN_GEIG_GEN is correct.'

        end if
      end if
      end
```

Output

```
Example 4 for LIN_GEIG_GEN is correct.
```

EVLRG

more...

Computes all of the eigenvalues of a real matrix.

Required Arguments

A — Real full matrix of order `N`. (Input)

EVAL — Complex vector of length `N` containing the eigenvalues of `A` in decreasing order of magnitude. (Output)

Optional Arguments

N — Order of the matrix. (Input)
Default: `N` = `SIZE` (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = `SIZE` (`A`,1).

FORTRAN 90 Interface

Generic:`CALL EVLRG (A, EVAL [,…])`

Specific:The specific interface names are `S_EVLRG` and `D_EVLRG`.

FORTRAN 77 Interface

Single:`CALL EVLRG (N, A, LDA, EVAL)`

Double:The double precision name is `DEVLRG`.

Description

Routine EVLRG computes the eigenvalues of a real matrix. The matrix is first balanced. Elementary or Gauss similarity transformations with partial pivoting are used to reduce this balanced matrix to a real upper Hessenberg matrix. A hybrid double — shifted LR — QR algorithm is used to compute the eigenvalues of the Hessenberg matrix, Watkins and Elsner (1990).

The underlying code is based on either EISPACK or LAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation, see "*Using ScaLAPACK, LAPACK, LINPACK, and EISPACK*" in the Introduction section of this manual. The LR— QR algorithm is based on software work of Watkins and Haag. Further details, some timing data, and credits are given in Hanson et al. (1990).

Comments

1. Workspace may be explicitly provided, if desired, by use of E3LRG/DE3LRG. The reference is:

   ```
   CALL E3LRG (N, A, LDA, EVAL, ACOPY, WK, IWK)
   ```

   The additional arguments are as follows:

   ACOPY — Real work array of length N^2. A and ACOPY may be the same, in which case the first N^2 elements of A will be destroyed.

   WK — Floating-point work array of size 4N.

   IWK — Integer work array of size 2N.

2. Informational error

Type	Code	Description
4	1	The iteration for an eigenvalue failed to converge.

3. *Integer Options* with *Chapter 11* Options Manager

   1 This option uses eight values to solve memory bank conflict (access inefficiency) problems. In routine E3LRG, the internal or working leading dimension of ACOPY is increased by IVAL(3) when N is a multiple of IVAL(4). The values IVAL(3) and IVAL(4) are temporarily replaced by IVAL(1) and IVAL(2), respectively, in routine EVLRG . Additional memory allocation and option value restoration are automatically done in EVLRG. There is no requirement that users change existing applications that use EVLRG or E3LRG. Default values for the option are IVAL(*) = 1, 16, 0, 1, 1, 16, 0, 1. Items 5-8 in IVAL(*) are for the generalized eigenvalue problem and are not used in EVLRG.

Example

In this example, a DATA statement is used to set *A* to a matrix given by Gregory and Karney (1969, page 85). The eigenvalues of this real matrix are computed and printed. The exact eigenvalues are known to be {4, 3, 2, 1}.

```
      USE EVLRG_INT
      USE WRCRN_INT

      IMPLICIT   NONE
!                                  Declare variables
      INTEGER    LDA, N
      PARAMETER  (N=4, LDA=N)
!
      REAL       A(LDA,N)
      COMPLEX    EVAL(N)

!                                  Set values of A
!
!                                  A = ( -2.0    2.0    2.0    2.0  )
!                                      ( -3.0    3.0    2.0    2.0  )
!                                      ( -2.0    0.0    4.0    2.0  )
!                                      ( -1.0    0.0    0.0    5.0  )
      DATA A/-2.0, -3.0, -2.0, -1.0, 2.0, 3.0, 0.0, 0.0, 2.0, 2.0, &
          4.0, 0.0, 2.0, 2.0, 2.0, 5.0/
!
!                                  Find eigenvalues of A
      CALL EVLRG (A, EVAL)
!                                  Print results
      CALL WRCRN ('EVAL', EVAL, 1, N, 1)
      END
```

Output

```
                          EVAL
              1                 2                 3                 4
 ( 4.000, 0.000)   ( 3.000, 0.000)   ( 2.000, 0.000)   ( 1.000, 0.000)
```

EVCRG

more...

Computes all of the eigenvalues and eigenvectors of a real matrix.

Required Arguments

A — Floating-point array containing the matrix. (Input)

EVAL — Complex array of size N containing the eigenvalues of A in decreasing order of magnitude. (Output)

EVEC — Complex array containing the matrix of eigenvectors. (Output)
The J-th eigenvector, corresponding to EVAL(J), is stored in the J-th column. Each vector is normalized to have Euclidean length equal to the value one.

Optional Arguments

N — Order of the matrix. (Input)
Default: N = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = SIZE (A,1).

LDEVEC — Leading dimension of EVEC exactly as specified in the dimension statement of the calling program. (Input)
Default: LDEVEC = SIZE (EVEC,1).

FORTRAN 90 Interface

Generic:CALL EVCRG (A, EVAL, EVEC [,…])

Specific:The specific interface names are S_EVCRG and D_EVCRG.

FORTRAN 77 Interface

Single: CALL EVCRG (N, A, LDA, EVAL, EVEC, LDEVEC)

Double: The double precision name is DEVCRG.

Description

Routine EVCRG computes the eigenvalues and eigenvectors of a real matrix. The matrix is first balanced. Orthogonal similarity transformations are used to reduce the balanced matrix to a real upper Hessenberg matrix. The implicit double – shifted QR algorithm is used to compute the eigenvalues and eigenvectors of this Hessenberg matrix. The eigenvectors are normalized such that each has Euclidean length of value one. The largest component is real and positive.

The underlying code is based on either EISPACK or LAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation, see "*Using ScaLAPACK, LAPACK, LINPACK, and EISPACK*" in the Introduction section of this manual. Further details, some timing data, and credits are given in Hanson et al. (1990).

Comments

1. Workspace may be explicitly provided, if desired, by use of E8CRG/DE8CRG. The reference is:

   CALL E8CRG (N, A, LDA, EVAL, EVEC, LDEVEC, ACOPY, ECOPY, WK, IWK)

   The additional arguments are as follows:

   ACOPY — Floating-point work array of size N by N. The arrays A and ACOPY may be the same, in which case the first N^2 elements of A will be destroyed. The array ACOPY can have its working row dimension increased from N to a larger value. An optional usage is required. See Item 3 below for further details.

   ECOPY — Floating-point work array of default size N by N + 1. The working, leading dimension of ECOPY is the same as that for ACOPY. To increase this value, an optional usage is required. See Item 3 below for further details.

   WK — Floating-point work array of size 6N.

   IWK — Integer work array of size N.

2. Informational error

Type	Code	Description
4	1	The iteration for the eigenvalues failed to converge. No eigenvalues or eigenvectors are computed.

3. *Integer Options* with *Chapter 11* Options Manager

1 This option uses eight values to solve memory bank conflict (access inefficiency) problems. In routine `E8CRG`, the internal or working leading dimensions of `ACOPY` and `ECOPY` are both increased by `IVAL`(3) when `N` is a multiple of `IVAL`(4). The values `IVAL`(3) and `IVAL`(4) are temporarily replaced by `IVAL`(1) and `IVAL`(2), respectively, in routine `EVCRG`. Additional memory allocation and option value restoration are automatically done in `EVCRG`. There is no requirement that users change existing applications that use `EVCRG` or `E8CRG`. Default values for the option are `IVAL(*)` = 1, 16, 0, 1, 1, 16, 0, 1. Items 5–8 in `IVAL(*)` are for the generalized eigenvalue problem and are not used in `EVCRG`.

Example

In this example, a `DATA` statement is used to set *A* to a matrix given by Gregory and Karney (1969, page 82). The eigenvalues and eigenvectors of this real matrix are computed and printed. The performance index is also computed and printed. This serves as a check on the computations. For more details, see IMSL routine `EPIRG`.

```
      USE EVCRG_INT
      USE EPIRG_INT
      USE UMACH_INT
      USE WRCRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    LDA, LDEVEC, N
      PARAMETER  (N=3, LDA=N, LDEVEC=N)
      INTEGER    NOUT
      REAL       PI
      COMPLEX    EVAL(N), EVEC(LDEVEC,N)
      REAL       A(LDA,N)

!                                 Define values of A:
!
!                                 A = (  8.0   -1.0   -5.0  )
!                                     ( -4.0    4.0   -2.0  )
!                                     ( 18.0   -5.0   -7.0  )
!
      DATA A/8.0, -4.0, 18.0, -1.0, 4.0, -5.0, -5.0, -2.0, -7.0/
!
!                                 Find eigenvalues and vectors of A
      CALL EVCRG (A, EVAL, EVEC)
!                                 Compute performance index
      PI = EPIRG(N,A,EVAL,EVEC)
!                                 Print results
      CALL UMACH (2, NOUT)
      CALL WRCRN ('EVAL', EVAL, 1, N, 1)
      CALL WRCRN ('EVEC', EVEC)
      WRITE (NOUT,'(/,A,F6.3)') ' Performance index = ', PI
      END
```

Output

```
                       EVAL
               1                  2                  3
 ( 2.000, 4.000)  ( 2.000,-4.000)  ( 1.000, 0.000)

                            EVEC
```

```
                     1                      2                      3
   1  ( 0.3162, 0.3162)  ( 0.3162,-0.3162)  ( 0.4082, 0.0000)
   2  (-0.0000, 0.6325)  (-0.0000,-0.6325)  ( 0.8165, 0.0000)
   3  ( 0.6325, 0.0000)  ( 0.6325, 0.0000)  ( 0.4082, 0.0000)

   Performance index =  0.026
```

EPIRG

This function computes the performance index for a real eigensystem.

Function Return Value

EPIRG — Performance index. (Output)

Required Arguments

NEVAL — Number of eigenvalue/eigenvector pairs on which the performance index computation is based. (Input)

A — Matrix of order `N`. (Input)

EVAL — Complex vector of length `NEVAL` containing eigenvalues of `A`. (Input)

EVEC — Complex `N` by `NEVAL` array containing eigenvectors of `A`. (Input)
The eigenvector corresponding to the eigenvalue `EVAL(J)` must be in the `J`-th column of `EVEC`.

Optional Arguments

N — Order of the matrix `A`. (Input)
Default: `N` = `SIZE` (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement in the calling program. (Input)
Default: `LDA` = `SIZE` (`A`,1).

LDEVEC — Leading dimension of `EVEC` exactly as specified in the dimension statement in the calling program. (Input)
Default: `LDEVEC` = `SIZE` (`EVEC`,1).

FORTRAN 90 Interface

Generic:`EPIRG` (`NEVAL`, `A`, `EVAL`, `EVEC` [,…])

Specific:The specific interface names are `S_EPIRG` and `D_EPIRG`.

FORTRAN 77 Interface

Single:EPIRG (N, NEVAL, A, LDA, EVAL, EVEC, LDEVEC)

Double:The double precision function name is DEPIRG.

Description

Let M = NEVAL, λ = EVAL, x_j = EVEC(*,J), the j-th column of EVEC. Also, let ε be the machine precision given by AMACH(4). The performance index τ is defined to be

$$\tau = \max_{1 \le j \le M} \frac{\|Ax_j - \lambda_j x_j\|_1}{10N\varepsilon\|A\|_1\|x_j\|_1}$$

The norms used are a modified form of the 1-norm. The norm of the complex vector v is

$$\|v\|_1 = \sum_{i=1}^{N} \left\{ |\Re\, v_i| + |\Im\, v_i| \right\}$$

While the exact value of τ is highly machine dependent, the performance of EVCSF is considered excellent if τ < 1, good if 1 ≤ τ ≤ 100, and poor if τ > 100.

The performance index was first developed by the EISPACK project at Argonne National Laboratory; see Smith et al. (1976, pages 124-125).

Comments

1. Workspace may be explicitly provided, if desired, by use of E2IRG/DE2IRG. The reference is:

   E2IRG (N, NEVAL, A, LDA, EVAL, EVEC, LDEVEC, CWK)

   The additional argument is:

   CWK — Complex work array of length N.

2. Informational errors

Type	Code	Description
3	1	The performance index is greater than 100.
3	2	An eigenvector is zero.
3	3	The matrix is zero.

Example

For an example of EPIRG, see IMSL routine EVCRG.

EVLCG

more...

Computes all of the eigenvalues of a complex matrix.

Required Arguments

A — Complex matrix of order `N`. (Input)

EVAL — Complex vector of length `N` containing the eigenvalues of `A` in decreasing order of magnitude. (Output)

Optional Arguments

N — Order of the matrix `A`. (Input)
Default: `N` = `SIZE` (A,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement in the calling program. (Input)
Default: `LDA` = `SIZE` (A,1).

FORTRAN 90 Interface

Generic:`CALL EVLCG` (A, EVAL [,…])

Specific:The specific interface names are `S_EVLCG` and `D_EVLCG`.

FORTRAN 77 Interface

Single:`CALL EVLCG (N, A, LDA, EVAL)`

Double:The double precision name is `EVLCG`.

Description

Routine EVLCG computes the eigenvalues of a complex matrix. The matrix is first balanced. Unitary similarity transformations are used to reduce this balanced matrix to a complex upper Hessenberg matrix. The shifted QR algorithm is used to compute the eigenvalues of this Hessenberg matrix.

The underlying code is based on either EISPACK or LAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation, see "*Using ScaLAPACK, LAPACK, LINPACK, and EISPACK*" in the Introduction section of this manual.

Comments

1. Workspace may be explicitly provided, if desired, by use of E3LCG/DE3LCG. The reference is:

   CALL E3LCG (N, A, LDA, EVAL, ACOPY, RWK, CWK, IWK)

   The additional arguments are as follows:

   ACOPY — Complex work array of length N^2. A and ACOPY may be the same, in which case the first N^2 elements of A will be destroyed.

   RWK — Work array of length N.

   CWK — Complex work array of length 2N.

   IWK — Integer work array of length N.

2. Informational error

Type	Code	Description
4	1	The iteration for an eigenvalue failed to converge.

3. *Integer Options* with *Chapter 11* Options Manager

   1 This option uses eight values to solve memory bank conflict (access inefficiency) problems. In routine E3LCG, the internal or working, leading dimension of ACOPY is increased by IVAL(3) when N is a multiple of IVAL(4). The values IVAL(3) and IVAL (4) are temporarily replaced by IVAL(1) and IVAL(2), respectively, in routine EVLCG. Additional memory allocation and option value restoration are automatically done in EVLCG. There is no requirement that users change existing applications that use EVLCG or E3LCG. Default values for the option are IVAL(*) = 1, 16, 0, 1, 1, 16, 0, 1. Items 5–8 in IVAL(*) are for the generalized eigenvalue problem and are not used in EVLCG.

Example

In this example, a DATA statement is used to set *A* to a matrix given by Gregory and Karney (1969, page 115). The program computes the eigenvalues of this matrix.

```
      USE EVLCG_INT
      USE WRCRN_INT

!                                 Declare variables
      INTEGER    LDA, N
      PARAMETER  (N=3, LDA=N)
!
      COMPLEX    A(LDA,N), EVAL(N)
!                                 Set values of A
!
!                                 A = ( 1+2i    3+4i   21+22i)
!                                     (43+44i  13+14i  15+16i)
!                                     ( 5+6i    7+8i   25+26i)
!
      DATA A/(1.0,2.0), (43.0,44.0), (5.0,6.0), (3.0,4.0), &
          (13.0,14.0), (7.0,8.0), (21.0,22.0), (15.0,16.0), &
          (25.0,26.0)/
!
!                                 Find eigenvalues of A
      CALL EVLCG (A, EVAL)
!                                 Print results
      CALL WRCRN ('EVAL', EVAL, 1, N, 1)
      END
```

Output

```
                        EVAL
              1                 2                 3
( 39.78, 43.00)  (  6.70, -7.88)  ( -7.48,  6.88)
```

EVCCG

more...

Computes all of the eigenvalues and eigenvectors of a complex matrix.

Required Arguments

A — Complex matrix of order `N`. (Input)

EVAL — Complex vector of length `N` containing the eigenvalues of `A` in decreasing order of magnitude. (Output)

EVEC — Complex matrix of order `N`. (Output)
The `J`-th eigenvector, corresponding to `EVAL(J)`, is stored in the `J`-th column. Each vector is normalized to have Euclidean length equal to the value one.

Optional Arguments

N — Order of the matrix `A`. (Input)
Default: `N` = `SIZE` (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement in the calling program. (Input)
Default: `LDA` = `SIZE` (`A`,1).

LDEVEC — Leading dimension of `EVEC` exactly as specified in the dimension statement in the calling program. (Input)
Default: `LDEVEC` = `SIZE` (`EVEC`,1).

FORTRAN 90 Interface

Generic:`CALL EVCCG` (`A`, `EVAL`, `EVEC` [,…])

Specific:The specific interface names are `S_EVCCG` and `D_EVCCG`.

FORTRAN 77 Interface

Single:CALL EVCCG (N, A, LDA, EVAL, EVEC, LDEVEC)

Double:The double precision name is DEVCCG.

Description

Routine EVCCG computes the eigenvalues and eigenvectors of a complex matrix. The matrix is first balanced. Unitary similarity transformations are used to reduce this balanced matrix to a complex upper Hessenberg matrix. The QR algorithm is used to compute the eigenvalues and eigenvectors of this Hessenberg matrix. The eigenvectors of the original matrix are computed by transforming the eigenvectors of the complex upper Hessenberg matrix.

The underlying code is based on either EISPACK or LAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation, see "*Using ScaLAPACK, LAPACK, LINPACK, and EISPACK*" in the Introduction section of this manual.

Comments

1. Workspace may be explicitly provided, if desired, by use of E6CCG/DE6CCG. The reference is:

   CALL E6CCG (N, A, LDA, EVAL, EVEC, LDEVEC, ACOPY, RWK, CWK, IWK)

   The additional arguments are as follows:

   ACOPY — Complex work array of length N^2. The arrays A and ACOPY may be the same, in which case the first N^2 elements of A will be destroyed.

   RWK — Work array of length N.

   CWK — Complex work array of length 2N.

   IWK — Integer work array of length N.

2. Informational error

Type	Code	Description
4	1	The iteration for the eigenvalues failed to converge. No eigenvalues or eigenvectors are computed.

3. *Integer Options* with *Chapter 11* Options Manager

1 This option uses eight values to solve memory bank conflict (access inefficiency) problems. In routine `E6CCG`, the internal or working leading dimensions of `ACOPY` and `ECOPY` are both increased by `IVAL`(3) when `N` is a multiple of `IVAL`(4). The values `IVAL`(3) and `IVAL`(4) are temporarily replaced by `IVAL`(1) and `IVAL`(2), respectively, in routine `EVCCG`. Additional memory allocation and option value restoration are automatically done in `EVCCG`. There is no requirement that users change existing applications that use `EVCCG` or `E6CCG`. Default values for the option are `IVAL(*)` = 1, 16, 0, 1, 1, 16, 0, 1. Items 5–8 in `IVAL(*)` are for the generalized eigenvalue problem and are not used in `EVCCG`.

Example

In this example, a `DATA` statement is used to set *A* to a matrix given by Gregory and Karney (1969, page 116). Its eigenvalues are known to be {1 + 5*i*, 2 + 6*i*, 3 + 7*i*, 4 + 8*i*}. The program computes the eigenvalues and eigenvectors of this matrix. The performance index is also computed and printed. This serves as a check on the computations, for more details, see IMSL routine `EPICG`.

```
      USE EVCCG_INT
      USE EPICG_INT
      USE WRCRN_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    LDA, LDEVEC, N
      PARAMETER  (N=4, LDA=N, LDEVEC=N)
!
      INTEGER    NOUT
      REAL       PI
      COMPLEX    A(LDA,N), EVAL(N), EVEC(LDEVEC,N)

!                                 Set values of A
!
!                                 A = (5+9i  5+5i  -6-6i  -7-7i)
!                                     (3+3i  6+10i -5-5i  -6-6i)
!                                     (2+2i  3+3i  -1+3i  -5-5i)
!                                     (1+i   2+2i  -3-3i     4i)
!
      DATA A/(5.0,9.0), (3.0,3.0), (2.0,2.0), (1.0,1.0), (5.0,5.0), &
          (6.0,10.0), (3.0,3.0), (2.0,2.0), (-6.0,-6.0), (-5.0,-5.0), &
          (-1.0,3.0), (-3.0,-3.0), (-7.0,-7.0), (-6.0,-6.0), &
          (-5.0,-5.0), (0.0,4.0)/
!
!                                 Find eigenvalues and vectors of A
      CALL EVCCG (A, EVAL, EVEC)
!                                 Compute performance index
      PI = EPICG(N,A,EVAL,EVEC)
!                                 Print results
      CALL UMACH (2, NOUT)
      CALL WRCRN ('EVAL', EVAL, 1, N, 1)
      CALL WRCRN ('EVEC', EVEC)

      WRITE (NOUT,'(/,A,F6.3)') ' Performance index = ', PI
      END
```

Output

```
                              EVAL
             1                 2                 3                 4
( 4.000, 8.000)  ( 3.000, 7.000)  ( 2.000, 6.000)  ( 1.000, 5.000)

                                    EVEC
                  1                   2                   3                   4
1  ( 0.5774, 0.0000)  ( 0.5774, 0.0000)  ( 0.3780, 0.0000)  ( 0.7559, 0.0000)
2  ( 0.5774,-0.0000)  ( 0.5773,-0.0000)  ( 0.7559, 0.0000)  ( 0.3780, 0.0000)
3  ( 0.5774,-0.0000)  (-0.0000,-0.0000)  ( 0.3780, 0.0000)  ( 0.3780, 0.0000)
4  ( 0.0000, 0.0000)  ( 0.5774, 0.0000)  ( 0.3780, 0.0000)  ( 0.3780, 0.0000)

Performance index =  0.016
```

EPICG

This function computes the performance index for a complex eigensystem.

Function Return Value

EPICG — Performance index. (Output)

Required Arguments

NEVAL — Number of eigenvalue/eigenvector pairs on which the performance index computation is based. (Input)

A — Complex matrix of order N. (Input)

EVAL — Complex vector of length N containing the eigenvalues of A. (Input)

EVEC — Complex matrix of order N containing the eigenvectors of A. (Input)
The J-th eigenvalue/eigenvector pair should be in EVAL(J) and in the J-th column of EVEC.

Optional Arguments

N — Order of the matrix A. (Input)
Default: N = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement in the calling program. (Input)
Default: LDA = SIZE (A,1).

LDEVEC — Leading dimension of EVEC exactly as specified in the dimension statement in the calling program. (Input)
Default: LDEVEC = SIZE (EVEC,1).

FORTRAN 90 Interface

Generic:EPICG (NEVAL, A, EVAL, EVEC [,…])

Specific:The specific interface names are S_EPICG and D_EPICG.

FORTRAN 77 Interface

Single:EPICG (N, NEVAL, A, LDA, EVAL, EVEC, LDEVEC)

Double:The double precision function name is DEPICG.

Description

Let M = NEVAL, λ = EVAL, x_j = EVEC(*, J), the j-th column of EVEC. Also, let ε be the machine precision given by AMACH(4). The performance index, τ, is defined to be

$$\tau = \max_{1 \le j \le M} \frac{\|Ax_j - \lambda_j x_j\|_1}{10N\varepsilon \|A\|_1 \|x_j\|_1}$$

The norms used are a modified form of the 1-norm. The norm of the complex vector v is

$$\|v\|_1 = \sum_{i=1}^{N} \left\{ |\,\Re\, v_i| + |\,\Im\, v_i| \right\}$$

While the exact value of τ is highly machine dependent, the performance of EVCCG is considered excellent if $\tau < 1$, good if $1 \le \tau \le 100$, and poor if $\tau > 100$. The performance index was first developed by the EISPACK project at Argonne National Laboratory; see Smith et al. (1976, pages 124-125).

Comments

1. Workspace may be explicitly provided, if desired, by use of E2ICG/DE2ICG. The reference is:

   E2ICG (N, NEVAL, A, LDA, EVAL, EVEC, LDEVEC, WK)

   The additional argument is:

   WK — Complex work array of length N.

2. Informational errors

Type	Code	Description
3	1	Performance index is greater than 100.
3	2	An eigenvector is zero.
3	3	The matrix is zero.

Example

For an example of EPICG, see IMSL routine EVCCG.

EVLSF

Computes all of the eigenvalues of a real symmetric matrix.

Required Arguments

A — Real symmetric matrix of order N. (Input)

EVAL — Real vector of length N containing the eigenvalues of A in decreasing order of magnitude. (Output)

Optional Arguments

N — Order of the matrix A. (Input)
Default: N = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement in the calling program. (Input)
Default: LDA = SIZE (A,1).

FORTRAN 90 Interface

Generic: CALL EVLSF (A, EVAL [,…])

Specific: The specific interface names are S_EVLSF and D_EVLSF.

FORTRAN 77 Interface

Single: CALL EVLSF (N, A, LDA, EVAL)

Double: The double precision name is DEVLSF.

Description

Routine EVLSF computes the eigenvalues of a real symmetric matrix. Orthogonal similarity transformations are used to reduce the matrix to an equivalent symmetric tridiagonal matrix. Then, an implicit rational QR algorithm is used to compute the eigenvalues of this tridiagonal matrix.

The underlying code is based on either EISPACK or LAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation, see "*Using ScaLAPACK, LAPACK, LINPACK, and EISPACK*" in the Introduction section of this manual.

Comments

1. Workspace may be explicitly provided, if desired, by use of `E4LSF/DE4LSF`. The reference is:

   `CALL E4LSF (N, A, LDA, EVAL, WORK, IWORK)`

   The additional arguments are as follows:

   WORK — Work array of length 2N.

   IWORK — Integer array of length N.

2. Informational error

Type	Code	Description
3	1	The iteration for the eigenvalue failed to converge in 100 iterations before deflating.

Example

In this example, the eigenvalues of a real symmetric matrix are computed and printed. This matrix is given by Gregory and Karney (1969, page 56).

```
      USE EVLSF_INT
      USE WRRRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    LDA, N
      PARAMETER  (N=4, LDA=N)
!
      REAL       A(LDA,N), EVAL(N)
!                                 Set values of A
!
!                                 A = (  6.0    4.0    4.0    1.0)
!                                     (  4.0    6.0    1.0    4.0)
!                                     (  4.0    1.0    6.0    4.0)
!                                     (  1.0    4.0    4.0    6.0)
!
      DATA A /6.0, 4.0, 4.0, 1.0, 4.0, 6.0, 1.0, 4.0, 4.0, 1.0, 6.0, &
             4.0, 1.0, 4.0, 4.0, 6.0 /
!
!                                 Find eigenvalues of A
      CALL EVLSF (A, EVAL)
!                                 Print results
      CALL WRRRN ('EVAL', EVAL, 1, N, 1)
      END
```

Output

```
               EVAL
      1         2         3         4
  15.00      5.00      5.00     -1.00
```

EVCSF

Computes all of the eigenvalues and eigenvectors of a real symmetric matrix.

Required Arguments

A — Real symmetric matrix of order N. (Input)

EVAL — Real vector of length N containing the eigenvalues of A in decreasing order of magnitude. (Output)

EVEC — Real matrix of order N. (Output)
The J-th eigenvector, corresponding to EVAL(J), is stored in the J-th column. Each vector is normalized to have Euclidean length equal to the value one.

Optional Arguments

N — Order of the matrix A. (Input)
Default: N = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement in the calling program. (Input)
Default: LDA = SIZE (A,1).

LDEVEC — Leading dimension of EVEC exactly as specified in the dimension statement in the calling program. (Input)
Default: LDEVEC = SIZE (EVEC,1).

FORTRAN 90 Interface

Generic: CALL EVCSF (A, EVAL, EVEC [,…])

Specific: The specific interface names are S_EVCSF and D_EVCSF.

FORTRAN 77 Interface

Single: CALL EVCSF (N, A, LDA, EVAL, EVEC, LDEVEC)

Double: The double precision name is DEVCSF.

Description

Routine EVCSF computes the eigenvalues and eigenvectors of a real symmetric matrix. Orthogonal similarity transformations are used to reduce the matrix to an equivalent symmetric tridiagonal matrix. These transformations are accumulated. An implicit rational QR algorithm is used to compute the eigenvalues of this tridiagonal matrix. The eigenvectors are computed using the eigenvalues as perfect shifts, Parlett (1980, pages 169, 172). The underlying code is based on either EISPACK or LAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation, see "*Using ScaLAPACK, LAPACK, LINPACK, and EISPACK*" in the Introduction section of this manual. Further details, some timing data, and credits are given in Hanson et al. (1990).

Comments

1. Workspace may be explicitly provided, if desired, by use of E5CSF/DE5CSF. The reference is:

   CALL E5CSF (N, A, LDA, EVAL, EVEC, LDEVEC, WORK, IWK)

   The additional argument is:

   WORK — Work array of length 3N.

   IWK — Integer array of length N.

2. Informational error

Type	Code	Description
3	1	The iteration for the eigenvalue failed to converge in 100 iterations before deflating.

Example

The eigenvalues and eigenvectors of this real symmetric matrix are computed and printed. The performance index is also computed and printed. This serves as a check on the computations. For more details, see EPISF.

```
      USE EVCSF_INT
      USE EPISF_INT
      USE UMACH_INT
      USE WRRRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    LDA, LDEVEC, N
      PARAMETER  (N=3, LDA=N, LDEVEC=N)
!
      INTEGER    NOUT
      REAL       A(LDA,N), EVAL(N), EVEC(LDEVEC,N), PI
!
!                                 Set values of A
!
```

```
!                                  A = (  7.0   -8.0   -8.0)
!                                      ( -8.0  -16.0  -18.0)
!                                      ( -8.0  -18.0   13.0)
!
      DATA A/7.0, -8.0, -8.0, -8.0, -16.0, -18.0, -8.0, -18.0, 13.0/
!
!                                  Find eigenvalues and vectors of A
      CALL EVCSF (A, EVAL, EVEC)
!                                  Compute performance index
      PI = EPISF (N, A, EVAL, EVEC)
!                                  Print results
      CALL UMACH (2, NOUT)
      CALL WRRRN ('EVAL', EVAL, 1, N, 1)
      CALL WRRRN ('EVEC', EVEC)

      WRITE (NOUT, '(/,A,F6.3)') ' Performance index = ', PI
      END
```

Output

```
         EVAL
     1       2       3
-27.90   22.68    9.22

            EVEC
         1         2         3
1   0.2945  -0.2722   0.9161
2   0.8521  -0.3591  -0.3806
3   0.4326   0.8927   0.1262

Performance index =  0.019
```

EVASF

Computes the largest or smallest eigenvalues of a real symmetric matrix.

Required Arguments

NEVAL — Number of eigenvalues to be computed. (Input)

A — Real symmetric matrix of order N. (Input)

SMALL — Logical variable. (Input)
If .TRUE., the smallest NEVAL eigenvalues are computed. If .FALSE., the largest NEVAL eigenvalues are computed.

EVAL — Real vector of length NEVAL containing the eigenvalues of A in decreasing order of magnitude. (Output)

Optional Arguments

N — Order of the matrix A. (Input)
Default: N = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement in the calling program. (Input)
Default: LDA = SIZE (A,1).

FORTRAN 90 Interface

Generic:	CALL EVASF (NEVAL, A, SMALL, EVAL [,…])
Specific:	The specific interface names are S_EVASF and D_EVASF.

FORTRAN 77 Interface

Single:	CALL EVASF (N, NEVAL, A, LDA, SMALL, EVAL)
Double:	The double precision name is DEVASF.

Description

Routine EVASF computes the largest or smallest eigenvalues of a real symmetric matrix. Orthogonal similarity transformations are used to reduce the matrix to an equivalent symmetric tridiagonal matrix. Then, an implicit rational QR algorithm is used to compute the eigenvalues of this tridiagonal matrix.

The reduction routine is based on the EISPACK routine TRED2. See Smith et al. (1976). The rational QR algorithm is called the PWK algorithm. It is given in Parlett (1980, page 169).

Comments

1. Workspace may be explicitly provided, if desired, by use of E4ASF/DE4ASF. The reference is:

   CALL E4ASF (N, NEVAL, A, LDA, SMALL, EVAL, WORK, IWK)

   Additional arguments are as follows:

   WORK — Work array of length 4N.

   IWK — Integer work array of length N.

2. Informational error

Type	Code	Description
3	1	The iteration for an eigenvalue failed to converge. The best estimate will be returned.

Example

In this example, the three largest eigenvalues of the computed Hilbert matrix $a_{ij} = 1/(i + j - 1)$ of order $N = 10$ are computed and printed.

```
      USE EVASF_INT
      USE WRRRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    LDA, N, NEVAL
      PARAMETER  (N=10, NEVAL=3, LDA=N)
!
      INTEGER    I, J
      REAL       A(LDA,N), EVAL(NEVAL), REAL
      LOGICAL    SMALL
      INTRINSIC  REAL
!                                 Set up Hilbert matrix
      DO 20  J=1, N
         DO 10  I=1, N
            A(I,J) = 1.0/REAL(I+J-1)
   10    CONTINUE
   20 CONTINUE
!                                 Find the 3 largest eigenvalues
      SMALL = .FALSE.
```

```
      CALL EVASF (NEVAL, A, SMALL, EVAL)
!                                Print results
      CALL WRRRN ('EVAL', EVAL, 1, NEVAL, 1)

     END
```

Output

```
         EVAL
     1       2       3
 1.752   0.343   0.036
```

EVESF

Computes the largest or smallest eigenvalues and the corresponding eigenvectors of a real symmetric matrix.

Required Arguments

NEVEC — Number of eigenvalues to be computed. (Input)

A — Real symmetric matrix of order N. (Input)

SMALL — Logical variable. (Input)
If .TRUE., the smallest NEVEC eigenvalues are computed. If .FALSE., the largest NEVEC eigenvalues are computed.

EVAL — Real vector of length NEVEC containing the eigenvalues of A in decreasing order of magnitude. (Output)

EVEC — Real matrix of dimension N by NEVEC. (Output)
The J-th eigenvector, corresponding to EVAL(J), is stored in the J-th column. Each vector is normalized to have Euclidean length equal to the value one.

Optional Arguments

N — Order of the matrix A. (Input)
Default: N = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement in the calling program. (Input)
Default: LDA = SIZE (A,1).

LDEVEC — Leading dimension of EVEC exactly as specified in the dimension statement in the calling program. (Input)
Default: LDEVEC = SIZE (EVEC,1).

FORTRAN 90 Interface

Generic: CALL EVESF (NEVEC, A, SMALL, EVAL, EVEC [,…])

Specific: The specific interface names are S_EVESF and D_EVESF.

FORTRAN 77 Interface

Single: `CALL EVESF (N, NEVEC, A, LDA, SMALL, EVAL, EVEC, LDEVEC)`

Double: The double precision name is `DEVESF`.

Description

Routine `EVESF` computes the largest or smallest eigenvalues and the corresponding eigenvectors of a real symmetric matrix. Orthogonal similarity transformations are used to reduce the matrix to an equivalent symmetric tridiagonal matrix. Then, an implicit rational QR algorithm is used to compute the eigenvalues of this tridiagonal matrix. Inverse iteration is used to compute the eigenvectors of the tridiagonal matrix. This is followed by orthogonalization of these vectors. The eigenvectors of the original matrix are computed by back transforming those of the tridiagonal matrix.

The reduction routine is based on the EISPACK routine `TRED2`. See Smith et al. (1976). The rational QR algorithm is called the PWK algorithm. It is given in Parlett (1980, page 169). The inverse iteration and orthogonalization computation is discussed in Hanson et al. (1990). The back transformation routine is based on the EISPACK routine `TRBAK1`.

Comments

1. Workspace may be explicitly provided, if desired, by use of `E5ESF/DE5ESF`. The reference is:

   ```
   CALL E5ESF (N, NEVEC, A, LDA, SMALL, EVAL, EVEC, LDEVEC, WK,
      IWK)
   ```

   The additional arguments are as follows:

   WK — Work array of length 9N.

   IWK — Integer array of length N.

2. Informational errors

Type	**Code**	**Description**
3	1	The iteration for an eigenvalue failed to converge. The best estimate will be returned.
3	2	Inverse iteration did not converge. Eigenvector is not correct for the specified eigenvalue.
3	3	The eigenvectors have lost orthogonality.

Example

In this example, a DATA statement is used to set *A* to a matrix given by Gregory and Karney (1969, page 55). The largest two eigenvalues and their eigenvectors are computed and printed. The performance index is also computed and printed. This serves as a check on the computations. For more details, see IMSL routine EPISF.

```
      USE EVESF_INT
      USE EPISF_INT
      USE UMACH_INT
      USE WRRRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    LDA, LDEVEC, N
      PARAMETER  (N=4, LDA=N, LDEVEC=N)
!
      INTEGER    NEVEC, NOUT
      REAL       A(LDA,N), EVAL(N), EVEC(LDEVEC,N), PI
      LOGICAL    SMALL
!
!                                 Set values of A
!
!                                 A = (  5.0    4.0    1.0    1.0)
!                                     (  4.0    5.0    1.0    1.0)
!                                     (  1.0    1.0    4.0    2.0)
!                                     (  1.0    1.0    2.0    4.0)
!
      DATA A/5.0, 4.0, 1.0, 1.0, 4.0, 5.0, 1.0, 1.0, 1.0, 1.0, 4.0, &
          2.0, 1.0, 1.0, 2.0, 4.0/
!
!                                 Find eigenvalues and vectors of A
      NEVEC = 2
      SMALL = .FALSE.
      CALL EVESF (NEVEC, A, SMALL, EVAL, EVEC)
!                                 Compute performance index
      PI = EPISF(NEVEC,A,EVAL,EVEC)
!                                 Print results
      CALL UMACH (2, NOUT)
      CALL WRRRN ('EVAL', EVAL, 1, NEVEC, 1)
      CALL WRRRN ('EVEC', EVEC, N, NEVEC, LDEVEC)

      WRITE (NOUT,'(/,A,F6.3)') ' Performance index = ', PI
      END
```

Output

```
      EVAL
      1       2
  10.00    5.00

        EVEC
           1         2
 1    0.6325   -0.3162
 2    0.6325   -0.3162
 3    0.3162    0.6325
 4    0.3162    0.6325

 Performance index =  0.031
```

EVBSF

Computes selected eigenvalues of a real symmetric matrix.

Required Arguments

MXEVAL — Maximum number of eigenvalues to be computed. (Input)

A — Real symmetric matrix of order N. (Input)

ELOW — Lower limit of the interval in which the eigenvalues are sought. (Input)

EHIGH — Upper limit of the interval in which the eigenvalues are sought. (Input)

NEVAL — Number of eigenvalues found. (Output)

EVAL — Real vector of length MXEVAL containing the eigenvalues of A in the interval (ELOW, EHIGH) in decreasing order of magnitude. (Output)

Only the first NEVAL elements of EVAL are significant.

Optional Arguments

N — Order of the matrix A. (Input)
Default: N = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement in the calling program. (Input)
Default: LDA = SIZE (A,1).

FORTRAN 90 Interface

Generic: CALL EVBSF (MXEVAL, A, ELOW, EHIGH, NEVAL, EVAL [,…])

Specific: The specific interface names are S_EVBSF and D_EVBSF.

FORTRAN 77 Interface

Single: CALL EVBSF (N, MXEVAL, A, LDA, ELOW, EHIGH, NEVAL, EVAL)

Double: The double precision name is DEVBSF.

Description

Routine EVBSF computes the eigenvalues in a given interval for a real symmetric matrix. Orthogonal similarity transformations are used to reduce the matrix to an equivalent symmetric tridiagonal matrix. Then, an implicit rational QR algorithm is used to compute the eigenvalues of this tridiagonal matrix. The reduction step is based on the EISPACK routine TRED1. See Smith et al. (1976). The rational QR algorithm is called the PWK algorithm. It is given in Parlett (1980, page 169).

Comments

1. Workspace may be explicitly provided, if desired, by use of E5BSF/DE5BSF. The reference is

   CALL E5BSF (N, MXEVAL, A, LDA, ELOW, EHIGH, NEVAL, EVAL, WK, IWK)

   The additional arguments are as follows:

   WK — Work array of length 5N.

   IWK — Integer work array of length 1N.

2. Informational error

Type	Code	Description
3	1	The number of eigenvalues in the specified interval exceeds MXEVAL. NEVAL contains the number of eigenvalues in the interval. No eigenvalues will be returned.

Example

In this example, a DATA statement is used to set *A* to a matrix given by Gregory and Karney (1969, page 56). The eigenvalues of *A* are known to be –1, 5, 5 and 15. The eigenvalues in the interval [1.5, 5.5] are computed and printed. As a test, this example uses MXEVAL = 4. The routine EVBSF computes NEVAL, the number of eigenvalues in the given interval. The value of NEVAL is 2.

```
      USE EVBSF_INT
      USE UMACH_INT
      USE WRRRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    LDA, MXEVAL, N
      PARAMETER  (MXEVAL=4, N=4, LDA=N)
!
      INTEGER    NEVAL, NOUT
      REAL       A(LDA,N), EHIGH, ELOW, EVAL(MXEVAL)
!
!                                 Set values of A
!
!                                 A = (   6.0    4.0    4.0    1.0)
```

```
!                                    (  4.0    6.0    1.0    4.0)
!                                    (  4.0    1.0    6.0    4.0)
!                                    (  1.0    4.0    4.0    6.0)
!
      DATA A/6.0, 4.0, 4.0, 1.0, 4.0, 6.0, 1.0, 4.0, 4.0, 1.0, 6.0, &
          4.0, 1.0, 4.0, 4.0, 6.0/
!
!                                Find eigenvalues of A
      ELOW  = 1.5
      EHIGH = 5.5
      CALL EVBSF (MXEVAL, A, ELOW, EHIGH, NEVAL, EVAL)
!                                Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,'(/,A,I2)') ' NEVAL = ', NEVAL
      CALL WRRRN ('EVAL', EVAL, 1, NEVAL, 1)
      END
```

Output

```
NEVAL =  2

      EVAL
      1       2
  5.000   5.000
```

EVFSF

Computes selected eigenvalues and eigenvectors of a real symmetric matrix.

Required Arguments

MXEVAL — Maximum number of eigenvalues to be computed. (Input)

A — Real symmetric matrix of order `N`. (Input)

ELOW — Lower limit of the interval in which the eigenvalues are sought. (Input)

EHIGH — Upper limit of the interval in which the eigenvalues are sought. (Input)

NEVAL — Number of eigenvalues found. (Output)

EVAL — Real vector of length `MXEVAL` containing the eigenvalues of `A` in the interval (`ELOW`, `EHIGH`) in decreasing order of magnitude. (Output)
Only the first `NEVAL` elements of `EVAL` are significant.

EVEC — Real matrix of dimension `N` by `MXEVAL`. (Output)
The `J`-th eigenvector corresponding to `EVAL(J)`, is stored in the `J`-th column. Only the first `NEVAL` columns of `EVEC` are significant. Each vector is normalized to have Euclidean length equal to the value one.

Optional Arguments

N — Order of the matrix `A`. (Input)
Default: `N` = `SIZE` (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement in the calling program. (Input)
Default: `LDA` = `SIZE` (`A`,1).

LDEVEC — Leading dimension of `EVEC` exactly as specified in the dimension statement in the calling program. (Input)
Default: `LDEVEC` = `SIZE` (`EVEC`,1).

FORTRAN 90 Interface

Generic: `CALL EVFSF (MXEVAL, A, ELOW, EHIGH, NEVAL, EVAL, EVEC [,…])`

Specific: The specific interface names are S_EVFSF and D_EVFSF.

FORTRAN 77 Interface

Single: CALL EVFSF (N, MXEVAL, A, LDA, ELOW, EHIGH, NEVAL, EVAL, EVEC, LDEVEC)

Double: The double precision name is DEVFSF.

Description

Routine EVFSF computes the eigenvalues in a given interval and the corresponding eigenvectors of a real symmetric matrix. Orthogonal similarity transformations are used to reduce the matrix to an equivalent symmetric tridiagonal matrix. Then, an implicit rational QR algorithm is used to compute the eigenvalues of this tridiagonal matrix. Inverse iteration is used to compute the eigenvectors of the tridiagonal matrix. This is followed by orthogonalization of these vectors. The eigenvectors of the original matrix are computed by back transforming those of the tridiagonal matrix.

The reduction step is based on the EISPACK routine TRED1. The rational QR algorithm is called the PWK algorithm. It is given in Parlett (1980, page 169). The inverse iteration and orthogonalization processes are discussed in Hanson et al. (1990). The transformation back to the users's input matrix is based on the EISPACK routine TRBAK1. See Smith et al. (1976) for the EISPACK routines.

Comments

1. Workspace may be explicitly provided, if desired, by use of E3FSF/DE3FSF. The reference is:

```
CALL E3FSF (N, MXEVAL, A, LDA, ELOW, EHIGH, NEVAL, VAL,
   EVEC, LDEVEC, WK, IWK)
```

The additional arguments are as follows:

WK — Work array of length 9N.

IWK — Integer work array of length N.

2. Informational errors

Type	Code	Description
3	1	The number of eigenvalues in the specified range exceeds MXEVAL. NEVAL contains the number of eigenvalues in the range. No eigenvalues will be computed.
3	2	Inverse iteration did not converge. Eigenvector is not correct for the specified eigenvalue.
3	3	The eigenvectors have lost orthogonality.

Example

In this example, *A* is set to the computed Hilbert matrix. The eigenvalues in the interval [0.001, 1] and their corresponding eigenvectors are computed and printed. This example uses MXEVAL = 3. The routine EVFSF computes the number of eigenvalues NEVAL in the given interval. The value of NEVAL is 2. The performance index is also computed and printed. For more details, see IMSL routine EPISF.

```
      USE EVFSF_INT
      USE EPISF_INT
      USE WRRRN_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    LDA, LDEVEC, MXEVAL, N, J, I
      PARAMETER  (MXEVAL=3, N=3, LDA=N, LDEVEC=N)
!
      INTEGER    NEVAL, NOUT
      REAL       A(LDA,N), EHIGH, ELOW, EVAL(MXEVAL), &
                EVEC(LDEVEC,MXEVAL), PI
!                                 Compute Hilbert matrix
      DO 20 J=1,N
         DO 10 I=1,N
            A(I,J) = 1.0/FLOAT(I+J-1)
   10    CONTINUE
   20 CONTINUE
!                                 Find eigenvalues and vectors
      ELOW  = 0.001
      EHIGH = 1.0
      CALL EVFSF (MXEVAL, A, ELOW, EHIGH, NEVAL, EVAL, EVEC, LDEVEC)
!                                 Compute performance index
      PI = EPISF(NEVAL,A,EVAL,EVEC)
!                                 Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,'(/,A,I2)') ' NEVAL = ', NEVAL
      CALL WRRRN ('EVAL', EVAL, 1, NEVAl, 1)
      CALL WRRRN ('EVEC', EVEC, N, NEVAL, LDEVEC)
      WRITE (NOUT,'(/,A,F6.3)') ' Performance index = ', PI
      END
```

Output

```
 NEVAL =  2

       EVAL
       1         2
  0.1223   0.0027

        EVEC
          1         2
 1  -0.5474  -0.1277
 2   0.5283   0.7137
 3   0.6490  -0.6887

 Performance index =  0.008
```

EPISF

This function computes the performance index for a real symmetric eigensystem.

Function Return Value

EPISF — Performance index. (Output)

Required Arguments

NEVAL — Number of eigenvalue/eigenvector pairs on which the performance index computation is based on. (Input)

A — Symmetric matrix of order `N`. (Input)

EVAL — Vector of length `NEVAL` containing eigenvalues of `A`. (Input)

EVEC — `N` by `NEVAL` array containing eigenvectors of `A`. (Input)
The eigenvector corresponding to the eigenvalue `EVAL`(`J`) must be in the `J`-th column of `EVEC`.

Optional Arguments

N — Order of the matrix `A`. (Input)
Default: `N` = `SIZE` (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement in the calling program. (Input)
Default: `LDA` = `SIZE` (`A`,1).

LDEVEC — Leading dimension of `EVEC` exactly as specified in the dimension statement in the calling program. (Input)
Default: `LDEVEC` = `SIZE` (`EVEC`,1).

FORTRAN 90 Interface

Generic: `EPISF` (`NEVAL`, `A`, `EVAL`, `EVEC` [,…])

Specific: The specific interface names are `S_EPISF` and `D_EPISF`.

FORTRAN 77 Interface

Single: EPISF (N, NEVAL, A, LDA, EVAL, EVEC, LDEVEC)

Double: The double precision function name is DEPISF.

Description

Let M = NEVAL, λ = EVAL, x_j = EVEC(*,J), the j-th column of EVEC. Also, let ε be the machine precision, given by AMACH(4), see the *Reference* chapter of this manual. The performance index, τ, is defined to be

$$\tau = \max_{1 \le j \le M} \frac{\left\| Ax_j - \lambda_j x_j \right\|_1}{10N\varepsilon \left\| A \right\|_1 \left\| x_j \right\|_1}$$

While the exact value of τ is highly machine dependent, the performance of EVCSF is considered excellent if $\tau < 1$, good if $1 \le \tau \le 100$, and poor if $\tau > 100$. The performance index was first developed by the EISPACK project at Argonne National Laboratory; see Smith et al. (1976, pages 124– 125).

Comments

1. Workspace may be explicitly provided, if desired, by use of E2ISF/DE2ISF. The reference is:

   ```
   E2ISF (N, NEVAL, A, LDA, EVAL, EVEC, LDEVEC, WORK)
   ```

   The additional argument is:

   WORK — Work array of length N.

   E2ISF — Performance Index.

2. Informational errors

Type	Code	Description
3	1	Performance index is greater than 100.
3	2	An eigenvector is zero.
3	3	The matrix is zero.

Example

For an example of EPISF, see routine EVCSF.

EVLSB

Computes all of the eigenvalues of a real symmetric matrix in band symmetric storage mode.

Required Arguments

A — Band symmetric matrix of order N. (Input)

NCODA — Number of codiagonals in A. (Input)

EVAL — Vector of length N containing the eigenvalues of A in decreasing order of magnitude. (Output)

Optional Arguments

N — Order of the matrix A. (Input)
Default: N = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement in the calling program. (Input)
Default: LDA = SIZE (A,1).

FORTRAN 90 Interface

Generic: CALL EVLSB (A, NCODA, EVAL [,…])

Specific: The specific interface names are S_EVLSB and D_EVLSB.

FORTRAN 77 Interface

Single: CALL EVLSB (N, A, LDA, NCODA, EVAL)

Double: The double precision name is DEVLSB.

Description

Routine EVLSB computes the eigenvalues of a real band symmetric matrix. Orthogonal similarity transformations are used to reduce the matrix to an equivalent symmetric tridiagonal matrix. The implicit QL algorithm is used to compute the eigenvalues of the resulting tridiagonal matrix.

The reduction routine is based on the EISPACK routine BANDR; see Garbow et al. (1977). The QL routine is based on the EISPACK routine IMTQL1; see Smith et al. (1976).

Comments

1. Workspace may be explicitly provided, if desired, by use of E3LSB/DE3LSB. The reference is:

   CALL E3LSB (N, A, LDA, NCODA, EVAL, ACOPY, WK)

   The additional arguments are as follows:

   ACOPY — Work array of length N(NCODA + 1). The arrays A and ACOPY may be the same, in which case the first N(NCODA + 1) elements of A will be destroyed.

   WK — Work array of length N.

2. Informational error

Type	Code	Description
4	1	The iteration for the eigenvalues failed to converge.

Example

In this example, a DATA statement is used to set *A* to a matrix given by Gregory and Karney (1969, page 77). The eigenvalues of this matrix are given by

$$\lambda_k = \left(1 - 2\cos\frac{k\pi}{N+1}\right)^2 - 3$$

Since the eigenvalues returned by EVLSB are in decreasing magnitude, the above formula for $k = 1, \ldots, N$ gives the values in a different order. The eigenvalues of this real band symmetric matrix are computed and printed.

```
      USE EVLSB_INT
      USE WRRRN_INT

      IMPLICIT   NONE
!                                  Declare variables
      INTEGER    LDA, LDEVEC, N, NCODA
      PARAMETER  (N=5, NCODA=2, LDA=NCODA+1, LDEVEC=N)
!
      REAL       A(LDA,N), EVAL(N)
!                                  Define values of A:
!                                  A = (-1   2   1        )
!                                      ( 2   0   2   1    )
!                                      ( 1   2   0   2   1 )
!                                      (     1   2   0   2 )
!                                      (         1   2  -1 )
!                                  Represented in band symmetric
!                                  form this is:
!                                  A = ( 0   0   1   1   1 )
!                                      ( 0   2   2   2   2 )
```

```
!                                     (-1  0  0  0 -1 )
!
      DATA A/0.0, 0.0, -1.0, 0.0, 2.0, 0.0, 1.0, 2.0, 0.0, 1.0, 2.0, &
          0.0, 1.0, 2.0, -1.0/
!
       CALL EVLSB (A, NCODA, EVAL)
!                                 Print results
      CALL WRRRN ('EVAL', EVAL, 1, N, 1)
      END
```

Output

```
                   EVAL
      1       2       3       4       5
  4.464  -3.000  -2.464  -2.000   1.000
```

EVCSB

Computes all of the eigenvalues and eigenvectors of a real symmetric matrix in band symmetric storage mode.

Required Arguments

A — Band symmetric matrix of order `N`. (Input)

NCODA — Number of codiagonals in `A`. (Input)

EVAL — Vector of length `N` containing the eigenvalues of `A` in decreasing order of magnitude. (Output)

EVEC — Matrix of order `N` containing the eigenvectors. (Output)
The `J`-th eigenvector, corresponding to `EVAL(J)`, is stored in the `J`-th column. Each vector is normalized to have Euclidean length equal to the value one.

Optional Arguments

N — Order of the matrix `A`. (Input)
Default: `N` = `SIZE` (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement in the calling program. (Input)
Default: `LDA` = `SIZE` (`A`,1).

LDEVEC — Leading dimension of `EVEC` exactly as specified in the dimension statement in the calling program. (Input)
Default: `LDEVEC` = `SIZE` (`EVEC`,1).

FORTRAN 90 Interface

Generic: `CALL EVCSB (A, NCODA, EVAL, EVEC [,…])`

Specific: The specific interface names are `S_EVCSB` and `D_EVCSB`.

FORTRAN 77 Interface

Single: `CALL EVCSB (N, A, LDA, NCODA, EVAL, EVEC, LDEVEC)`

Double: The double precision name is `DEVCSB`.

Description

Routine EVCSB computes the eigenvalues and eigenvectors of a real band symmetric matrix. Orthogonal similarity transformations are used to reduce the matrix to an equivalent symmetric tridiagonal matrix. These transformations are accumulated. The implicit QL algorithm is used to compute the eigenvalues and eigenvectors of the resulting tridiagonal matrix.

The reduction routine is based on the EISPACK routine BANDR; see Garbow et al. (1977). The QL routine is based on the EISPACK routine IMTQL2; see Smith et al. (1976).

Comments

1. Workspace may be explicitly provided, if desired, by use of E4CSB/DE4CSB. The reference is:

   CALL E4CSB (N, A, LDA, NCODA, EVAL, EVEC, LDEVEC, COPY, WK, IWK)

   The additional arguments are as follows:

   ACOPY — Work array of length N(NCODA + 1). A and ACOPY may be the same, in which case the first N * NCODA elements of A will be destroyed.

   WK — Work array of length N.

   IWK — Integer work array of length N.

2. Informational error

Type	Code	Description
4	1	The iteration for the eigenvalues failed to converge.

3. The success of this routine can be checked using EPISB.

Example

In this example, a DATA statement is used to set A to a band matrix given by Gregory and Karney (1969, page 75). The eigenvalues, λ_k, of this matrix are given by

$$\lambda_k = 16\sin^4\left(\frac{k\pi}{2N+2}\right)$$

The eigenvalues and eigenvectors of this real band symmetric matrix are computed and printed. The performance index is also computed and printed. This serves as a check on the computations; for more details, see IMSL routine EPISB.

```
USE EVCSB_INT
USE EPISB_INT
```

```
      USE UMACH_INT
      USE WRRRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    LDA, LDEVEC, N, NCODA
      PARAMETER  (N=6, NCODA=2, LDA=NCODA+1, LDEVEC=N)
!
      INTEGER    NOUT
      REAL       A(LDA,N), EVAL(N), EVEC(LDEVEC,N), PI
!                                 Define values of A:
!                                 A = (  5  -4   1             )
!                                     ( -4   6  -4   1         )
!                                     (  1  -4   6  -4   1     )
!                                     (      1  -4   6  -4   1 )
!                                     (          1  -4   6  -4 )
!                                     (              1  -4   5 )
!                                 Represented in band symmetric
!                                 form this is:
!                                 A = (  0   0   1   1   1   1 )
!                                     (  0  -4  -4  -4  -4  -4 )
!                                     (  5   6   6   6   6   5 )
!
      DATA A/0.0, 0.0, 5.0, 0.0, -4.0, 6.0, 1.0, -4.0, 6.0, 1.0, -4.0, &
          6.0, 1.0, -4.0, 6.0, 1.0, -4.0, 5.0/
!
!                                 Find eigenvalues and vectors
      CALL EVCSB (A, NCODA, EVAL, EVEC)
!                                 Compute performance index
      PI = EPISB(N,A,NCODA,EVAL,EVEC)
!                                 Print results
      CALL UMACH (2, NOUT)
      CALL WRRRN ('EVAL', EVAL, 1, N, 1)
      CALL WRRRN ('EVEC', EVEC)
      WRITE (NOUT,'(/,A,F6.3)') ' Performance index = ', PI
      END
```

Output

```
                        EVAL
      1       2       3       4       5       6
  14.45   10.54    5.98    2.42    0.57    0.04

                            EVEC
          1         2         3         4         5         6
 1  -0.2319   -0.4179   -0.5211    0.5211   -0.4179    0.2319
 2   0.4179    0.5211    0.2319    0.2319   -0.5211    0.4179
 3  -0.5211   -0.2319    0.4179   -0.4179   -0.2319    0.5211
 4   0.5211   -0.2319   -0.4179   -0.4179    0.2319    0.5211
 5  -0.4179    0.5211   -0.2319    0.2319    0.5211    0.4179
 6   0.2319   -0.4179    0.5211    0.5211    0.4179    0.2319

 Performance index =  0.029
```

EVASB

Computes the largest or smallest eigenvalues of a real symmetric matrix in band symmetric storage mode.

Required Arguments

NEVAL — Number of eigenvalues to be computed. (Input)

A — Band symmetric matrix of order N. (Input)

NCODA — Number of codiagonals in A. (Input)

SMALL — Logical variable. (Input)
If .TRUE., the smallest NEVAL eigenvalues are computed. If .FALSE., the largest NEVAL eigenvalues are computed.

EVAL — Vector of length NEVAL containing the computed eigenvalues in decreasing order of magnitude. (Output)

Optional Arguments

N — Order of the matrix A. (Input)
Default: N = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement in the calling program. (Input)
Default: LDA = SIZE (A,1).

FORTRAN 90 Interface

Generic: CALL EVASB (NEVAL, A, NCODA, SMALL, EVAL [,…])

Specific: The specific interface names are S_EVASB and D_EVASB.

FORTRAN 77 Interface

Single: CALL EVASB (N, NEVAL, A, LDA, NCODA, SMALL, EVAL)

Double: The double precision name is DEVASB.

Description

Routine EVASB computes the largest or smallest eigenvalues of a real band symmetric matrix. Orthogonal similarity transformations are used to reduce the matrix to an equivalent symmetric tridiagonal matrix. The rational QR algorithm with Newton corrections is used to compute the extreme eigenvalues of this tridiagonal matrix.

The reduction routine is based on the EISPACK routine BANDR; see Garbow et al. (1978). The QR routine is based on the EISPACK routine RATQR; see Smith et al. (1976).

Comments

1. Workspace may be explicitly provided, if desired, by use of E3ASB/DE3ASB. The reference is:

   CALL E3ASB (N, NEVAL, A, LDA, NCODA, SMALL, EVAL, ACOPY, WK)

   The additional arguments are as follows:

   ACOPY — Work array of length N(NCODA + 1). A and ACOPY may be the same, in which case the first N(NCODA + 1) elements of A will be destroyed.

   WK — Work array of length 3N.

2. Informational error

Type	Code	Description
3	1	The iteration for an eigenvalue failed to converge. The best estimate will be returned.

Example

The following example is given in Gregory and Karney (1969, page 63). The smallest four eigenvalues of the matrix

$$A = \begin{bmatrix} 5 & 2 & 1 & 1 & & & & & & & \\ 2 & 6 & 3 & 1 & 1 & & & & & & \\ 1 & 3 & 6 & 3 & 1 & 1 & & & & & \\ 1 & 1 & 3 & 6 & 3 & 1 & 1 & & & & \\ & 1 & 1 & 3 & 6 & 3 & 1 & 1 & & & \\ & & 1 & 1 & 3 & 6 & 3 & 1 & 1 & & \\ & & & 1 & 1 & 3 & 6 & 3 & 1 & 1 & \\ & & & & 1 & 1 & 3 & 6 & 3 & 1 & 1 \\ & & & & & 1 & 1 & 3 & 6 & 3 & 1 \\ & & & & & & 1 & 1 & 3 & 6 & 2 \\ & & & & & & & 1 & 1 & 2 & 5 \end{bmatrix}$$

are computed and printed.

```
      USE EVASB_INT
      USE WRRRN_INT
      USE SSET_INT

      IMPLICIT   NONE
!                                  Declare variables
      INTEGER    LDA, N, NCODA, NEVAL
      PARAMETER  (N=11, NCODA=3, NEVAL=4, LDA=NCODA+1)
!
      REAL       A(LDA,N), EVAL(NEVAL)
      LOGICAL    SMALL
!                                  Set up matrix in band symmetric
!                                  storage mode
      CALL SSET (N, 6.0, A(4:,1), LDA)
      CALL SSET (N-1, 3.0, A(3:,2), LDA)
      CALL SSET (N-2, 1.0, A(2:,3), LDA)
      CALL SSET (N-3, 1.0, A(1:,4), LDA)
      CALL SSET (NCODA, 0.0, A(1:,1), 1)
      CALL SSET (NCODA-1, 0.0, A(1:,2), 1)
      CALL SSET (NCODA-2, 0.0, A(1:,3), 1)
      A(4,1) = 5.0
      A(4,N) = 5.0
      A(3,2) = 2.0
      A(3,N) = 2.0
!                                  Find the 4 smallest eigenvalues
      SMALL = .TRUE.
      CALL EVASB (NEVAL, A, NCODA, SMALL, EVAL)
!                                  Print results
      CALL WRRRN ('EVAL', EVAL, 1, NEVAL, 1)
      END
```

Output

```
             EVAL
      1       2       3       4
  4.000   3.172   1.804   0.522
```

EVESB

Computes the largest or smallest eigenvalues and the corresponding eigenvectors of a real symmetric matrix in band symmetric storage mode.

Required Arguments

NEVEC — Number of eigenvectors to be calculated. (Input)

A — Band symmetric matrix of order N. (Input)

NCODA — Number of codiagonals in A. (Input)

SMALL — Logical variable. (Input)
If .TRUE. , the smallest NEVEC eigenvectors are computed. If .FALSE. , the largest NEVEC eigenvectors are computed.

EVAL — Vector of length NEVEC containing the eigenvalues of A in decreasing order of magnitude. (Output)

EVEC — Real matrix of dimension N by NEVEC. (Output)
The J-th eigenvector, corresponding to EVAL(J), is stored in the J-th column. Each vector is normalized to have Euclidean length equal to the value one.

Optional Arguments

N — Order of the matrix A. (Input)
Default: N = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement in the calling program. (Input)
Default: LDA = SIZE (A,1).

LDEVEC — Leading dimension of EVEC exactly as specified in the dimension statement in the calling program. (Input)
Default: LDEVEC = SIZE (EVEC,1).

FORTRAN 90 Interface

Generic: CALL EVESB (NEVEC, A, NCODA, SMALL, EVAL, EVEC,…)

Specific: The specific interface names are `S_EVESB` and `D_EVESB`.

FORTRAN 77 Interface

Single: `CALL EVESB (N, NEVEC, A, LDA, NCODA, SMALL, EVAL, EVEC, LDEVEC)`

Double: The double precision name is `DEVESB`.

Description

Routine `EVESB` computes the largest or smallest eigenvalues and the corresponding eigenvectors of a real band symmetric matrix. Orthogonal similarity transformations are used to reduce the matrix to an equivalent symmetric tridiagonal matrix. The rational QR algorithm with Newton corrections is used to compute the extreme eigenvalues of this tridiagonal matrix. Inverse iteration and orthogonalization are used to compute the eigenvectors of the given band matrix. The reduction routine is based on the EISPACK routine `BANDR`; see Garbow et al. (1977). The QR routine is based on the EISPACK routine `RATQR`; see Smith et al. (1976). The inverse iteration and orthogonalization steps are based on EISPACK routine `BANDV` using the additional steps given in Hanson et al. (1990).

Comments

1. Workspace may be explicitly provided, if desired, by use of `E4ESB/DE4ESB`. The reference is:

   ```
   CALL E4ESB (N, NEVEC, A, LDA, NCODA, SMALL, EVAL, EVEC, LDE-
     VEC, ACOPY, WK, IWK)
   ```

   The additional argument is:

   ACOPY — Work array of length `N(NCODA + 1)`.

   WK — Work array of length `N(2NCODA + 5)`.

   IWK — Integer work array of length `N`.

2. Informational errors

Type	Code	Description
3	1	Inverse iteration did not converge. Eigenvector is not correct for the specified eigenvalue.
3	2	The eigenvectors have lost orthogonality.

3. The success of this routine can be checked using `EPISB`.

Example

The following example is given in Gregory and Karney (1969, page 75). The largest three eigenvalues and the corresponding eigenvectors of the matrix are computed and printed.

```
      USE EVESB_INT
      USE EPISB_INT
      USE UMACH_INT
      USE WRRRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    LDA, LDEVEC, N, NCODA, NEVEC
      PARAMETER  (N=6, NCODA=2, NEVEC=3, LDA=NCODA+1, LDEVEC=N)
!
      INTEGER    NOUT
      REAL       A(LDA,N), EVAL(NEVEC), EVEC(LDEVEC,NEVEC), PI
      LOGICAL    SMALL
!                                 Define values of A:
!                                 A = (  5  -4   1             )
!                                     ( -4   6  -4   1         )
!                                     (  1  -4   6  -4   1     )
!                                     (      1  -4   6  -4   1 )
!                                     (          1  -4   6  -4 )
!                                     (              1  -4   5 )
!                                 Represented in band symmetric
!                                 form this is:
!                                 A = (  0   0   1   1   1   1 )
!                                     (  0  -4  -4  -4  -4  -4 )
!                                     (  5   6   6   6   6   5 )
!
      DATA A/0.0, 0.0, 5.0, 0.0, -4.0, 6.0, 1.0, -4.0, 6.0, 1.0, -4.0, &
          6.0, 1.0, -4.0, 6.0, 1.0, -4.0, 5.0/
!
!                                 Find the 3 largest eigenvalues
!                                 and their eigenvectors.
      SMALL = .FALSE.
      CALL EVESB (NEVEC, A, NCODA, SMALL, EVAL, EVEC)
!                                 Compute performance index
      PI = EPISB(NEVEC,A,NCODA,EVAL,EVEC)
!                                 Print results
      CALL UMACH (2, NOUT)
      CALL WRRRN ('EVAL', EVAL, 1, NEVEC, 1)
      CALL WRRRN ('EVEC', EVEC)
      WRITE (NOUT,'(/,A,F6.3)') ' Performance index = ', PI
      END
```

Output

```
        EVAL
    1       2       3
14.45   10.54    5.98

              EVEC
          1         2         3
1    0.2319   -0.4179    0.5211
2   -0.4179    0.5211   -0.2319
3    0.5211   -0.2319   -0.4179
4   -0.5211   -0.2319    0.4179
5    0.4179    0.5211    0.2319
6   -0.2319   -0.4179   -0.5211
```

```
   Performance index =  0.175
```

EVBSB

Computes the eigenvalues in a given interval of a real symmetric matrix stored in band symmetric storage mode.

Required Arguments

MXEVAL — Maximum number of eigenvalues to be computed. (Input)

A — Band symmetric matrix of order N. (Input)

NCODA — Number of codiagonals in A. (Input)

ELOW — Lower limit of the interval in which the eigenvalues are sought. (Input)

EHIGH — Upper limit of the interval in which the eigenvalues are sought. (Input)

NEVAL — Number of eigenvalues found. (Output)

EVAL — Real vector of length MXEVAL containing the eigenvalues of A in the interval (ELOW, EHIGH) in decreasing order of magnitude. (Output)
Only the first NEVAL elements of EVAL are set.

Optional Arguments

N — Order of the matrix A. (Input)
Default: N = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement in the calling program. (Input)
Default: LDA = SIZE (A,1).

FORTRAN 90 Interface

Generic:	CALL EVBSB (MXEVAL, A, NCODA, ELOW, EHIGH, NEVAL, EVAL [,…])
Specific:	The specific interface names are S_EVBSB and D_EVBSB.

FORTRAN 77 Interface

Single:	CALL EVBSB (N, MXEVAL, A, LDA, NCODA, ELOW, EHIGH, NEVAL, EVAL)
Double:	The double precision name is DEVBSB.

Description

Routine EVBSB computes the eigenvalues in a given range of a real band symmetric matrix. Orthogonal similarity transformations are used to reduce the matrix to an equivalent symmetric tridiagonal matrix. A bisection algorithm is used to compute the eigenvalues of the tridiagonal matrix in a given range.

The reduction routine is based on the EISPACK routine BANDR; see Garbow et al. (1977). The bisection routine is based on the EISPACK routine BISECT; see Smith et al. (1976).

Comments

1. Workspace may be explicitly provided, if desired, by use of E3BSB/DE3BSB. The reference is:

   CALL E3BSB (N, MXEVAL, A, LDA, NCODA, ELOW, EHIGH, NEVAL, EVAL, ACOPY, WK)

   The additional arguments are as follows:

   ACOPY — Work matrix of size NCODA + 1 by N. A and ACOPY may be the same, in which case the first N(NCODA + 1) elements of A will be destroyed.

   WK — Work array of length 5N.

2. Informational error

Type	Code	Description
3	1	The number of eigenvalues in the specified interval exceeds MXEVAL. NEVAL contains the number of eigenvalues in the interval. No eigenvalues will be returned.

Example

In this example, a DATA statement is used to set *A* to a matrix given by Gregory and Karney (1969, page 77). The eigenvalues in the range (-2.5, 1.5) are computed and printed. As a test, this example uses MXEVAL = 5. The routine EVBSB computes NEVAL, the number of eigenvalues in the given range, has the value 3.

```
      USE EVBSB_INT
      USE UMACH_INT
      USE WRRRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    LDA, MXEVAL, N, NCODA
      PARAMETER  (MXEVAL=5, N=5, NCODA=2, LDA=NCODA+1)
!
      INTEGER    NEVAL, NOUT
      REAL       A(LDA,N), EHIGH, ELOW, EVAL(MXEVAL)
!
!                                 Define values of A:
!                                 A = ( -1   2   1          )
```

```
!                                     (  2   0   2   1       )
!                                     (  1   2   0   2   1  )
!                                     (      1   2   0   2  )
!                                     (          1   2  -1  )
!                                 Representedin band symmetric
!                                 form this is:
!                                 A = (  0   0   1   1   1 )
!                                     (  0   2   2   2   2 )
!                                     ( -1   0   0   0  -1 )
      DATA A/0.0, 0.0, -1.0, 0.0, 2.0, 0.0, 1.0, 2.0, 0.0, 1.0, 2.0, &
          0.0, 1.0, 2.0, -1.0/
!
      ELOW  = -2.5
      EHIGH = 1.5
      CALL EVBSB (MXEVAL, A, NCODA, ELOW, EHIGH, NEVAL, EVAL)
!                                 Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,'(/,A,I1)') ' NEVAL = ', NEVAL
      CALL WRRRN ('EVAL', EVAL, 1, NEVAl, 1)
      END
```

Output

```
NEVAL = 3

          EVAL
      1       2       3
 -2.464  -2.000   1.000
```

EVFSB

Computes the eigenvalues in a given interval and the corresponding eigenvectors of a real symmetric matrix stored in band symmetric storage mode.

Required Arguments

MXEVAL — Maximum number of eigenvalues to be computed. (Input)

A — Band symmetric matrix of order `N`. (Input)

NCODA — Number of codiagonals in `A`. (Input)

ELOW — Lower limit of the interval in which the eigenvalues are sought. (Input)

EHIGH — Upper limit of the interval in which the eigenvalues are sought. (Input)

NEVAL — Number of eigenvalues found. (Output)

EVAL — Real vector of length `MXEVAL` containing the eigenvalues of `A` in the interval (`ELOW`, `EHIGH`) in decreasing order of magnitude. (Output)
Only the first `NEVAL` elements of `EVAL` are significant.

EVEC — Real matrix containing in its first `NEVAL` columns the eigenvectors associated with the eigenvalues found and stored in `EVAL`. Eigenvector `J` corresponds to eigenvalue `J` for `J` = 1 to `NEVAL`. Each vector is normalized to have Euclidean length equal to the value one. (Output)

Optional Arguments

N — Order of the matrix `A`. (Input)
Default: `N` = `SIZE` (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement in the calling program. (Input)
Default: `LDA` = `SIZE` (`A`,1).

LDEVEC — Leading dimension of `EVEC` exactly as specified in the dimension statement in the calling program. (Input)
Default: `LDEVEC` = `SIZE` (`EVEC`,1).

FORTRAN 90 Interface

Generic: CALL EVFSB (MXEVEL, A, NCODA, ELOW, EHIGH, NEVAL, EVAL, EVEC [,…])

Specific: The specific interface names are S_EVFSB and D_EVFSB.

FORTRAN 77 Interface

Single: CALL EVFSB (N, MXEVAL, A, LDA, NCODA, ELOW, EHIGH, NEVAL, EVAL, EVEC, LDEVEC)

Double: The double precision name is DEVFSB.

Description

Routine EVFSB computes the eigenvalues in a given range and the corresponding eigenvectors of a real band symmetric matrix. Orthogonal similarity transformations are used to reduce the matrix to an equivalent tridiagonal matrix. A bisection algorithm is used to compute the eigenvalues of the tridiagonal matrix in the required range. Inverse iteration and orthogonalization are used to compute the eigenvectors of the given band symmetric matrix.

The reduction routine is based on the EISPACK routine BANDR; see Garbow et al. (1977). The bisection routine is based on the EISPACK routine BISECT; see Smith et al. (1976). The inverse iteration and orthogonalization steps are based on the EISPACK routine BANDV using remarks from Hanson et al. (1990).

Comments

1. Workspace may be explicitly provided, if desired, by use of E3FSB/DE3FSB. The reference is:

   CALL E3FSB (N, MXEVAL, A, LDA, NCODA, ELOW, EHIGH, NEVAL, EVAL, EVEC, LDEVEC, ACOPY, WK1, WK2, IWK)

   The additional arguments are as follows:

   ACOPY — Work matrix of size NCODA + 1 by N.

   WK1 — Work array of length 6N.

   WK2 — Work array of length 2N * NCODA + N

   IWK — Integer work array of length N.

2. Informational errors

Type	Code	Description
3	1	The number of eigenvalues in the specified interval exceeds MXEVAL. NEVAL contains the number of eigenvalues in the interval. No eigenvalues will be returned.
3	2	Inverse iteration did not converge. Eigenvector is not correct for the specified eigenvalue.
3	3	The eigenvectors have lost orthogonality.

Example

In this example, a DATA statement is used to set *A* to a matrix given by Gregory and Karney (1969, page 75). The eigenvalues in the range [1, 6] and their corresponding eigenvectors are computed and printed. As a test, this example uses MXEVAL = 4. The routine EVFSB computes NEVAL, the number of eigenvalues in the given range has the value 2. As a check on the computations, the performance index is also computed and printed. For more details, see IMSL routine EPISB.

```
      USE EVFSB_INT
      USE EPISB_INT
      USE WRRRN_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    LDA, LDEVEC, MXEVAL, N, NCODA
      PARAMETER  (MXEVAL=4, N=6, NCODA=2, LDA=NCODA+1, LDEVEC=N)
!
      INTEGER    NEVAL, NOUT
      REAL       A(LDA,N), EHIGH, ELOW, EVAL(MXEVAL), &
                 EVEC(LDEVEC,MXEVAL), PI
!                                 Define values of A:
!                                 A = (  5  -4   1              )
!                                     ( -4   6  -4   1          )
!                                     (  1  -4   6  -4   1      )
!                                     (      1  -4   6  -4   1  )
!                                     (          1  -4   6  -4  )
!                                     (              1  -4   5  )
!                                 Represented in band symmetric
!                                 form this is:
!                                 A = (  0   0   1   1   1   1  )
!                                     (  0  -4  -4  -4  -4  -4  )
!                                     (  5   6   6   6   6   5  )
      DATA A/0.0, 0.0, 5.0, 0.0, -4.0, 6.0, 1.0, -4.0, 6.0, 1.0, -4.0, &
          6.0, 1.0, -4.0, 6.0, 1.0, -4.0, 5.0/
!
!                                 Find eigenvalues and vectors
      ELOW  = 1.0
      EHIGH = 6.0
      CALL EVFSB (MXEVAL, A, NCODA, ELOW, EHIGH, NEVAL, EVAL, EVEC)
!                                 Compute performance index
      PI = EPISB(NEVAL,A,NCODA,EVAL,EVEC)
!                                 Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,'(/,A,I1)') ' NEVAL = ', NEVAL
      CALL WRRRN ('EVAL', EVAL, 1, NEVAL, 1)
      CALL WRRRN ('EVEC', EVEC, N, NEVAL, LDEVEC)
```

```
      WRITE (NOUT,'(/,A,F6.3)') ' Performance index = ', PI
      END
```

Output

```
NEVAL = 2

      EVAL
      1       2
  5.978   2.418

        EVEC
          1        2
 1   0.5211   0.5211
 2  -0.2319   0.2319
 3  -0.4179  -0.4179
 4   0.4179  -0.4179
 5   0.2319   0.2319
 6  -0.5211   0.5211

 Performance index =  0.083
```

EPISB

This function computes the performance index for a real symmetric eigensystem in band symmetric storage mode.

Required Arguments

EPISB — Performance index. (Output)

Required Arguments

NEVAL — Number of eigenvalue/eigenvector pairs on which the performance is based. (Input)

A — Band symmetric matrix of order `N`. (Input)

NCODA — Number of codiagonals in `A`. (Input)

EVAL — Vector of length `NEVAL` containing eigenvalues of `A`. (Input)

EVEC — `N` by `NEVAL` array containing eigenvectors of `A`. (Input)
The eigenvector corresponding to the eigenvalue `EVAL`(`J`) must be in the `J`-th column of `EVEC`.

Optional Arguments

N — Order of the matrix `A`. (Input)
Default: `N` = `SIZE` (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement in the calling program. (Input)
Default: `LDA` = `SIZE` (`A`,1).

LDEVEC — Leading dimension of `EVEC` exactly as specified in the dimension statement in the calling program. (Input)
Default: `LDEVEC` = `SIZE` (`EVEC`,1).

FORTRAN 90 Interface

Generic: `EPISB` (`NEVAL`, `A`, `NCODA`, `EVAL`, `EVEC`, …)

Specific: The specific interface names are `S_EPISB` and `D_EPISB`.

FORTRAN 77 Interface

Single: EPISB (N, NEVAL, A, LDA, NCODA, EVAL, EVEC, LDEVEC)

Double: The double precision function name is DEPISB.

Description

Let M = NEVAL, λ = EVAL, x_j = EVEC(*,J), the j-th column of EVEC. Also, let ε be the machine precision, given by AMACH(4), see the *Reference* chapter of the manual. The performance index, τ, is defined to be

$$\tau = \max_{1 \le j \le M} \frac{\left\| Ax_j - \lambda_j x_j \right\|_1}{10N\varepsilon \left\| A \right\|_1 \left\| x_j \right\|_1}$$

While the exact value of τ is highly machine dependent, the performance of EVCSF is considered excellent if $\tau < 1$, good if $1 \le \tau \le 100$, and poor if $\tau > 100$. The performance index was first developed by the EISPACK project at Argonne National Laboratory; see Smith et al. (1976, pages 124 – 125).

Comments

1. Workspace may be explicitly provided, if desired, by use of E2ISB/DE2ISB. The reference is:

   E2ISB (N, NEVAL, A, LDA, NCODA, EVAL, EVEC, LDEVEC, WK)

   The additional argument is:

   WK — Work array of length N.

2. Informational errors

Type	Code	Description
3	1	Performance index is greater than 100.
3	2	An eigenvector is zero.
3	3	The matrix is zero.

Example

For an example of EPISB, see IMSL routine EVCSB.

EVLHF

more...

Computes all of the eigenvalues of a complex Hermitian matrix.

Required Arguments

A — Complex Hermitian matrix of order `N`. (Input)
Only the upper triangle is used.

EVAL — Real vector of length `N` containing the eigenvalues of `A` in decreasing order of magnitude. (Output)

Optional Arguments

N — Order of the matrix `A`. (Input)
Default: `N` = `SIZE` (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement in the calling program. (Input)
Default: `LDA` = `SIZE` (`A`,1).

FORTRAN 90 Interface

Generic: `CALL EVLHF` (`A`, `EVAL` [,...])

Specific: The specific interface names are `S_EVLHF` and `D_EVLHF`.

FORTRAN 77 Interface

Single: `CALL EVLHF` (`N`, `A`, `LDA`, `EVAL`)

Double: The double precision name is `DEVLHF`.

Description

Routine EVLHF computes the eigenvalues of a complex Hermitian matrix. Unitary similarity transformations are used to reduce the matrix to an equivalent real symmetric tridiagonal matrix. The implicit QL algorithm is used to compute the eigenvalues of this tridiagonal matrix.

The underlying code is based on either EISPACK or LAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation, see "*Using ScaLAPACK, LAPACK, LINPACK, and EISPACK*" in the Introduction section of this manual.

Comments

1. Workspace may be explicitly provided, if desired, by use of E3LHF/DE3LHF. The reference is:

   CALL E3LHF (N, A, LDA, EVAL, ACOPY, RWK, CWK, IWK)

   The additional arguments are as follows:

   ACOPY — Complex work array of length N^2. A and ACOPY may be the same in which case A will be destroyed.

   RWK — Work array of length N.

   CWK — Complex work array of length 2N.

   IWK — Integer work array of length N.

2. Informational errors

Type	**Code**	**Description**
3	1	The matrix is not Hermitian. It has a diagonal entry with a small imaginary part.
4	1	The iteration for an eigenvalue failed to converge.
4	2	The matrix is not Hermitian. It has a diagonal entry with an imaginary part.

3. *Integer Options* with *Chapter 11* Options Manager

   1 This option uses eight values to solve memory bank conflict (access inefficiency) problems. In routine E3LHF, the internal or working leading dimensions of ACOPY and ECOPY are both increased by IVAL(3) when N is a multiple of IVAL(4). The values IVAL(3) and IVAL(4) are temporarily replaced by IVAL(1) and IVAL(2), respectively, in routine EVLHF. Additional memory allocation and option value restoration are automatically done in EVLHF. There is no requirement that users change existing applications that use EVLHF or E3LHF. Default values for the option are IVAL(*) = 1, 16, 0, 1, 1, 16, 0, 1. Items 5 – 8 in IVAL(*) are for the generalized eigenvalue problem and are not used in EVLHF.

Example

In this example, a DATA statement is used to set *A* to a matrix given by Gregory and Karney (1969, page 114). The eigenvalues of this complex Hermitian matrix are computed and printed.

```
      USE EVLHF_INT
      USE WRRRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    LDA, N
      PARAMETER  (N=2, LDA=N)
!
      REAL       EVAL(N)
      COMPLEX    A(LDA,N)
!                                 Set values of A
!
!                                 A = (  1      -i  )
!                                     (  i       1  )
!
      DATA A/(1.0,0.0), (0.0,1.0), (0.0,-1.0), (1.0,0.0)/
!
!                                 Find eigenvalues of A
      CALL EVLHF (A, EVAL)
!                                 Print results
      CALL WRRRN ('EVAL', EVAL, 1, N, 1)
      END
```

Output

```
      EVAL
      1       2
  2.000   0.000
```

EVCHF

more...

Computes all of the eigenvalues and eigenvectors of a complex Hermitian matrix.

Required Arguments

A — Complex Hermitian matrix of order `N`. (Input)
Only the upper triangle is used.

EVAL — Real vector of length `N` containing the eigenvalues of `A` in decreasing order of magnitude. (Output)

EVEC — Complex matrix of order `N`. (Output)
The `J`-th eigenvector, corresponding to `EVAL(J)`, is stored in the `J`-th column. Each vector is normalized to have Euclidean length equal to the value one.

Optional Arguments

N — Order of the matrix `A`. (Input)
Default: `N` = `SIZE` (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement in the calling program. (Input)
Default: `LDA` = `SIZE` (`A`,1).

LDEVEC — Leading dimension of `EVEC` exactly as specified in the dimension statement in the calling program. (Input)
Default: `LDEVEC` = `SIZE` (`EVEC`,1).

FORTRAN 90 Interface

Generic: `CALL EVCHF` (`A`, `EVAL`, `EVEC` [,…])

Specific: The specific interface names are `S_EVCHF` and `D_EVCHF`.

FORTRAN 77 Interface

Single: CALL EVCHF (N, A, LDA, EVAL, EVEC, LDEVEC)

Double: The double precision name is DEVCHF.

Description

Routine EVCHF computes the eigenvalues and eigenvectors of a complex Hermitian matrix. Unitary similarity transformations are used to reduce the matrix to an equivalent real symmetric tridiagonal matrix. The implicit QL algorithm is used to compute the eigenvalues and eigenvectors of this tridiagonal matrix. These eigenvectors and the transformations used to reduce the matrix to tridiagonal form are combined to obtain the eigenvectors for the user's problem. The underlying code is based on either EISPACK or LAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation, see "*Using ScaLAPACK, LAPACK, LINPACK, and EISPACK*" in the Introduction section of this manual.

Comments

1. Workspace may be explicitly provided, if desired, by use of E5CHF/DE5CHF. The reference is:

   CALL E5CHF (N, A, LDA, EVAL, EVEC, LDEVEC, ACOPY, RWK, CWK, IWK)

   The additional arguments are as follows:

   ACOPY — Complex work array of length N^2. A and ACOPY may be the same, in which case A will be destroyed.

   RWK — Work array of length $N^2 + N$.

   CWK — Complex work array of length 2N.

   IWK — Integer work array of length N.

2. Informational error

Type	Code	Description
3	1	The matrix is not Hermitian. It has a diagonal entry with a small imaginary part.
4	1	The iteration for an eigenvalue failed to converge.
4	2	The matrix is not Hermitian. It has a diagonal entry with an imaginary part.

3. The success of this routine can be checked using EPIHF.

4. *Integer Options* with *Chapter 11* Options Manager

1 This option uses eight values to solve memory bank conflict (access inefficiency) problems. In routine E5CHF, the internal or working leading dimensions of ACOPY and ECOPY are both increased by IVAL(3) when N is a multiple of IVAL(4). The values IVAL(3) and IVAL(4) are temporarily replaced by IVAL(1) and IVAL(2), respectively, in routine EVCHF. Additional memory allocation and option value restoration are automatically done in EVCHF. There is no requirement that users change existing applications that use EVCHF or E5CHF. Default values for the option are IVAL(*) = 1, 16, 0, 1, 1, 16, 0, 1. Items 5–8 in IVAL(*) are for the generalized eigenvalue problem and are not used in EVCHF.

Example

In this example, a DATA statement is used to set *A* to a complex Hermitian matrix. The eigenvalues and eigenvectors of this matrix are computed and printed. The performance index is also computed and printed. This serves as a check on the computations, for more details, see routine EPIHF.

```
      USE IMSL_libraries

      IMPLICIT   NONE

!                                 Declare variables
      INTEGER    LDA, LDEVEC, N
      PARAMETER  (N=3, LDA=N, LDEVEC=N)
!
      INTEGER    NOUT
      REAL       EVAL(N), PI
      COMPLEX    A(LDA,N), EVEC(LDEVEC,N)
!                                 Set values of A
!
!                                 A = ((1, 0)  (  1,-7i)  ( 0,- i))
!                                     ((1,7i)  (  5,   0)  (10,-3i))
!                                     ((0, i)  ( 10, 3i)  (-2,   0))
!
      DATA A/(1.0,0.0), (1.0,7.0), (0.0,1.0), (1.0,-7.0), (5.0,0.0), &
          (10.0, 3.0), (0.0,-1.0), (10.0,-3.0), (-2.0,0.0)/
!
!                                 Find eigenvalues and vectors of A
      CALL EVCHF (A, EVAL, EVEC)
!                                 Compute performance index
      PI = EPIHF(N,A,EVAL,EVEC)
!                                 Print results
      CALL UMACH (2, NOUT)
      CALL WRRRN ('EVAL', EVAL, 1, N, 1)
      CALL WRCRN ('EVEC', EVEC)
      WRITE (NOUT,'(/,A,F6.3)') ' Performance index = ', PI
      END
```

Output

```
          EVAL
      1        2        3
  15.38   -10.63    -0.75

                                  EVEC
                         1                      2                      3
 1  ( 0.0631,-0.4075)  (-0.0598,-0.3117)  ( 0.8539, 0.0000)
 2  ( 0.7703, 0.0000)  (-0.5939, 0.1841)  (-0.0313,-0.1380)
```

```
   3  ( 0.4668, 0.1366)  ( 0.7160, 0.0000)  ( 0.0808,-0.4942)

   Performance index =  0.093
```

EVAHF

Computes the largest or smallest eigenvalues of a complex Hermitian matrix.

Required Arguments

NEVAL — Number of eigenvalues to be calculated. (Input)

A — Complex Hermitian matrix of order N. (Input)
Only the upper triangle is used.

SMALL — Logical variable. (Input)
If .TRUE., the smallest NEVAL eigenvalues are computed. If .FALSE., the largest NEVAL eigenvalues are computed.

EVAL — Real vector of length N containing the extreme eigenvalues of A in decreasing order of magnitude in the first NEVAL elements. (Output)

Optional Arguments

N — Order of the matrix A. (Input)
Default: N = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement in the calling program. (Input)
Default: LDA = SIZE (A,1).

FORTRAN 90 Interface

Generic: CALL EVAHF (NEVAL, A, SMALL, EVAL [,…])

Specific: The specific interface names are S_EVAHF and D_EVAHF.

FORTRAN 77 Interface

Single: CALL EVAHF (N, NEVAL, A, LDA, SMALL, EVAL)

Double: The double precision name is DEVAHF.

Description

Routine EVAHF computes the largest or smallest eigenvalues of a complex Hermitian matrix. Unitary transformations are used to reduce the matrix to an equivalent symmetric tridiagonal matrix. The rational QR algorithm with Newton corrections is used to compute the extreme eigenvalues of this tridiagonal matrix.

The reduction routine is based on the EISPACK routine HTRIDI. The QR routine is based on the EISPACK routine RATQR. See Smith et al. (1976) for the EISPACK routines.

Comments

1. Workspace may be explicitly provided, if desired, by use of E3AHF/DE3AHF. The reference is

   CALL E3AHF (N, NEVAL, A, LDA, SMALL, EVAL, ACOPY, RWK, CWK, IWK)

   The additional arguments are as follows:

   ACOPY — Complex work array of length N^2. A and ACOPY may be the same in which case A will be destroyed.

   RWK — Work array of length 2N.

   CWK — Complex work array of length 2N.

   IWK — Work array of length N.

2. Informational errors

Type	**Code**	**Description**
3	1	The iteration for an eigenvalue failed to converge. The best estimate will be returned.
3	2	The matrix is not Hermitian. It has a diagonal entry with a small imaginary part.
4	2	The matrix is not Hermitian. It has a diagonal entry with an imaginary part.

Example

In this example, a DATA statement is used to set *A* to a matrix given by Gregory and Karney (1969, page 114). Its largest eigenvalue is computed and printed.

```
      USE EVAHF_INT
      USE WRRRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    LDA, N
      PARAMETER  (N=2, LDA=N)
```

```
!
      INTEGER    NEVAL
      REAL       EVAL(N)
      COMPLEX    A(LDA,N)
      LOGICAL    SMALL
!                                  Set values of A
!
!                                  A = (  1      -i  )
!                                      (  i       1  )
!
      DATA A/(1.0,0.0), (0.0,1.0), (0.0,-1.0), (1.0,0.0)/
!
!                                  Find the largest eigenvalue of A
      NEVAL = 1
      SMALL = .FALSE.
      CALL EVAHF (NEVAL, A, SMALL, EVAL)
!                                  Print results
      CALL WRRRN ('EVAL', EVAL, 1, NEVAl, 1)
      END
```

Output

```
  EVAL
  2.000
```

EVEHF

Computes the largest or smallest eigenvalues and the corresponding eigenvectors of a complex Hermitian matrix.

Required Arguments

NEVEC — Number of eigenvectors to be computed. (Input)

A — Complex Hermitian matrix of order N. (Input)
Only the upper triangle is used.

SMALL — Logical variable. (Input)
If .TRUE., the smallest NEVEC eigenvectors are computed. If .FALSE., the largest NEVEC eigenvectors are computed.

EVAL — Real vector of length N containing the eigenvalues of A in decreasing order of magnitude. (Output)

EVEC — Complex matrix of dimension N by NEVEC. (Output)
The J-th eigenvector corresponding to EVAL(J), is stored in the J-th column. Each vector is normalized to have Euclidean length equal to the value one.

Optional Arguments

N — Order of the matrix A. (Input)
Default: N = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement in the calling program. (Input)
Default: LDA = SIZE (A,1).

LDEVEC — Leading dimension of EVEC exactly as specified in the dimension statement in the calling program. (Input)
Default: LDEVEC = SIZE (EVEC,1).

FORTRAN 90 Interface

Generic: CALL EVEHF (NEVEC, A, SMALL, EVAL, EVEC [,…])

Specific: The specific interface names are S_EVEHF and D_EVEHF.

FORTRAN 77 Interface

Single: `CALL EVEHF (N, NEVEC, A, LDA, SMALL, EVAL, EVEC, LDEVEC)`

Double: The double precision name is `DEVEHF`.

Description

Routine EVEHF computes the largest or smallest eigenvalues and the corresponding eigenvectors of a complex Hermitian matrix. Unitary transformations are used to reduce the matrix to an equivalent real symmetric tridiagonal matrix. The rational QR algorithm with Newton corrections is used to compute the extreme eigenvalues of the tridiagonal matrix. Inverse iteration is used to compute the eigenvectors of the tridiagonal matrix. Eigenvectors of the original matrix are found by back transforming the eigenvectors of the tridiagonal matrix.

The reduction routine is based on the EISPACK routine HTRIDI. The QR routine used is based on the EISPACK routine RATQR. The inverse iteration routine is based on the EISPACK routine TINVIT. The back transformation routine is based on the EISPACK routine HTRIBK. See Smith et al. (1976) for the EISPACK routines.

Comments

1. Workspace may be explicitly provided, if desired, by use of E3EHF/DE3EHF. The reference is:

```
CALL E3EHF (N, NEVEC, A, LDA, SMALL, EVAL, EVEC, LDEVEC,
   ACOPY, RW1, RW2, CWK, IWK)
```

The additional arguments are as follows:

ACOPY — Complex work array of length N^2. A and ACOPY may be the same, in which case A will be destroyed.

RW1 — Work array of length N * NEVEC. Used to store the real eigenvectors of a symmetric tridiagonal matrix.

RW2 — Work array of length 8N.

CWK — Complex work array of length 2N.

IWK — Work array of length N.

2. Informational errors

Type	Code	Description
3	1	The iteration for an eigenvalue failed to converge. The best estimate will be returned.
3	2	The iteration for an eigenvector failed to converge. The eigenvector will be set to 0.

Type	Code	Description
3	3	The matrix is not Hermitian. It has a diagonal entry with a small imaginary part.
4	2	The matrix is not Hermitian. It has a diagonal entry with an imaginary part.

3. The success of this routine can be checked using EPIHF.

Example

In this example, a DATA statement is used to set *A* to a matrix given by Gregory and Karney (1969, page 115). The smallest eigenvalue and its corresponding eigenvector is computed and printed. The performance index is also computed and printed. This serves as a check on the computations. For more details, see IMSL routine EPIHF.

```
      USE IMSL_LIBRARIES

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    LDA, LDEVEC, N, NEVEC
      PARAMETER  (N=3, NEVEC=1, LDA=N, LDEVEC=N)
!
      INTEGER    NOUT
      REAL       EVAL(N), PI
      COMPLEX    A(LDA,N), EVEC(LDEVEC,NEVEC)
      LOGICAL    SMALL
!                                 Set values of A
!
!                                 A = (  2      -i      0  )
!                                     (  i       2      0  )
!                                     (  0       0      3  )
!
      DATA A/(2.0,0.0), (0.0,1.0), (0.0,0.0), (0.0,-1.0), (2.0,0.0), &
          (0.0,0.0), (0.0,0.0), (0.0,0.0), (3.0,0.0)/
!
!                                 Find smallest eigenvalue and its
!                                 eigenvectors
      SMALL = .TRUE.
      CALL EVEHF (NEVEC, A, SMALL, EVAL, EVEC)
!                                 Compute performance index
      PI = EPIHF(NEVEC,A,EVAL,EVEC)
!                                 Print results
      CALL UMACH (2, NOUT)
      CALL WRRRN ('EVAL', EVAL, 1, NEVEC, 1)
      CALL WRCRN ('EVEC', EVEC)
      WRITE (NOUT,'(/,A,F6.3)') ' Performance index = ', PI
      END
```

Output

```
    EVAL
    1.000

           EVEC
   1   ( 0.0000, 0.7071)
   2   ( 0.7071, 0.0000)
```

```
   3  ( 0.0000, 0.0000)

   Performance index =  0.031
```

EVBHF

Computes the eigenvalues in a given range of a complex Hermitian matrix.

Required Arguments

MXEVAL — Maximum number of eigenvalues to be computed. (Input)

A — Complex Hermitian matrix of order N. (Input)
Only the upper triangle is used.

ELOW — Lower limit of the interval in which the eigenvalues are sought. (Input)

EHIGH – Upper limit of the interval in which the eigenvalues are sought. (Input)

NEVAL — Number of eigenvalues found. (Output)

EVAL — Real vector of length MXEVAL containing the eigenvalues of A in the interval (ELOW, EHIGH) in decreasing order of magnitude. (Output)
Only the first NEVAL elements of EVAL are significant.

Optional Arguments

N — Order of the matrix A. (Input)
Default: N = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement in the calling program. (Input)
Default: LDA = SIZE (A,1).

FORTRAN 90 Interface

Generic: CALL EVBHF (MXEVAL, A, ELOW, EHIGH, NEVAL, EVAL [,…])

Specific: The specific interface names are S_EVBHF and D_EVBHF.

FORTRAN 77 Interface

Single: CALL EVBHF (N, MXEVAL, A, LDA, ELOW, EHIGH, NEVAL, EVAL)

Double: The double precision name is DEVBHF.

Description

Routine EVBHF computes the eigenvalues in a given range of a complex Hermitian matrix. Unitary transformations are used to reduce the matrix to an equivalent symmetric tridiagonal matrix. A bisection algorithm is used to compute the eigenvalues in the given range of this tridiagonal matrix.

The reduction routine is based on the EISPACK routine HTRIDI. The bisection routine used is based on the EISPACK routine BISECT. See Smith et al. (1976) for the EISPACK routines.

Comments

1. Workspace may be explicitly provided, if desired, by use of E3BHF/DE3BHF. The reference is:

   ```
   CALL E3BHF (N, MXEVAL, A, LDA, ELOW, EHIGH, NEVAL, EVAL,
      ACOPY, RWK, CWK, IWK)
   ```

   The additional arguments are as follows:

   ACOPY — Complex work matrix of size N by N. A and ACOPY may be the same, in which case the first N^2 elements of A will be destroyed.

   RWK — Work array of length 5N.

   CWK — Complex work array of length 2N.

   IWK — Work array of length MXEVAL.

2. Informational errors

Type	**Code**	**Description**
3	1	The number of eigenvalues in the specified range exceeds MXEVAL. NEVAL contains the number of eigenvalues in the range. No eigenvalues will be computed.
3	2	The matrix is not Hermitian. It has a diagonal entry with a small imaginary part.
4	2	The matrix is not Hermitian. It has a diagonal entry with an imaginary part.

Example

In this example, a DATA statement is used to set *A* to a matrix given by Gregory and Karney (1969, page 114). The eigenvalues in the range [1.5, 2.5] are computed and printed. This example allows a maximum number of eigenvalues MXEVAL = 2. The routine computes that there is one eigenvalue in the given range. This value is returned in NEVAL.

```
      USE EVBHF_INT
      USE UMACH_INT
```

```
      USE WRRRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    LDA, MXEVAL, N
      PARAMETER  (MXEVAL=2, N=2, LDA=N)
!
      INTEGER    NEVAL, NOUT
      REAL       EHIGH, ELOW, EVAL(MXEVAL)
      COMPLEX    A(LDA,N)
!                                 Set values of A
!
!                                 A = (  1       -i  )
!                                     (  i        1  )
!
      DATA A/(1.0,0.0), (0.0,1.0), (0.0,-1.0), (1.0,0.0)/
!
!                                 Find eigenvalue
      ELOW  = 1.5
      EHIGH = 2.5
      CALL EVBHF (MXEVAL, A, ELOW, EHIGH, NEVAL, EVAL)
!
!                                 Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,'(/,A,I3)') ' NEVAL = ', NEVAL
      CALL WRRRN ('EVAL', EVAL, 1, NEVAL, 1)
      END
```

Output

```
 NEVAL =   1

  EVAL
  2.000
```

EVFHF

Computes the eigenvalues in a given range and the corresponding eigenvectors of a complex Hermitian matrix.

Required Arguments

MXEVAL — Maximum number of eigenvalues to be computed. (Input)

A — Complex Hermitian matrix of order `N`. (Input)
Only the upper triangle is used.

ELOW — Lower limit of the interval in which the eigenvalues are sought. (Input)

EHIGH — Upper limit of the interval in which the eigenvalues are sought. (Input)

NEVAL — Number of eigenvalues found. (Output)

EVAL — Real vector of length `MXEVAL` containing the eigenvalues of `A` in the interval (`ELOW`, `EHIGH`) in decreasing order of magnitude. (Output)
Only the first `NEVAL` elements of `EVAL` are significant.

EVEC — Complex matrix containing in its first `NEVAL` columns the eigenvectors associated with the eigenvalues found stored in `EVAL`. Each vector is normalized to have Euclidean length equal to the value one. (Output)

Optional Arguments

N — Order of the matrix `A`. (Input)
Default: `N` = `SIZE` (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement in the calling program. (Input)
Default: `LDA` = `SIZE` (`A`,1).

LDEVEC — Leading dimension of `EVEC` exactly as specified in the dimension statement in the calling program. (Input)
Default: `LDEVEC` = `SIZE` (`EVEC`,1).

FORTRAN 90 Interface

Generic: `CALL EVFHF (MXEVAL, A, ELOW, EHIGH, NEVAL, EVAL, EVEC [,…])`

Specific: The specific interface names are S_EVFHF and D_EVFHF.

FORTRAN 77 Interface

Single: CALL EVFHF (N, MXEVAL, A, LDA, ELOW, EHIGH, NEVAL, EVAL, EVEC, LDEVEC)

Double: The double precision name is DEVHFH.

Description

Routine EVFHF computes the eigenvalues in a given range and the corresponding eigenvectors of a complex Hermitian matrix. Unitary transformations are used to reduce the matrix to an equivalent symmetric tridiagonal matrix. A bisection algorithm is used to compute the eigenvalues in the given range of this tridiagonal matrix. Inverse iteration is used to compute the eigenvectors of the tridiagonal matrix. The eigenvectors of the original matrix are computed by back transforming the eigenvectors of the tridiagonal matrix.

The reduction routine is based on the EISPACK routine HTRIDI. The bisection routine is based on the EISPACK routine BISECT. The inverse iteration routine is based on the EISPACK routine TINVIT. The back transformation routine is based on the EISPACK routine HTRIBK. See Smith et al. (1976) for the EISPACK routines.

Comments

1. Workspace may be explicitly provided, if desired, by use of E3FHF/DE3FHF. The reference is:

```
CALL E3FHF (N, MXEVAL, A, LDA, ELOW, EHIGH, NEVAL, EVAL,
   EVEC, LDEVEC, ACOPY, ECOPY, RWK, CWK, IWK)
```

   The additional arguments are as follows:

   ACOPY — Complex work matrix of size N by N. A and ACOPY may be the same, in which case the first N^2 elements of A will be destroyed.

   ECOPY — Work matrix of size N by MXEVAL. Used to store eigenvectors of a real tridiagonal matrix.

   RWK — Work array of length 8N.

   CWK — Complex work array of length 2N.

   IWK — Work array of length MXEVAL.

2. Informational errors

Type	Code	Description
3	1	The number of eigenvalues in the specified range exceeds MXEVAL. NEVAL contains the number of eigenvalues in the range. No eigenvalues will be computed.
3	2	The iteration for an eigenvector failed to converge. The eigenvector will be set to 0.
3	3	The matrix is not Hermitian. It has a diagonal entry with a small imaginary part.
4	2	The matrix is not Hermitian. It has a diagonal entry with an imaginary part.

Example

In this example, a DATA statement is used to set *A* to a complex Hermitian matrix. The eigenvalues in the range [–15, 0] and their corresponding eigenvectors are computed and printed. As a test, this example uses MXEVAL = 3. The routine EVFHF computes the number of eigenvalues in the given range. That value, NEVAL, is two. As a check on the computations, the performance index is also computed and printed. For more details, see routine EPIHF.

```
      USE IMSL_LIBRARIES

      IMPLICIT   NONE

!                                 Declare variables
      INTEGER    LDA, LDEVEC, MXEVAL, N
      PARAMETER  (MXEVAL=3, N=3, LDA=N, LDEVEC=N)
!
      INTEGER    NEVAL, NOUT
      REAL       EHIGH, ELOW, EVAL(MXEVAL), PI
      COMPLEX    A(LDA,N), EVEC(LDEVEC,MXEVAL)
!                                 Set values of A
!
!                                 A = ((1, 0)  (  1,-7i)  ( 0,- i))
!                                     ((1,7i)  (  5,   0)  (10,-3i))
!                                     ((0, i)  ( 10, 3i)  (-2,   0))
!
      DATA A/(1.0,0.0), (1.0,7.0), (0.0,1.0), (1.0,-7.0), (5.0,0.0), &
          (10.0,3.0), (0.0,-1.0), (10.0,-3.0), (-2.0,0.0)/
!
!                                 Find eigenvalues and vectors
      ELOW  = -15.0
      EHIGH = 0.0
      CALL EVFHF (MXEVAL, A, ELOW, EHIGH, NEVAL, EVAL, EVEC)
!                                 Compute performance index
      PI = EPIHF(NEVAL,A,EVAL,EVEC)
!                                 Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,'(/,A,I3)') ' NEVAL = ', NEVAL
      CALL WRRRN ('EVAL', EVAL, 1, NEVAL, 1)
      CALL WRCRN ('EVEC', EVEC, N, NEVAL, LDEVEC)
      WRITE (NOUT,'(/,A,F6.3)') ' Performance index = ', PI
      END
```

Output

```
NEVAL =   2

     EVAL
     1       2
-10.63   -0.75

                 EVEC
                   1                  2
1  (-0.0598,-0.3117)  ( 0.8539, 0.0000)
2  (-0.5939, 0.1841)  (-0.0313,-0.1380)
3  ( 0.7160, 0.0000)  ( 0.0808,-0.4942)

Performance index =  0.057
```

EPIHF

This function computes the performance index for a complex Hermitian eigensystem.

Function Return Value

EPIHF — Performance index. (Output)

Required Arguments

NEVAL — Number of eigenvalue/eigenvector pairs on which the performance index computation is based. (Input)

A — Complex Hermitian matrix of order N. (Input)

EVAL — Vector of length NEVAL containing eigenvalues of A. (Input)

EVEC — Complex N by NEVAL array containing eigenvectors of A. (Input)
The eigenvector corresponding to the eigenvalue EVAL(J) must be in the J-th column of EVEC.

Optional Arguments

N — Order of the matrix A. (Input)
Default: N = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement in the calling program. (Input)
Default: LDA = SIZE (A,1).

LDEVEC — Leading dimension of EVEC exactly as specified in the dimension statement in the calling program. (Input)
Default: LDEVEC = SIZE (EVEC,1).

FORTRAN 90 Interface

Generic: EPIHF (NEVAL, A, EVAL, EVEC [,…])

Specific: The specific interface names are S_EPIHF and D_EPIHF.

FORTRAN 77 Interface

Single: `EPIHF (N, NEVAL, A, LDA, EVAL, EVEC, LDEVEC)`

Double: The double precision function name is `DEPIHF`.

Description

Let M = NEVAL, λ = EVAL, x_j = EVEC(*, J), the j-th column of EVEC. Also, let ε be the machine precision, given by AMACH(4), see the *Reference* chapter of this manual. The performance index, τ, is defined to be

$$\tau = \max_{1 \le j \le M} \frac{\|Ax_j - \lambda_j x_j\|_1}{10 N \varepsilon \|A\|_1 \|x_j\|_1}$$

The norms used are a modified form of the 1-norm. The norm of the complex vector v is

$$\|v\|_1 = \sum_{i=1}^{N} \left\{ |\Re\, v_i| + |\Im\, v_i| \right\}$$

While the exact value of τ is highly machine dependent, the performance of EVCSF is considered excellent if $\tau < 1$, good if $1 \le \tau \le 100$, and poor if $\tau > 100$. The performance index was first developed by the EISPACK project at Argonne National Laboratory; see Smith et al. (1976, pages 124 – 125).

Comments

1. Workspace may be explicitly provided, if desired, by use of E2IHF/DE2IHF. The reference is:

   `E2IHF(N, NEVAL, A, LDA, EVAL, EVEC, LDEVEC, WK)`

   The additional argument is

   WK — Complex work array of length N.

2. Informational errors

Type	Code	Description
3	1	Performance index is greater than 100.
3	2	An eigenvector is zero.
3	3	The matrix is zero.

Example

For an example of EPIHF, see IMSL routine EVCHF.

EVLRH

Computes all of the eigenvalues of a real upper Hessenberg matrix.

Required Arguments

A — Real upper Hessenberg matrix of order N. (Input)

EVAL — Complex vector of length N containing the eigenvalues in decreasing order of magnitude. (Output)

Optional Arguments

N — Order of the matrix A. (Input)
Default: N = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement in the calling program. (Input)
Default: LDA = SIZE (A,1).

FORTRAN 90 Interface

Generic: CALL EVLRH (A, EVAL [,…])

Specific: The specific interface names are S_EVLRH and D_EVLRH.

FORTRAN 77 Interface

Single: CALL EVLRH (N, A, LDA, EVAL)

Double: The double precision name is DEVLRH.

Description

Routine EVLRH computes the eigenvalues of a real upper Hessenberg matrix by using the QR algorithm. The QR Algorithm routine is based on the EISPACK routine HQR, Smith et al. (1976).

Comments

1. Workspace may be explicitly provided, if desired, by use of E3LRH/DE3LRH. The reference is:

   CALL E3LRH (N, A, LDA, EVAL, ACOPY, WK, IWK)

   The additional arguments are as follows:

   ACOPY — Real N by N work matrix.

   WK — Real vector of length 3*n*.

   IWK — Integer vector of length *n*.

2. Informational error

Type	Code	Description
4	1	The iteration for the eigenvalues failed to converge.

Example

In this example, a DATA statement is used to set A to an upper Hessenberg matrix of integers. The eigenvalues of this matrix are computed and printed.

```
      USE EVLRH_INT
      USE UMACH_INT
      USE WRCRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    LDA, N
      PARAMETER  (N=4, LDA=N)
!
      INTEGER    NOUT
      REAL       A(LDA,N)
      COMPLEX    EVAL(N)
!                                 Set values of A
!
!                                 A = (  2.0    1.0    3.0    4.0  )
!                                     (  1.0    0.0    0.0    0.0  )
!                                     (         1.0    0.0    0.0  )
!                                     (                1.0    0.0  )
!
      DATA A/2.0, 1.0, 0.0, 0.0, 1.0, 0.0, 1.0, 0.0, 3.0, 0.0, 0.0, &
          1.0, 4.0, 0.0, 0.0, 0.0/
!
!                                 Find eigenvalues of A
      CALL EVLRH (A, EVAL)
!                                 Print results
      CALL UMACH (2, NOUT)
      CALL WRCRN ('EVAL', EVAL, 1, N, 1)
      END
```

Output

```
                            EVAL
                 1                 2                 3                 4
```

```
   ( 2.878, 0.000)  ( 0.011, 1.243)  ( 0.011,-1.243)  (-0.900, 0.000)
```

EVCRH

Computes all of the eigenvalues and eigenvectors of a real upper Hessenberg matrix.

Required Arguments

A — Real upper Hessenberg matrix of order N. (Input)

EVAL — Complex vector of length N containing the eigenvalues in decreasing order of magnitude. (Output)

EVEC — Complex matrix of order N. (Output)
The J-th eigenvector, corresponding to EVAL(J), is stored in the J-th column. Each vector is normalized to have Euclidean length equal to the value one.

Optional Arguments

N — Order of the matrix A. (Input)
Default: N = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement in the calling program. (Input)
Default: LDA = SIZE (A,1).

LDEVEC — Leading dimension of EVEC exactly as specified in the dimension statement in the calling program. (Input)
Default: LDEVEC = SIZE (EVEC,1).

FORTRAN 90 Interface

Generic: CALL EVCRH (A, EVAL, EVEC [,…])

Specific: The specific interface names are S_EVCRH and D_EVCRH.

FORTRAN 77 Interface

Single: CALL EVCRH (N, A, LDA, EVAL, EVEC, LDEVEC)

Double: The double precision name is DEVCRH.

Description

Routine EVCRH computes the eigenvalues and eigenvectors of a real upper Hessenberg matrix by using the QR algorithm. The QR algorithm routine is based on the EISPACK routine HQR2; see Smith et al. (1976).

Comments

1. Workspace may be explicitly provided, if desired, by use of E6CRH/DE6CRH. The reference is:

   CALL E6CRH (N, A, LDA, EVAL, EVEC, LDEVEC, ACOPY, ECOPY, RWK, IWK)

   The additional arguments are as follows:

   ACOPY — Real N by N work matrix.

   ECOPY — Real N by N work matrix.

   RWK — Real array of length 3N.

   IWK — Integer array of length N.

2. Informational error

Type	Code	Description
4	1	The iteration for the eigenvalues failed to converge.

Example

In this example, a DATA statement is used to set *A* to a Hessenberg matrix with integer entries. The values are returned in decreasing order of magnitude. The eigenvalues, eigenvectors and performance index of this matrix are computed and printed. See routine EPIRG for details.

```
      USE EVCRH_INT
      USE EPIRG_INT
      USE UMACH_INT
      USE WRCRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    LDA, LDEVEC, N
      PARAMETER  (N=4, LDA=N, LDEVEC=N)
!
      INTEGER    NOUT
      REAL       A(LDA,N), PI
      COMPLEX    EVAL(N), EVEC(LDEVEC,N)
!                                 Define values of A:
!
!                                 A = ( -1.0   -1.0   -1.0   -1.0  )
!                                     (  1.0    0.0    0.0    0.0  )
!                                     (         1.0    2.0    0.0  )
!                                     (                1.0    0.0  )
!
```

```
      DATA A/-1.0, 1.0, 0.0, 0.0, -1.0, 0.0, 1.0, 0.0, -1.0, 0.0, 2.0, &
          1.0, -1.0, 0.0, 0.0, 0.0/
!
!                                 Find eigenvalues and vectors of A
      CALL EVCRH (A, EVAL, EVEC)
!                                 Compute performance index
      PI = EPIRG(N,A,EVAL,EVEC)
!                                 Print results
      CALL UMACH (2, NOUT)
      CALL WRCRN ('EVAL', EVAL, 1, N, 1)
      CALL WRCRN ('EVEC', EVEC)
      WRITE (NOUT,'(/,A,F6.3)') ' Performance index = ', PI
      END
```

Output

```
                                    EVAL
                    1                  2                  3                  4
      (1.722, 0.000)    (-0.651,0.759)    (-0.651, -0.759)    (0.581,0.000)

                                     EVEC
                       1                   2                   3                   4
   1  (-0.3733, 0.0000)  (-0.4330, 0.5044)  (-0.4330,-0.5044)  (-0.3194, 0.0000)
   2  (-0.2168, 0.0000)  ( 0.6648, 0.0000)  ( 0.6648, 0.0000)  (-0.5500, 0.0000)
   3  ( 0.7800, 0.0000)  (-0.2317,-0.0663)  (-0.2317, 0.0663)  ( 0.3875, 0.0000)
   4  ( 0.4530, 0.0000)  ( 0.1006, 0.2190)  ( 0.1006,-0.2190)  ( 0.6673, 0.0000)

   Performance index =  0.026
```

EVLCH

Computes all of the eigenvalues of a complex upper Hessenberg matrix.

Required Arguments

A — Complex upper Hessenberg matrix of order N. (Input)

EVAL — Complex vector of length N containing the eigenvalues of A in decreasing order of magnitude. (Output)

Required Arguments

N — Order of the matrix A. (Input)
Default: N = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement in the calling program. (Input)
Default: LDA = SIZE (A,1).

FORTRAN 90 Interface

Generic: CALL EVLCH (A, EVAL [,…])

Specific: The specific interface names are S_EVLCH and D_EVLCH.

FORTRAN 77 Interface

Single: CALL EVLCH (N, A, LDA, EVAL)

Double: The double precision name is DEVLCH.

Description

Routine EVLCH computes the eigenvalues of a complex upper Hessenberg matrix using the QR algorithm. This routine is based on the EISPACK routine COMQR2; see Smith et al. (1976).

Comments

1. Workspace may be explicitly provided, if desired, by use of E3LCH/DE3LCH. The reference is:

   CALL E3LCH (N, A, LDA, EVAL, ACOPY, RWK, IWK)

   The additional arguments are as follows:

   ACOPY — Complex N by N work array. A and ACOPY may be the same, in which case A is destroyed.

   RWK — Real work array of length N.

   IWK — Integer work array of length N.

2. Informational error

Type	Code	Description
4	1	The iteration for the eigenvalues failed to converge.

Example

In this example, a DATA statement is used to set the matrix A. The program computes and prints the eigenvalues of this matrix.

```
      USE EVLCH_INT
      USE WRCRN_INT

      IMPLICIT NONE
!                                 Declare variables
      INTEGER LDA, N
      PARAMETER (N=4, LDA=N)
      COMPLEX A(LDA,N), EVAL(N)
!                                 Set values of A
!
!                                 A = (5+9i  5+5i  -6-6i  -7-7i)
!                                     (3+3i  6+10i -5-5i  -6-6i)
!                                     ( 0    3+3i  -1+3i  -5-5i)
!                                     ( 0     0    -3-3i     4i)
!
      DATA A /(5.0,9.0), (3.0,3.0), (0.0,0.0), (0.0,0.0), &
             (5.0,5.0), (6.0,10.0), (3.0,3.0), (0.0,0.0), &
             (-6.0,-6.0), (-5.0,-5.0), (-1.0,3.0), (-3.0,-3.0), &
             (-7.0,-7.0), (-6.0,-6.0), (-5.0,-5.0), (0.0,4.0)/
!
!                                 Find the eigenvalues of A
      CALL EVLCH (A, EVAL)
!                                 Print results
      CALL WRCRN ('EVAL', EVAL, 1, N, 1)
      END
```

Output

```
                                EVAL
                 1                     2                     3                     4
 (   8.22, 12.22)  (   3.40,   7.40)  (   1.60,   5.60)  ( -3.22,   0.78)
```

EVCCH

Computes all of the eigenvalues and eigenvectors of a complex upper Hessenberg matrix.

Required Arguments

A — Complex upper Hessenberg matrix of order `N`. (Input)

EVAL — Complex vector of length `N` containing the eigenvalues of `A` in decreasing order of magnitude. (Output)

EVEC — Complex matrix of order `N`. (Output)
The `J`-th eigenvector, corresponding to `EVAL(J)`, is stored in the `J`-th column. Each vector is normalized to have Euclidean length equal to the value one.

Optional Arguments

N — Order of the matrix `A`. (Input)
Default: `N` = `SIZE` (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement in the calling program. (Input)
Default: `LDA` = `SIZE` (`A`,1).

LDEVEC — Leading dimension of `EVEC` exactly as specified in the dimension statement in the calling program. (Input)
Default: `LDEVEC` = `SIZE` (`EVEC`,1).

FORTRAN 90 Interface

Generic: `CALL EVCCH (A, EVAL, EVEC [,…])`

Specific: The specific interface names are `S_EVCCH` and `D_EVCCH`.

FORTRAN 77 Interface

Single: `CALL EVCCH (N, A, LDA, EVAL, EVEC, LDEVEC)`

Double: The double precision name is `DEVCCH`.

Description

Routine EVCCH computes the eigenvalues and eigenvectors of a complex upper Hessenberg matrix using the QR algorithm. This routine is based on the EISPACK routine COMQR2; see Smith et al. (1976).

Comments

1. Workspace may be explicitly provided, if desired, by use of E4CCH/DE4CCH. The reference is:

   CALL E4CCH (N, A, LDA, EVAL, EVEC, LDEVEC, ACOPY, CWORK, RWK, IWK)

   The additional arguments are as follows:

   ACOPY — Complex N by N work array. A and ACOPY may be the same, in which case A is destroyed.

   CWORK — Complex work array of length 2N.

   RWK — Real work array of length N.

   IWK — Integer work array of length N.

2 Informational error

Type	Code	Description
4	1	The iteration for the eigenvalues failed to converge.

3. The results of EVCCH can be checked using EPICG. This requires that the matrix A explicitly contains the zeros in A(I, J) for (I – 1) > J which are assumed by EVCCH.

Example

In this example, a DATA statement is used to set the matrix *A*. The program computes the eigenvalues and eigenvectors of this matrix. The performance index is also computed and printed. This serves as a check on the computations; for more details, see IMSL routine EPICG. The zeros in the lower part of the matrix are not referenced by EVCCH, but they are required by EPICG.

```
      USE EVCCH_INT
      USE EPICG_INT
      USE UMACH_INT
      USE WRCRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    LDA, LDEVEC, N
      PARAMETER  (N=4, LDA=N, LDEVEC=N)
!
      INTEGER    NOUT
      REAL       PI
```

```
      COMPLEX    A(LDA,N), EVAL(N), EVEC(LDEVEC,N)
!                               Set values of A
!
!                               A = (5+9i  5+5i  -6-6i  -7-7i)
!                                   (3+3i  6+10i -5-5i  -6-6i)
!                                   ( 0    3+3i  -1+3i  -5-5i)
!                                   ( 0     0    -3-3i     4i)
!
      DATA A/(5.0,9.0), (3.0,3.0), (0.0,0.0), (0.0,0.0), (5.0,5.0), &
          (6.0,10.0), (3.0,3.0), (0.0,0.0), (-6.0,-6.0), (-5.0,-5.0), &
          (-1.0,3.0), (-3.0,-3.0), (-7.0,-7.0), (-6.0,-6.0), &
          (-5.0,-5.0), (0.0,4.0)/
!
!                               Find eigenvalues and vectors of A
      CALL EVCCH (A, EVAL, EVEC)
!                               Compute performance index
      PI = EPICG(N,A,EVAL,EVEC)
!                               Print results
      CALL UMACH (2, NOUT)
      CALL WRCRN ('EVAL', EVAL, 1, N, 1)
      CALL WRCRN ('EVEC', EVEC)
      WRITE (NOUT,'(/,A,F6.3)') ' Performance index = ', PI
      END
```

Output

```
                                 EVAL
               1                 2                 3                 4
 (  8.22, 12.22)  (  3.40,  7.40)  (  1.60,  5.60)  ( -3.22,  0.78)

                                     EVEC
                      1                   2                   3                   4
 1  ( 0.7167, 0.0000)  (-0.0704, 0.0000)  (-0.3678, 0.0000)  ( 0.5429, 0.0000)
 2  ( 0.6402,-0.0000)  (-0.0046,-0.0000)  ( 0.6767, 0.0000)  ( 0.4298,-0.0000)
 3  ( 0.2598, 0.0000)  ( 0.7477, 0.0000)  (-0.3005, 0.0000)  ( 0.5277,-0.0000)
 4  (-0.0948,-0.0000)  (-0.6603,-0.0000)  ( 0.5625, 0.0000)  ( 0.4920,-0.0000)

 Performance index =  0.020
```

GVLRG

Computes all of the eigenvalues of a generalized real eigensystem $Az = \lambda Bz$.

Required Arguments

A — Real matrix of order N. (Input)

B — Real matrix of order N. (Input)

ALPHA — Complex vector of size N containing scalars α_i , $i = 1, \ldots, n$. If $\beta_i \neq 0$, $\lambda_i = \alpha_i / \beta_i$ the eigenvalues of the system in decreasing order of magnitude. (Output)

BETAV — Vector of size N containing scalars β_i. (Output)

Optional Arguments

N — Order of the matrices A and B. (Input)
Default: N = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement in the calling program. (Input)
Default: LDA = SIZE (A,1).

LDB — Leading dimension of B exactly as specified in the dimension statement in the calling program. (Input)
Default: LDB = SIZE (B,1).

FORTRAN 90 Interface

Generic: CALL GVLRG (A, B, ALPHA, BETAV [,…])

Specific: The specific interface names are S_GVLRG and D_GVLRG.

FORTRAN 77 Interface

Single: CALL GVLRG (N, A, LDA, B, LDB, ALPHA, BETAV)

Double: The double precision name is DGVLRG.

Description

Routine GVLRG computes the eigenvalues of the generalized eigensystem $Ax = \lambda Bx$ where A and B are real matrices of order N. The eigenvalues for this problem can be infinite; so instead of returning λ, GVLRG returns α and β. If β is nonzero, then $\lambda = \alpha/\beta$.

The first step of the QZ algorithm is to simultaneously reduce A to upper Hessenberg form and B to upper triangular form. Then, orthogonal transformations are used to reduce A to quasi-upper-triangular form while keeping B upper triangular. The generalized eigenvalues are then computed.

The underlying code is based on either EISPACK or LAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation, see "*Using ScaLAPACK, LAPACK, LINPACK, and EISPACK*" in the Introduction section of this manual.

Comments

1. Workspace may be explicitly provided, if desired, by use of G3LRG/DG3LRG. The reference is:

```
CALL G3LRG (N, A, LDA, B, LDB, ALPHA, BETAV, ACOPY, BCOPY,
   RWK, CWK, IWK)
```

   The additional arguments are as follows:

   ACOPY — Work array of size N^2. The arrays A and ACOPY may be the same, in which case the first N^2 elements of A will be destroyed.

   BCOPY — Work array of size N^2. The arrays B and BCOPY may be the same, in which case the first N^2 elements of B will be destroyed.

   RWK — Real work array of size N.

   CWK — Complex work array of size N.

   IWK — Integer work array of size N.

2. *Integer Options* with *Chapter 11* Options Manager

   1 This option uses eight values to solve memory bank conflict (access inefficiency) problems. In routine G3LRG, the internal or working leading dimension of ACOPY is increased by IVAL(3) when N is a multiple of IVAL(4). The values IVAL(3) and IVAL (4) are temporarily replaced by IVAL(1) and IVAL(2), respectively, in routine GVLRG. Analogous comments hold for BCOPY and the values IVAL(5) IVAL(8). Additional memory allocation and option value restoration are automatically done in GVLRG. There is no requirement that users change existing applications that use GVLRG or G3LRG. Default values for the option are IVAL(*) = 1, 16, 0, 1, 1, 16, 0, 1.

Example

In this example, DATA statements are used to set *A* and *B*. The eigenvalues are computed and printed.

```
      USE IMSL_LIBRARIES

      IMPLICIT   NONE
      INTEGER    LDA, LDB, N
      PARAMETER  (N=3, LDA=N, LDB=N)
!
      INTEGER    I
      REAL       A(LDA,N), B(LDB,N), BETAV(N)
      COMPLEX    ALPHA(N), EVAL(N)
!
!                                 Set values of A and B
!                                 A = (  1.0     0.5    0.0  )
!                                     (-10.0     2.0    0.0  )
!                                     (  5.0     1.0    0.5  )
!
!                                 B = (  0.5     0.0    0.0  )
!                                     (  3.0     3.0    0.0  )
!                                     (  4.0     0.5    1.0  )
!
!                                 Declare variables
      DATA A/1.0, -10.0, 5.0, 0.5, 2.0, 1.0, 0.0, 0.0, 0.5/
      DATA B/0.5, 3.0, 4.0, 0.0, 3.0, 0.5, 0.0, 0.0, 1.0/
!
      CALL GVLRG (A, B, ALPHA, BETAV)
!                                 Compute eigenvalues
      DO 10  I=1, N
            EVAL(I) = ALPHA(I)/BETAV(I)
   10 CONTINUE
!                                 Print results
      CALL WRCRN ('EVAL', EVAL, 1, N, 1)
      END
```

Output

```
                         EVAL
               1                 2                 3
 ( 0.833, 1.993)   ( 0.833,-1.993)   ( 0.500, 0.000)
```

GVCRG

more...

Computes all of the eigenvalues and eigenvectors of a generalized real eigensystem $Az = \lambda Bz$.

Required Arguments

A — Real matrix of order `N`. (Input)

B — Real matrix of order `N`. (Input)

ALPHA — Complex vector of size `N` containing scalars α_i. If $\beta_i \neq 0$, $\lambda_i = \alpha_i / \beta_i$, $i = 1, \ldots, n$ are the eigenvalues of the system.

BETAV — Vector of size `N` containing scalars β_i. (Output)

EVEC — Complex matrix of order `N`. (Output)
The J-th eigenvector, corresponding to λ_J, is stored in the J-th column. Each vector is normalized to have Euclidean length equal to the value one.

Optional Arguments

N — Order of the matrices `A` and `B`. (Input)
Default: `N` = `SIZE` (A,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement in the calling program. (Input)
Default: `LDA` = `SIZE` (A,1).

LDB — Leading dimension of `B` exactly as specified in the dimension statement in the calling program. (Input)
Default: `LDB` = `SIZE` (B,1).

LDEVEC — Leading dimension of EVEC exactly as specified in the dimension statement in the calling program. (Input)
Default: LDEVEC = SIZE (EVEC,1).

FORTRAN 90 Interface

Generic: CALL GVCRG (A, B, ALPHA, BETAV, EVEC [,…])

Specific: The specific interface names are S_GVCRG and D_GVCRG.

FORTRAN 77 Interface

Single: CALL GVCRG (N, A, LDA, B, LDB, ALPHA, BETAV, EVEC, LDEVEC)

Double: The double precision name is DGVCRG.

Description

Routine GVCRG computes the complex eigenvalues and eigenvectors of the generalized eigensystem $Ax = \lambda Bx$ where A and B are real matrices of order N. The eigenvalues for this problem can be infinite; so instead of returning λ, GVCRG returns complex numbers α and real numbers β. If β is nonzero, then $\lambda = \alpha/\beta$. For problems with small $|\beta|$ users can choose to solve the mathematically equivalent problem $Bx = \mu Ax$ where $\mu = \lambda^{-1}$.

The first step of the QZ algorithm is to simultaneously reduce A to upper Hessenberg form and B to upper triangular form. Then, orthogonal transformations are used to reduce A to quasi-upper-triangular form while keeping B upper triangular. The generalized eigenvalues and eigenvectors for the reduced problem are then computed.

The underlying code is based on either EISPACK or LAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation, see "*Using ScaLAPACK, LAPACK, LINPACK, and EISPACK*" in the Introduction section of this manual.

Comments

1. Workspace may be explicitly provided, if desired, by use of G8CRG/DG8CRG. The reference is:

```
CALL G8CRG (N, A, LDA, B, LDB, ALPHA, BETAV, EVEC, LDEVEC,
   ACOPY, BCOPY, ECOPY, RWK, CWK, IWK)
```

   The additional arguments are as follows:

   ACOPY — Work array of size N^2. The arrays A and ACOPY may be the same, in which case the first N^2 elements of A will be destroyed.

   BCOPY — Work array of size N^2. The arrays B and BCOPY may be the same, in which case the first N^2 elements of B will be destroyed.

ECOPY — Work array of size N^2.

RWK — Work array of size N.

CWK — Complex work array of size N.

IWK — Integer work array of size N.

2. *Integer Options* with *Chapter 11* Options Manager

1 This option uses eight values to solve memory bank conflict (access inefficiency) problems. In routine G8CRG, the internal or working leading dimensions of ACOPY and ECOPY are both increased by IVAL(3) when N is a multiple of IVAL(4). The values IVAL(3) and IVAL(4) are temporarily replaced by IVAL(1) and IVAL(2), respectively, in routine GVCRG. Analogous comments hold for the array BCOPY and the option values IVAL(5) – IVAL(8). Additional memory allocation and option value restoration are automatically done in GVCRG. There is no requirement that users change existing applications that use GVCRG or G8CRG. Default values for the option are IVAL(*) = 1, 16, 0, 1, 1, 16, 0, 1. Items 5–8 in IVAL(*) are for the generalized eigenvalue problem and are not used in GVCRG.

Example

In this example, DATA statements are used to set *A* and *B*. The eigenvalues, eigenvectors and performance index are computed and printed for the systems $Ax = \lambda Bx$ and $Bx = \mu Ax$ where $\mu = \lambda^{-1}$. For more details about the performance index, see routine GPIRG.

```
      USE IMSL_LIBRARIES

      IMPLICIT   NONE
      INTEGER    LDA, LDB, LDEVEC, N
      PARAMETER  (N=3, LDA=N, LDB=N, LDEVEC=N)
!
      INTEGER    I, NOUT
      REAL       A(LDA,N), B(LDB,N), BETAV(N), PI
      COMPLEX    ALPHA(N), EVAL(N), EVEC(LDEVEC,N)
!
!                                 Define values of A and B:
!                                 A = (  1.0     0.5    0.0  )
!                                     (-10.0     2.0    0.0  )
!                                     (  5.0     1.0    0.5  )
!
!                                 B = (  0.5     0.0    0.0  )
!                                     (  3.0     3.0    0.0  )
!                                     (  4.0     0.5    1.0  )
!
!                                 Declare variables
      DATA A/1.0, -10.0, 5.0, 0.5, 2.0, 1.0, 0.0, 0.0, 0.5/
      DATA B/0.5, 3.0, 4.0, 0.0, 3.0, 0.5, 0.0, 0.0, 1.0/
!
      CALL GVCRG (A, B, ALPHA, BETAV, EVEC)
!                                 Compute eigenvalues
      DO 10  I=1, N
            EVAL(I) = ALPHA(I)/BETAV(I)
   10 CONTINUE
!                                 Compute performance index
      PI = GPIRG(N,A,B,ALPHA,BETAV,EVEC)
!                                 Print results
```

```
      CALL UMACH (2, NOUT)
      CALL WRCRN ('EVAL', EVAL, 1, N, 1)
      CALL WRCRN ('EVEC', EVEC)
      WRITE (NOUT,'(/,A,F6.3)') ' Performance index = ', PI
!                                Solve for reciprocals of values
      CALL GVCRG (B, A, ALPHA, BETAV, EVEC)

!                                Compute reciprocals
      DO 20  I=1, N
            EVAL(I) = ALPHA(I)/BETAV(I)
   20 CONTINUE
!                                Compute performance index
      PI = GPIRG(N,B,A,ALPHA,BETAV,EVEC)
!                                Print results
      CALL WRCRN ('EVAL reciprocals', EVAL, 1, N, 1)
      CALL WRCRN ('EVEC', EVEC)
      WRITE (NOUT,'(/,A,F6.3)') ' Performance index = ', PI
      END
```

Output

```
                      EVAL
              1                2                3
( 0.833, 1.993)  ( 0.833,-1.993)  ( 0.500, 0.000)

                        EVEC
                1                2                3
1  (-0.197, 0.150)  (-0.197,-0.150)  (-0.000, 0.000)
2  (-0.069,-0.568)  (-0.069, 0.568)  (-0.000, 0.000)
3  ( 0.782, 0.000)  ( 0.782, 0.000)  ( 1.000, 0.000)

Performance index =  0.384

                EVAL reciprocals
              1                2                3
( 2.000, 0.000)  ( 0.179, 0.427)  ( 0.179,-0.427)

                        EVEC
                1                2                3
1  ( 0.000, 0.000)  (-0.197,-0.150)  (-0.197, 0.150)
2  ( 0.000, 0.000)  (-0.069, 0.568)  (-0.069,-0.568)
3  ( 1.000, 0.000)  ( 0.782, 0.000)  ( 0.782, 0.000)

Performance index =  0.283
```

GPIRG

This function computes the performance index for a generalized real eigensystem $Az = \lambda Bz$.

Function Return Value

GPIRG — Performance index. (Output)

Required Arguments

NEVAL — Number of eigenvalue/eigenvector pairs performance index computation is based on. (Input)

A — Real matrix of order N. (Input)

B — Real matrix of order N. (Input)

ALPHA — Complex vector of length NEVAL containing the numerators of eigenvalues. (Input)

BETAV — Real vector of length NEVAL containing the denominators of eigenvalues. (Input)

EVEC — Complex N by NEVAL array containing the eigenvectors. (Input)

Optional Arguments

N — Order of the matrices A and B. (Input)
Default: N = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement in the calling program. (Input)
Default: LDA = SIZE (A,1).

LDB — Leading dimension of B exactly as specified in the dimension statement in the calling program. (Input)
Default: LDB = SIZE (B,1).

LDEVEC — Leading dimension of EVEC exactly as specified in the dimension statement in the calling program. (Input)
Default: LDEVEC = SIZE (EVEC,1).

FORTRAN 90 Interface

Generic: GPIRG (NEVAL, A, B, ALPHA, BETAV, EVEC, GPIRG [,…])

Specific: The specific interface names are S_GPIRG and D_GPIRG.

FORTRAN 77 Interface

Single: GPIRG (N, NEVAL, A, LDA, B, LDB, ALPHA, BETAV, EVEC, LDEVEC)

Double: The double precision function name is DGPIRG.

Description

Let M = NEVAL, x_j = EVEC(*,J) , the j-th column of EVEC. Also, let ε be the machine precision given by AMACH(4), see the *Reference* chapter of this manual. The performance index, τ , is defined to be

$$\tau = \max_{1 \le j \le M} \frac{\| \beta_j A x_j - \alpha_j B x_j \|_1}{\varepsilon \left(|\beta_j| \, \|A\|_1 + |\alpha_j| \, \|B\|_1 \right) \|x_j\|_1}$$

The norms used are a modified form of the 1-norm. The norm of the complex vector v is

$$\|v\|_1 = \sum_{i=1}^{N} \left\{ |\,\Re\, v_i| + |\,\Im\, v_i| \right\}$$

While the exact value of τ is highly machine dependent, the performance of GVCRG is considered excellent if $\tau < 1$, good if $1 \le \tau \le 100$, and poor if $\tau > 100$. The performance index was first developed by the EISPACK project at Argonne National Laboratory; see Garbow et al. (1977, pages 77– 79).

Comments

1. Workspace may be explicitly provided, if desired, by use of G2IRG/DG2IRG. The reference is:

   G2IRG (N, NEVAL, A, LDA, B, LDB, ALPHA, BETAV, EVEC, LDEVEC, WK)

   The additional argument is:

   WK — Complex work array of length 2N.

2. Informational errors

Type	Code	Description
3	1	Performance index is greater than 100.
3	2	An eigenvector is zero.
3	3	The matrix A is zero.
3	4	The matrix B is zero.

3. The J-th eigenvalue should be ALPHA(J)/BETAV(J), its eigenvector should be in the J-th column of EVEC.

Example

For an example of GPIRG, see routine GVCRG.

GVLCG

Computes all of the eigenvalues of a generalized complex eigensystem $Az = \lambda Bz$.

Required Arguments

A — Complex matrix of order N. (Input)

B — Complex matrix of order N. (Input)

ALPHA — Complex vector of length N. Ultimately, alpha(*i*)/betav(*i*) (for *i* = 1, *n*), will be the eigenvalues of the system in decreasing order of magnitude. (Output)

BETAV — Complex vector of length N. (Output)

Optional Arguments

N — Order of the matrices A and B. (Input)
Default: N = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement in the calling program. (Input)
Default: LDA = SIZE (A,1).

LDB — Leading dimension of B exactly as specified in the dimension statement in the calling program. (Input)
Default: LDB = SIZE (B,1).

FORTRAN 90 Interface

Generic: CALL GVLCG (A, B, ALPHA, BETAV [,…])

Specific: The specific interface names are S_GVLCG and D_GVLCG.

FORTRAN 77 Interface

Single: CALL GVLCG (N, A, LDA, B, LDB, ALPHA, BETAV)

Double: The double precision name is DGVLCG.

Description

Routine GVLCG computes the eigenvalues of the generalized eigensystem $Ax = \lambda Bx$, where A and B are complex matrices of order n. The eigenvalues for this problem can be infinite; so instead of returning λ, GVLCG returns α and β. If β is nonzero, then $\lambda = \alpha/\beta$. If the eigenvectors are needed, then use GVCCG.

The underlying code is based on either EISPACK or LAPACK code depending upon which supporting libraries are used during linking. For a detailed explanation, see "*Using ScaLAPACK, LAPACK, LINPACK, and EISPACK*" in the Introduction section of this manual. Some timing information is given in Hanson et al. (1990).

Comments

1. Workspace may be explicitly provided, if desired, by use of G3LCG/DG3LCG. The reference is:

   CALL G3LCG (N, A, LDA, B, LDB, ALPHA, BETAV, ACOPY, BCOPY, CWK, WK, IWK)

   The additional arguments are as follows:

   ACOPY — Complex work array of length N^2. A and ACOPY may be the same, in which case A will be destroyed.

   BCOPY — Complex work array of length N^2. B and BCOPY may be the same, in which case B will be destroyed.

   CWK — Complex work array of length N.

   WK — Real work array of length N.

   IWK — Integer work array of length N.

2. Informational error

Type	Code	Description
4	1	The iteration for the eigenvalues failed to converge.

Example

In this example, DATA statements are used to set A and B. Then, the eigenvalues are computed and printed.

```
      USE GVLCG_INT
      USE WRCRN_INT

      IMPLICIT   NONE
!                                 Declaration of variables
      INTEGER    LDA, LDB, N
      PARAMETER  (N=5, LDA=N, LDB=N)
!
      INTEGER    I
      COMPLEX    A(LDA,N), ALPHA(N), B(LDB,N), BETAV(N), EVAL(N)
!
```

```
!                                  Define values of A and B
!
      DATA A/(-238.0,-344.0), (76.0,152.0), (118.0,284.0), &
          (-314.0,-160.0), (-54.0,-24.0), (86.0,178.0), &
          (-96.0,-128.0), (55.0,-182.0), (132.0,78.0), &
          (-205.0,-400.0), (164.0,240.0), (40.0,-32.0), &
          (-13.0,460.0), (114.0,296.0), (109.0,148.0), &
          (-166.0,-308.0), (60.0,184.0), (34.0,-192.0), &
          (-90.0,-164.0), (158.0,312.0), (56.0,158.0), &
          (-60.0,-136.0), (-176.0,-214.0), (-424.0,-374.0), &
          (-38.0,-96.0)/
      DATA B/(388.0,94.0), (-304.0,-76.0), (-658.0,-136.0), &
          (-640.0,-10.0), (-162.0,-72.0), (-386.0,-122.0), &
          (384.0,64.0), (-73.0,100.0), (204.0,-42.0), (631.0,158.0), &
          (-250.0,-14.0), (-160.0,16.0), (-109.0,-250.0), &
          (-692.0,-90.0), (131.0,52.0), (556.0,130.0), &
          (-240.0,-92.0), (-118.0,100.0), (288.0,66.0), &
          (-758.0,-184.0), (-396.0,-62.0), (240.0,68.0), &
          (406.0,96.0), (-192.0,154.0), (278.0,76.0)/
!
      CALL GVLCG (A, B, ALPHA, BETAV)
!                                  Compute eigenvalues
      EVAL = ALPHA/BETAV

!                                  Print results
      CALL WRCRN ('EVAL', EVAL, 1, N, 1)

      STOP
      END
```

Output

```
                                EVAL
                1                 2                 3                 4
(-1.000,-1.333)  ( 0.765, 0.941)  (-0.353, 0.412)  (-0.353,-0.412)

                5
(-0.353,-0.412)
```

GVCCG

Computes all of the eigenvalues and eigenvectors of a generalized complex eigensystem $Az = \lambda Bz$.

Required Arguments

A — Complex matrix of order N. (Input)

B — Complex matrix of order N. (Input)

ALPHA — Complex vector of length N. Ultimately, alpha(i)/betav(i) (for i = 1, …, n), will be the eigenvalues of the system in decreasing order of magnitude. (Output)

BETAV — Complex vector of length N. (Output)

EVEC — Complex matrix of order N. (Output)
The J-th eigenvector, corresponding to ALPHA(J)/BETAV(J), is stored in the J-th column. Each vector is normalized to have Euclidean length equal to the value one.

Optional Arguments

N — Order of the matrices A and B. (Input)
Default: N = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = SIZE (A,1).

LDB — Leading dimension of B exactly as specified in the dimension statement of the calling program. (Input)
Default: LDB = SIZE (B,1).

LDEVEC — Leading dimension of EVEC exactly as specified in the dimension statement of the calling program. (Input)
Default: LDEVEC = SIZE (EVEC,1).

FORTRAN 90 Interface

Generic: CALL GVCCG (A, B, ALPHA, BETAV, EVEC [,…])

Specific: The specific interface names are S_GVCCG and D_GVCCG.

FORTRAN 77 Interface

Single: CALL GVCCG (N, A, LDA, B, LDB, ALPHA, BETAV, EVEC, LDEVEC)

Double: The double precision name is DGVCCG.

Description

Routine GVCCG computes the eigenvalues and eigenvectors of the generalized eigensystem $Ax = \lambda Bx$. Here, A and B, are complex matrices of order n. The eigenvalues for this problem can be infinite; so instead of returning λ, GVCCG returns α and β. If β is nonzero, then $\lambda = \alpha/\beta$.

The routine GVCCG uses the QZ algorithm described by Moler and Stewart (1973). The implementation is based on routines of Garbow (1978). Some timing results are given in Hanson et al. (1990).

Comments

1. Workspace may be explicitly provided, if desired, by use of G6CCG/DG6CCG. The reference is:

```
CALL G6CCG (N, A, LDA, B, LDB, ALPHA, BETAV, EVEC, LDEVEC,
   ACOPY, BCOPY, CWK, WK, IWK)
```

   The additional arguments are as follows:

   ACOPY — Complex work array of length N^2. A and ACOPY may be the same in which case the first N^2 elements of A will be destroyed.

   BCOPY — Complex work array of length N^2. B and BCOPY may be the same in which case the first N^2 elements of B will be destroyed.

   CWK — Complex work array of length N.

   WK — Real work array of length N.

   IWK — Integer work array of length N.

2. Informational error

Type	Code	Description
4	1	The iteration for an eigenvalue failed to converge.

3. The success of this routine can be checked using GPICG.

Example

In this example, DATA statements are used to set *A* and *B*. The eigenvalues and eigenvectors are computed and printed. The performance index is also computed and printed. This serves as a check on the computations. For more details, see routine GPICG.

```
      USE IMSL_LIBRARIES

      IMPLICIT   NONE
      INTEGER    LDA, LDB, LDEVEC, N
      PARAMETER  (N=3, LDA=N, LDB=N, LDEVEC=N)
!
      INTEGER    I, NOUT
      REAL       PI
      COMPLEX    A(LDA,N), ALPHA(N), B(LDB,N), BETAV(N), EVAL(N), &
                EVEC(LDEVEC,N)
!
!                                 Define values of A and B
!                                 A = (  1+0i   0.5+i   0+5i    )
!                                     (-10+0i     2+i   0+0i    )
!                                     (  5+i     1+0i   0.5+3i  )
!
!                                 B = ( 0.5+0i     0+0i  0+0i   )
!                                     (   3+3i     3+3i   0+i   )
!                                     (   4+2i    0.5+i   1+i   )
!
!                                 Declare variables
      DATA A/(1.0,0.0), (-10.0,0.0), (5.0,1.0), (0.5,1.0), (2.0,1.0), &
          (1.0,0.0), (0.0,5.0), (0.0,0.0), (0.5,3.0)/
      DATA B/(0.5,0.0), (3.0,3.0), (4.0,2.0), (0.0,0.0), (3.0,3.0), &
          (0.5,1.0), (0.0,0.0), (0.0,1.0), (1.0,1.0)/
!                                 Compute eigenvalues
      CALL GVCCG (A, B, ALPHA, BETAV, EVEC)

                        EVAL = ALPHA/BETAV
!                                 Compute performance index
      PI = GPICG(N,A,B,ALPHA,BETAV,EVEC)
!                                 Print results
      CALL UMACH (2, NOUT)
      CALL WRCRN ('EVAL', EVAL, 1, N, 1)
      CALL WRCRN ('EVEC', EVEC)
      WRITE (NOUT, '(/,A,F6.3)') ' Performance index = ', PI
      END
```

Output

```
                        EVAL
              1                 2                 3
( -8.18,-25.38)  (  2.18,  0.61)  (  0.12, -0.39)

                             EVEC
                   1                   2                   3
1  (-0.3267,-0.1245)  (-0.3007,-0.2444)  ( 0.0371, 0.1518)
2  ( 0.1767, 0.0054)  ( 0.8959, 0.0000)  ( 0.9577, 0.0000)
3  ( 0.9201, 0.0000)  (-0.2019, 0.0801)  (-0.2215, 0.0968)

Performance index =  0.709
```

GPICG

This function computes the performance index for a generalized complex eigensystem $Az = \lambda Bz$.

Function Return Value

GPICG — Performance index. (Output)

Required Arguments

NEVAL — Number of eigenvalue/eigenvector pairs performance index computation is based on. (Input)

A — Complex matrix of order `N`. (Input)

B — Complex matrix of order `N`. (Input)

ALPHA — Complex vector of length `NEVAL` containing the numerators of eigenvalues. (Input)

BETAV — Complex vector of length `NEVAL` containing the denominators of eigenvalues. (Input)

EVEC — Complex `N` by `NEVAL` array containing the eigenvectors. (Input)

Optional Arguments

N — Order of the matrices `A` and `B`. (Input)
Default: `N` = `SIZE` (A,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement in the calling program. (Input)
Default: `LDA` = `SIZE` (A,1).

LDB — Leading dimension of `B` exactly as specified in the dimension statement in the calling program. (Input)
Default: `LDB` = `SIZE` (B,1).

LDEVEC — Leading dimension of `EVEC` exactly as specified in the dimension statement in the calling program. (Input)
Default: `LDEVEC` = `SIZE` (`EVEC`,1).

FORTRAN 90 Interface

Generic: GPICG (NEVAL, A, B, ALPHA, BETAV, EVEC [,…])

Specific: The specific interface names are S_GPICG and D_GPICG.

FORTRAN 77 Interface

Single: GPICG (N, NEVAL, A, LDA, B, LDB, ALPHA, BETAV, EVEC, LDEVEC)

Double: The double precision name is DGPICG.

Description

Let M = NEVAL, x_j = EVEC(*, J) , the j-th column of EVEC. Also, let ε be the machine precision given by AMACH(4). The performance index, τ , is defined to be

$$\tau = \max_{1 \le j \le M} \frac{\|\beta_j A x_j - \alpha_j B x_j\|_1}{\varepsilon\left(|\beta_j| \|A\|_1 + |\alpha_j| \|B\|_1\right) \|x_j\|_1}$$

The norms used are a modified form of the 1-norm. The norm of the complex vector v is

$$\|v\|_1 = \sum_{i=1}^{N} \left\{ |\, \Re\, v_i| + |\, \Im\, v_i| \right\}$$

While the exact value of τ is highly machine dependent, the performance of GVCCG is considered excellent if $\tau < 1$, good if $1 \le \tau \le 100$, and poor if $\tau > 100$.

The performance index was first developed by the EISPACK project at Argonne National Laboratory; see Garbow et al. (1977, pages 77-79).

Comments

1. Workspace may be explicitly provided, if desired, by use of G2ICG/DG2ICG. The reference is:

   G2ICG (N, NEVAL, A, LDA, B, LDB, ALPHA, BETAV, EVEC, LDEVEC, WK)

   The additional argument is:

   WK — Complex work array of length 2N.

2. Informational errors

Type	Code	Description
3	1	Performance index is greater than 100.
3	2	An eigenvector is zero.
3	3	The matrix A is zero.
3	4	The matrix B is zero.

3. The J-th eigenvalue should be ALPHA(J)/BETAV (J), its eigenvector should be in the J-th column of EVEC.

Example

For an example of GPICG, see routine GVCCG.

GVLSP

more...

Computes all of the eigenvalues of the generalized real symmetric eigenvalue problem $Az = \lambda Bz$, with B symmetric positive definite.

Required Arguments

A — Real symmetric matrix of order `N`. (Input)

B — Positive definite symmetric matrix of order `N`. (Input)

EVAL — Vector of length `N` containing the eigenvalues in decreasing order of magnitude. (Output)

Optional Arguments

N — Order of the matrices `A` and `B`. (Input)
Default: `N` = `SIZE` (A,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement in the calling program. (Input)
Default: `LDA` = `SIZE` (A,1).

LDB — Leading dimension of `B` exactly as specified in the dimension statement in the calling program. (Input)
Default: `LDB` = `SIZE` (B,1).

FORTRAN 90 Interface

Generic: `CALL GVLSP (A, B, EVAL [,…])`

Specific: The specific interface names are `S_GVLSP` and `D_GVLSP`.

FORTRAN 77 Interface

Single: `CALL GVLSP (N, A, LDA, B, LDB, EVAL)`

Double: The double precision name is `DGVLSP`.

Description

Routine `GVLSP` computes the eigenvalues of $Ax = \lambda Bx$ with A symmetric and B symmetric positive definite. The Cholesky factorization $B = R^T R$, with R a triangular matrix, is used to transform the equation $Ax = \lambda Bx$ to

$$(R^{-T} AR^{-1})(Rx) = \lambda\,(Rx)$$

The eigenvalues of $C = R^{-T} AR^{-1}$ are then computed. This development is found in Martin and Wilkinson (1968). The Cholesky factorization of B is computed based on IMSL routine `LFTDS`, (see *Chapter 1, "Linear Systems"*). The eigenvalues of C are computed based on routine `EVLSF`. Further discussion and some timing results are given Hanson et al. (1990).

Comments

1. Workspace may be explicitly provided, if desired, by use of `G3LSP/DG3LSP`. The reference is:

   `CALL G3LSP (N, A, LDA, B, LDB, EVAL, IWK, WK1, WK2)`

   The additional arguments are as follows:

   IWK — Integer work array of length `N`.

   WK1 — Work array of length `2N`.

   WK2 — Work array of length $N^2 + N$.

2. Informational errors

Type	Code	Description
4	1	The iteration for an eigenvalue failed to converge.
4	2	Matrix B is not positive definite.

Example

In this example, a `DATA` statement is used to set the matrices A and B. The eigenvalues of the system are computed and printed.

```
      USE GVLSP_INT
      USE WRRRN_INT

      IMPLICIT   NONE
```

```
!                                  Declare variables
      INTEGER    LDA, LDB, N
      PARAMETER  (N=3, LDA=N, LDB=N)
!
      REAL       A(LDA,N), B(LDB,N), EVAL(N)
!                                  Define values of A:
!                                  A = (  2    3    5  )
!                                      (  3    2    4  )
!                                      (  5    4    2  )
      DATA A/2.0, 3.0, 5.0, 3.0, 2.0, 4.0, 5.0, 4.0, 2.0/
!
!                                  Define values of B:
!                                  B = (  3    1    0  )
!                                      (  1    2    1  )
!                                      (  0    1    1  )
      DATA B/3.0, 1.0, 0.0, 1.0, 2.0, 1.0, 0.0, 1.0, 1.0/
!
!                                  Find eigenvalues
      CALL GVLSP (A, B, EVAL)
!                                  Print results
      CALL WRRRN ('EVAL', EVAL, 1, N, 1)
      END
```

Output

```
          EVAL
      1        2        3
 -4.717    4.393   -0.676
```

GVCSP

more...

Computes all of the eigenvalues and eigenvectors of the generalized real symmetric eigenvalue problem $Az = \lambda Bz$, with B symmetric positive definite.

Required Arguments

A — Real symmetric matrix of order `N`. (Input)

B — Positive definite symmetric matrix of order `N`. (Input)

EVAL — Vector of length `N` containing the eigenvalues in decreasing order of magnitude. (Output)

EVEC — Matrix of order `N`. (Output)
The `J`-th eigenvector, corresponding to `EVAL(J)`, is stored in the `J`-th column. Each vector is normalized to have Euclidean length equal to the value one.

Optional Arguments

N — Order of the matrices `A` and `B`. (Input)
Default: `N` = `SIZE` (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement in the calling program. (Input)
Default: `LDA` = `SIZE` (`A`,1).

LDB — Leading dimension of `B` exactly as specified in the dimension statement in the calling program. (Input)
Default: `LDB` = `SIZE` (`B`,1).

LDEVEC — Leading dimension of `EVEC` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDEVEC` = `SIZE` (`EVEC`,1).

FORTRAN 90 Interface

Generic: `CALL GVCSP (A, B, EVAL, EVEC [,…])`

Specific: The specific interface names are `S_GVCSP` and `D_GVCSP`.

FORTRAN 77 Interface

Single: `CALL GVCSP (N, A, LDA, B, LDB, EVAL, EVEC, LDEVEC)`

Double: The double precision name is `DGVCSP`.

Description

Routine `GVLSP` computes the eigenvalues and eigenvectors of $Az = \lambda Bz$, with A symmetric and B symmetric positive definite. The Cholesky factorization $B = R^T R$, with R a triangular matrix, is used to transform the equation $Az = \lambda Bz$, to

$$(R^{-T} AR^{-1})(Rz) = \lambda\,(Rz)$$

The eigenvalues and eigenvectors of $C = R^{-T} AR^{-1}$ are then computed. The generalized eigenvectors of A are given by $z = R^{-1}\,x$, where x is an eigenvector of C. This development is found in Martin and Wilkinson (1968). The Cholesky factorization is computed based on IMSL routine `LFTDS`, see *Chapter 1, "Linear Systems"*. The eigenvalues and eigenvectors of C are computed based on routine `EVCSF`. Further discussion and some timing results are given Hanson et al. (1990).

Comments

1. Workspace may be explicitly provided, if desired, by use of `G3CSP/DG3CSP`. The reference is:

   ```
   CALL G3CSP (N, A, LDA, B, LDB, EVAL, EVEC, LDEVEC, IWK, WK1,
     WK2)
   ```

   The additional arguments are as follows:

   IWK — Integer work array of length `N`.

   WK1 — Work array of length `3N`.

   WK2 — Work array of length $N^2 + N$.

2. Informational errors

Type	Code	Description
4	1	The iteration for an eigenvalue failed to converge.
4	2	Matrix B is not positive definite.

3. The success of this routine can be checked using GPISP.

Example

In this example, a DATA statement is used to set the matrices *A* and *B*. The eigenvalues, eigenvectors and performance index are computed and printed. For details on the performance index, see IMSL routine GPISP.

```
      USE GVCSP_INT
      USE GPISP_INT
      USE UMACH_INT
      USE WRRRN_INT

      IMPLICIT   NONE
!                                  Declare variables
      INTEGER    LDA, LDB, LDEVEC, N
      PARAMETER  (N=3, LDA=N, LDB=N, LDEVEC=N)
!
      INTEGER    NOUT
      REAL       A(LDA,N), B(LDB,N), EVAL(N), EVEC(LDEVEC,N), PI
!                                  Define values of A:
!                                  A = (  1.1    1.2    1.4   )
!                                      (  1.2    1.3    1.5   )
!                                      (  1.4    1.5    1.6   )
      DATA A/1.1, 1.2, 1.4, 1.2, 1.3, 1.5, 1.4, 1.5, 1.6/
!
!                                  Define values of B:
!                                  B = (  2.0    1.0    0.0   )
!                                      (  1.0    2.0    1.0   )
!                                      (  0.0    1.0    2.0   )
      DATA B/2.0, 1.0, 0.0, 1.0, 2.0, 1.0, 0.0, 1.0, 2.0/
!
!                                  Find eigenvalues and vectors
      CALL GVCSP (A, B, EVAL, EVEC)
!                                  Compute performance index
      PI = GPISP(N,A,B,EVAL,EVEC)
!                                  Print results
      CALL UMACH (2, NOUT)
      CALL WRRRN ('EVAL', EVAL)
      CALL WRRRN ('EVEC', EVEC)
      WRITE (NOUT,'(/,A,F6.3)') ' Performance index = ', PI
      END
```

Output

```
EVAL
 1   1.386
 2  -0.058
 3  -0.003

            EVEC
         1         2         3
 1   0.6431   -0.1147   -0.6817
 2  -0.0224   -0.6872    0.7266
 3   0.7655    0.7174   -0.0858

 Performance index =  0.417
```

GPISP

This function computes the performance index for a generalized real symmetric eigensystem problem.

Function Return Value

GPISP — Performance index. (Output)

Required Arguments

NEVAL — Number of eigenvalue/eigenvector pairs that the performance index computation is based on. (Input)

A — Symmetric matrix of order N. (Input)

B — Symmetric matrix of order N. (Input)

EVAL — Vector of length NEVAL containing eigenvalues. (Input)

EVEC — N by NEVAL array containing the eigenvectors. (Input)

Optional Arguments

N — Order of the matrices A and B. (Input)
Default: N = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement in the calling program. (Input)
Default: LDA = SIZE (A,1).

LDB — Leading dimension of B exactly as specified in the dimension statement in the calling program. (Input)
Default: LDB = SIZE (B,1).

LDEVEC — Leading dimension of EVEC exactly as specified in the dimension statement in the calling program. (Input)
Default: LDEVEC = SIZE (EVEC,1).

FORTRAN 90 Interface

Generic: GPISP (NEVAL, A, B, EVAL, EVEC [,…])

Specific: The specific interface names are S_GPISP and D_GPISP.

FORTRAN 77 Interface

Single: GPISP (N, NEVAL, A, LDA, B, LDB, EVAL, EVEC, LDEVEC)

Double: The double precision name is DGPISP.

Description

Let M = NEVAL, λ = EVAL, x_j = EVEC(*, J) , the j-th column of EVEC. Also, let ε be the machine precision given by AMACH(4). The performance index, τ , is defined to be

$$\tau = \max_{1 \le j \le M} \frac{\|Ax_j - \lambda_j Bx_j\|_1}{\varepsilon\left(\|A\|_1 + |\lambda_j| \|B\|_1 \right) \|x_j\|_1}$$

The norms used are a modified form of the 1-norm. The norm of the complex vector v is

$$\|v\|_1 = \sum_{i=1}^{N} \left\{ |\Re\, v_i| + |\Im\, v_i| \right\}$$

While the exact value of τ is highly machine dependent, the performance of GVCSP is considered excellent if $\tau < 1$, good if $1 \le \tau \le 100$, and poor if $\tau > 100$.. The performance index was first developed by the EISPACK project at Argonne National Laboratory; see Garbow et al. (1977, pages 77-79).

Comments

1. Workspace may be explicitly provided, if desired, by use of G2ISP/DG2ISP. The reference is:

   G2ISP (N, NEVAL, A, LDA, B, LDB, EVAL, EVEC, LDEVEC, WORK)

   The additional argument is:

   WORK — Work array of length 2 * N.

2. Informational errors

Type	Code	Description
3	1	Performance index is greater than 100.
3	2	An eigenvector is zero.

Type	Code	Description
3	3	The matrix A is zero.
3	4	The matrix B is zero.

3. The `J`-th eigenvalue should be `ALPHA`(`J`)/`BETAV`(`J`), its eigenvector should be in the `J`-th column of `EVEC`.

Example

For an example of GPISP, see routine `GVCSP`.

Eigenvalues and Eigenvectors Computed with ARPACK

First see *Using ARPACK for Ordinary and Generalized Eigenvalue Problems* in the Usage Notes section of this chapter. We describe here the Fortran 2003 usage of four basic problem types. There must be compiler support for the object-oriented features of Fortran 2003 to use these routines.

The generalized eigenvalue problem $Ax = \lambda Bx$ requires that some eigenvalues and eigenvectors be computed. The organization of the user-written function for matrix-vector products depends on the part of the eigenvalue spectrum that is desired.

For an ordinary problem with A symmetric and $B = I$, the eigenvalues of largest or smallest magnitude can be computed by providing the operator products $\omega = Ax$. Here x is an input vector and ω is the result of applying the linear operator A to x. This process is repeated several times within the Arnoldi algorithm, and the net result is a few eigenvalues of A and the corresponding eigenvectors.

For a generalized problem, it is useful and efficient to consider a shift value σ and the ordinary eigenvalue problem $Cx \equiv (A - \sigma B)^{-1} Bx = vx$. The matrix pencil $A - \sigma B$ is non-singular. The purpose of the user-written function is to provide results for the individual operator products $\omega = Bx$, $\omega = (A - \sigma B)^{-1}x$, and $\omega = Ax$. Usually the inverse matrix product will be computed by solving linear systems, where the matrix pencil is the coefficient matrix. The desired eigenvalues of this ordinary problem satisfy $\lambda_j = \sigma + v_j^{-1}$.

In the special case that B is positive definite, well-conditioned, and symmetric, one may compute the Cholesky decomposition $B = R^T R$ and then solve the ordinary eigenvalue problem $Cy \equiv R^{-T} AR^{-1} y = \lambda y$. The product operation required by the Arnoldi algorithm, $\omega = Cx$, is performed in steps: Solve $Rz = x$ for z, compute $y = Az$, and solve $R^T x = y$ for ω. The eigenvectors, Y, of C are transformed to those of the generalized problem, X, by solving $RX = Y$ for X.

The operations required by ARPACK codes are returned as array functions. An array of input values, x, will yield an output array, y. These functions are written by the user. They must be written according to an *abstract interface*, given below. There are two user functions, double precision real and complex, that we support for the eigenvalue problem, and a third for the singular value decomposition, using double precision real data only. This interface, the named or enumerated constants that describe what is needed, and the eigenvalue codes are in the module `ARPACK_INT`. We use the notation: `DKIND=kind(1.D0)` to specify two double precision data types: `REAL(DKIND)` and `COMPLEX(DKIND)`. The interface `SVDMV(…)` is for the singular value decomposition products only. For that problem the components `EXTYPE%MROWS` and `EXTYPE%NCOLS` are switched between the operator sizes M and N to account for computing $y = A_{MxN}x$ or $y = A^T x$.

The Abstract Interfaces for User-Written Array Functions

```
     Abstract Interface

          FUNCTION DMV(X, TASK, EXTYPE)RESULT(Y)
              IMPORT DKIND,  ARPACKBASE
              REAL(DKIND), INTENT(INOUT) :: X(:)
              INTEGER, INTENT(IN) :: TASK
              CLASS (ARPACKBASE), INTENT(INOUT) :: EXTYPE
              REAL(DKIND) Y(SIZE(X))
          END FUNCTION

          FUNCTION ZMV (X, TASK, EXTYPE) RESULT(Y)
              IMPORT DKIND,  ARPACKBASE
              CLASS (ARPACKBASE), INTENT(INOUT) :: EXTYPE
              COMPLEX (DKIND), INTENT(INOUT) :: X(:)
              INTEGER, INTENT(IN) :: TASK
              COMPLEX (DKIND) Y(SIZE(X))
          END FUNCTION

          FUNCTION SVDMV (X, TASK, EXTYPE) RESULT(Y)
              IMPORT DKIND,  ARPACKBASE
              CLASS (ARPACKBASE), INTENT(INOUT) :: EXTYPE
              REAL (DKIND), INTENT(INOUT) :: X(EXTYPE%NCOLS)
              INTEGER, INTENT(IN) :: TASK
              REAL (DKIND) Y(EXTYPE%MROWS)
          END FUNCTION

      End Interface
```

The Base Class ARPACKBASE

The components of the derived type ARPACKBASE contain data used by the ARPACK routines. These will have initial or default values assigned. The default values can usually be left unchanged with a first use of our codes. They are used as arguments to the original routines of the ARPACK package. The more experienced user may wish to change the components marked with '=>' to new values, depending on their application. These can be changed prior to calling the ARPACK interface codes we provide. This base class can be extended to pass user data or procedure pointers for use within the array function.

Note that the derived type argument EXTYPE, is optional in all the ARPACK_ eigenvalue routines, but it is not optional for the user-written array functions. If EXTYPE is not included in the argument list of the ARPACK_ eigenvalue routine, an internally declared type is passed to the array functions as the argument, EXTYPE. Although the user may choose not to use this optional argument when calling our interface routines, they must include this argument in their user-supplied array function code. In this case, the array function code does not need to reference this argument.

```
TYPE, PUBLIC :: ARPACKBASE
        INTEGER :: TASK   = 0                    ! Local store in Class for compute
                                                 ! tasks to follow. Used in ARPACK_SVD.
        INTEGER :: MROWS=0                       ! Defines output vector size
        INTEGER :: NCOLS=0                       ! Defines input/output vector size
     => COMPLEX(DKIND) :: SHIFT=&
          (0._DKIND, 0._DKIND)                   ! Shift factor
        REAL(DKIND) :: TOL=EPSILON(0._DKIND)     ! Error tolerance
        INTEGER :: ISHFTS = 1                    ! Number of shifts - don't change
     => INTEGER :: MAXITR = HUGE(1)              ! Max number of iterations (many!)
     => INTEGER :: MAXMV  = HUGE(1)              ! Max number of matrix ops (many!)
     => INTEGER :: INFO   = 0                    ! ARPACK error flag, = 0 is OK
     => INTEGER :: NACC   = 0                    ! Number of accurate eigenvalues or
                                                 ! singular values computed.
        INTEGER :: IPARAM(11)=0                  ! ARPACK array of direction and
                                                 ! result flags
     => REAL(DKIND) ::  FACTOR_MAXNCV = 2.5_DKIND ! Factor for the Number of Ritz
                                                 ! vectors > the number of requested
                                                 ! eigenvalues
        LOGICAL :: RALEIGH_QUOTIENT = .TRUE.     ! Compute eigenvalues using the
                                                 ! computed eigenvectors and Raleigh
                                                 ! quotients.
        REAL(DKIND), ALLOCATABLE :: RESID(:)     ! REAL Starting vector for Arnoldi
                                                 ! iteration, if allocated; else
                                                 ! random
        COMPLEX(DKIND), ALLOCATABLE :: ZRESID(:) ! COMPLEX Starting vector for Arnoldi
                                                 ! iteration, if allocated; else
                                                 ! random
    END TYPE
```

ARPACK_SYMMETRIC

Computes some eigenvalues and eigenvectors of the generalized real symmetric eigenvalue problem $Ax = \lambda Bx$. This can be used for the case $B = I$.

Required Arguments

N — The dimension of the problem. (Input)

F — User-supplied FUNCTION to return matrix-vector operations or linear solutions. This user function is written corresponding to the *abstract interface* for the function DMV(…). The usage is F (X, TASK, EXTYPE), where

Function Return Value

F — An array of length N containing matrix-vector operations or linear equations solutions. Operations provided as code in the function F will be made depending upon the value of argument TASK.

Required Arguments

X — An array of length N containing the vector to which the operator will be applied. (Input)

TASK — An enumerated type which specifies the operation to be performed. (Input) TASK is an enumerated integer value, use-associated from the module ARPACK_INT. It will be one of the following:

Value	Description
ARPACK_Prepare	Take initial steps to prepare for the operations that follow. These steps can include defining the data for the matrices, factorizations for upcoming linear system solves, or recording the vectors used in the operations.
ARPACK_A_x	$y = Ax$
ARPACK_B_x	$y = Bx$
ARPACK_inv_A_minus_Shift_x	$y = (A - \sigma I)^{-1}x$
ARPACK_inv_B_x	$y = B^{-1}x$
ARPACK_inv_A_minus_Shift_B_x	$y = (A - \sigma B)^{-1}x$

EXTYPE — A derived type of the extensible class ARPACKBASE, which may be used to pass additional information to/from the user-supplied function. (Input/Output)
The user must include a USE ARPACK_INT statement in the calling program to define this derived type. If EXTYPE is not included as an argument to ARPACK_SYMMETRIC it should be ignored in the user-function, F.

The function F must be written according to the abstract interface for DMV. If F is not use-associated nor contained in the calling program, declare it with PROCEDURE(DMV) F.

VALUES — An array of eigenvalues. (Output)
The value NEV=size(VALUES) defines the number of eigenvalues to be computed. The calling program declares or allocates the array VALUES(1:NEV). The number of eigenvalues computed accurately is optionally available as the component EXTYPE%NACC of the base class EXTYPE.

Optional Arguments

PLACE — Defines the output content of VALUES. (Input)
PLACE specifies the placement within the spectrum for the required eigenvalues. PLACE can be one of the following enumerated integers as defined in ARPACK_INT:

Value
ARPACK_Largest_Algebraic
ARPACK_Smallest_Algebraic
ARPACK_Largest_Magnitude
ARPACK_inv_A_minus_Shift_x
ARPACK_Smallest_Magnitude
ARPACK_Both_Ends

Default: PLACE = ARPACK_Largest_Algebraic.

TYPE — Defines the eigenvalue problem as either a standard or generalized eigenvalue problem. (Input)
TYPE can be one of the following enumerated integers as defined in ARPACK_INT:

Value	Description
ARPACK_Standard	$Ax = \lambda x$
ARPACK_Generalized	$Ax = \lambda Bx$

Default: TYPE = ARPACK_Standard.

CATEGORY — CATEGORY and TYPE define the operation sequence provided in the user-written function. (Input)

CATEGORY can be one of the following enumerated integers as defined in ARPACK_INT:

Value	Description
ARPACK_Regular	$y = Ax$
ARPACK_Regular_Inverse	$y = Ax, y = Bx, y = B^{-1}x$
ARPACK_Shift_Invert	$y = Ax, y = (A - \sigma I)^{-1}x$
ARPACK_Buckling	$y = Ax, y = Bx, y = (A - \sigma B)^{-1}x$
ARPACK_Cayley	$y = Ax, y = Bx, y = (A - \sigma B)^{-1}x$

Default: CATEGORY = ARPACK_Regular.

EXTYPE — A derived type of the extensible class ARPACKBASE, which may be used to pass additional information to/from the user-supplied function. (Input/Output)

The user must include a USE ARPACK_INT statement in the calling program to define this derived type. If EXTYPE is not included as an argument to ARPACK_SYMMETRIC it must still be supplied as an argument to user-function, F, but is not used.

VECTORS — An allocatable array of approximate eigenvectors. (Output)

It is not necessary to allocate VECTORS(:,:). If this argument is used the allocation occurs within the routine ARPACK_SYMMETRIC. The output sizes are VECTORS(1:N,1:NCV). The second dimension value is NCV=min(N, max(FACTOR_MAXNCV*NEV,NEV+1)), where the value FACTOR_MAXNCV is a component of the base class, ARPACKBASE. The first NEV columns of VECTORS(:,:) are the eigenvectors.

FORTRAN 2003 Interface

Generic: ARPACK_SYMMETRIC (N, F, VALUES [,…])

Specific: The specific interface name is D_ARPACK_SYMMETRIC.

Fortran 90 Interface

A Fortran 90 compiler version is not available for this routine.

Description

Routine ARPACK_SYMMETRIC calls ARPACK subroutines to compute partial eigenvalue-eigenvector decompositions for symmetric real matrices. The ARPACK routines are dsaupd and dseupd (see *ARPACK Users' Guide*, SIAM Publications, (1998)), which use "reverse communication" to obtain the required matrix-vector operations for this approximation. Responses to these requests are made by calling the user-written function F. By including the class object EXTYPE as an argument to this function, user data and procedure pointers are available for the evaluations. A user code must extend the base class EXTYPE to include the extra data and procedure pointers.

Comments

The user function F is written to supply requests for the matrix operations. The following psuedo-code outlines the required responses of F depending on the circumstances. Only those cases that follow from the settings of PLACE, TYPE and CATEGORY need to be provided in the user code. The enumerated constants, ARPACK_A_x, etc., are available by use-association from the module ARPACK_INT.

```
FUNCTION F (X, TASK, EXTYPE) RESULT(Y)
USE ARPACK_INT
IMPLICIT NONE

CLASS(ARPACKBASE), INTENT(INOUT) :: EXTYPE
REAL(DKIND), INTENT(INOUT) :: X(:)
INTEGER, INTENT(IN) :: TASK
REAL(DKIND) Y(SIZE(X))

SELECT CASE (TASK)

      CASE (ARPACK_Prepare)
      …{Take initial steps to prepare for the operations that follow.}
      CASE (ARPACK_A_x)
      …y = Ax
      CASE (ARPACK_B_x)
      …y = Bx
      CASE (ARPACK_inv_A_minus_Shift_x)
      …y = (A − σI)^-1 x
      CASE (ARPACK_inv_B_x)
      …y = B^-1 x
      CASE (ARPACK_inv_A_minus_Shift_B_x)
      …y = (A − σB)^-1 x
      CASE DEFAULT
      …{This is an error condition. }
END SELECT
END FUNCTION
```

Examples

Example 1

We approximate eigenvalues and eigenfunctions of the Laplacian operator

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \equiv \Delta u, -\Delta u = \lambda u$$

on the unit square, [0,1] × [0,1], with zero Dirichlet boundary values. The full set of eigenvalues and their eigenfunctions are given by the sequence $\lambda_{m,n} = (m^2 + n^2)\pi^2$, $u_{m,n}(x,y) = \sin(m\pi) \sin(n\pi)$, where m,n are positive integers.

This provides a check on the accuracy of the numerical results. Equally spaced divided differences on the unit square are used to approximate $-\Delta u$. A few eigenvalues of *smallest magnitude*, and their eigenvectors, are requested. This application requires the optional argument PLACE=ARPACK_Smallest_Magnitude. The user function code provides the second order divided difference operator applied to an input vector. The problem is a symmetric matrix eigenvalue computation. It involves only the single TASK, ARPACK_A_x, in the user functions.

The function FCN defines a grid of values and provides the operation that derives from this eigenvalue problem. The class argument EXTYPE must be declared but need not be used. Within the main program, the function interface for the external function FCN is specified with the declaration PROCEDURE (DMV) FCN.

(Example arpack_symmetric_ex1.f90)

```
      PROGRAM ARPACK_SYMMETRIC_EX1
      USE ARPACK_INT
      USE UMACH_INT
      USE WRRRN_INT
      IMPLICIT NONE
!     Compute the smallest eigenvalues of a discrete Laplacian,
!     based on second order divided differences.
!     The matrix used is the 2 dimensional discrete Laplacian on
!     the unit square with zero Dirichlet boundary condition.
      INTEGER                   :: J, NOUT
      INTEGER, parameter        :: NEV=5   !number of Eigenvalues required
      INTEGER, parameter        :: NV=0, NX=10
      INTEGER, parameter        :: N=NX**2 !size of matrix problem
      REAL(DKIND)               :: VALUES(NEV), RES(N), EF(NX, NX)
      REAL(DKIND), ALLOCATABLE  :: VECTORS(:,:)
      REAL(DKIND)               :: NORM
      LOGICAL                   :: SMALL, SOLVED
      TYPE(ARPACKBASE)          :: Q
      PROCEDURE(DMV)            :: FCN

      CALL UMACH(2, NOUT)
! Note that VECTORS(:,:) does not need to be allocated
! in the calling program.  That happens within the
! routine ARPACK_SYMMETRIC().  It is OK to do this but
! the sizes (N,NCV) are determined in ARPACK_SYMMETRIC.
      CALL ARPACK_SYMMETRIC(N, FCN, VALUES, &
           PLACE=ARPACK_Smallest_Magnitude,  VECTORS=VECTORS)
      WRITE(NOUT, *) 'Number of eigenvalues requested, and declared accurate'
      WRITE(NOUT, *) '-------------------------------------------------------'
      WRITE(NOUT, '(5X, I4, 5X, I4)') NEV, Q%NACC
      WRITE(NOUT, *) 'Number of Matrix-Vector Products Recorded, EX-11'
      WRITE(NOUT, *) '------------------------------------------------'
      WRITE(NOUT, '(5X, I4)') NV
      CALL WRRRN('Smallest Laplacian Eigenvalues', VALUES)
```

```
! Check residuals, A*vectors = values*vectors:
      DO J=1,NEV
! Necessary to have an unused TYPE(ARPACKBASE) :: Q as an argument:
          RES=FCN(VECTORS(:,J), ARPACK_A_x, Q)-VALUES(J)*VECTORS(:,J)
          NORM=maxval(abs(RES))
          SMALL=(NORM <= ABS(VALUES(J))*SQRT(EPSILON(NORM)))
          IF(J==1) SOLVED=SMALL
          SOLVED=SOLVED .and. SMALL
      END DO
      IF(SOLVED) THEN
         WRITE(nout,'(A///)') &
              'All Ritz Values and Vectors have small residuals.'
      ELSE
         WRITE(nout,'(A///)') &
               'Some Ritz Values and Vectors have large residuals.'
      ENDIF

! The first eigenvector is scaled to be positive.
! It defines the eigenfunction for the smallest
! eigenvalue at the grid defined by the differencing.
      EF=reshape(VECTORS(:,1),(/NX,NX/))
      CALL WRRRN('First 2D Laplacian Eigenfunction at Grid Points', EF)

      END

      FUNCTION FCN(X, TASK, EX)RESULT(Y)
         USE ARPACK_INT

         CLASS(ARPACKBASE),INTENT(INOUT) :: EX
         REAL(DKIND), INTENT(INOUT) :: X(:)
         INTEGER, INTENT(IN) :: TASK
         REAL(DKIND) Y(SIZE(X))

! Local variables:
         INTEGER J
         INTEGER, SAVE :: NX
         REAL(DKIND), SAVE :: HSQ

         SELECT CASE(TASK)
            CASE(ARPACK_A_x)
!     Computes y <-- A*x, where A is the N**2 by N**2 block
!     tridiagonal matrix
!
!                    | T -I          |
!                    |-I  T -I       |
!                A = |   -I  T       |
!                    |        ...  -I|
!                    |           -I T|
               Y(1:NX)=T(NX,X(1:NX)) - X(NX+1:2*NX)
               DO J=NX+1,NX**2-NX,NX
                  Y(J:J+NX-1)=T(NX,X(J:J+NX-1))&
                            - X(J-NX:J-1)-X(J+NX:J+2*NX-1)
               END DO
               Y((NX-1)*NX+1:NX**2)= - X((NX-1)*NX-NX+1:(NX-1)*NX)&
                                   + T(NX,X((NX-1)*NX+1:NX**2))
! Note that HSQ is passed as a component of the extended type.
               Y=(1._DKIND/HSQ)*Y

            CASE(ARPACK_Prepare)
! Define NX, 1/H**2 so they are later available in the evaluator.
               NX=10 ! This value is fixed in the evaluator.
               HSQ = 1._DKIND/REAL(NX+1,DKIND)**2
               Y=0._DKIND
            CASE DEFAULT
               WRITE(NOUT,*) TASK, ': INVALID TASK REQUESTED'
               STOP 'IMSL_ERROR_WRONG_OPERATION'
```

```
            END SELECT
      CONTAINS
         FUNCTION T(NX, X)RESULT(V)
            INTEGER, INTENT(IN) :: NX
            REAL(DKIND), INTENT(IN) :: X(:)
            REAL(DKIND) :: V(NX)
            REAL(DKIND) :: MONE=-1._DKIND, FOUR=4._DKIND
            INTEGER J

            V(1)=FOUR*X(1)+MONE*X(2)
            DO J=2,NX-1
               V(J)=MONE*X(J-1)+FOUR*X(J)+MONE*X(J+1)
            END DO
            V(NX)=MONE*X(NX-1)+FOUR*X(NX)
         END FUNCTION
      END FUNCTION
```

Output

```
 Number of eigenvalues requested, and declared accurate
  ------------------------------------------------------
         5        0
  Number of Matrix-Vector Products Recorded, EX-11
  ------------------------------------------------
         0

  Smallest Laplacian Eigenvalues
            1   19.61
            2   48.22
            3   48.22
            4   76.83
            5   93.33
 All Ritz Values and Vectors have small residuals.



               First 2D Laplacian Eigenfunction at Grid Points
             1        2        3        4        5        6        7        8
  1     0.0144   0.0277   0.0387   0.0466   0.0507   0.0507   0.0466   0.0387
  2     0.0277   0.0531   0.0743   0.0894   0.0973   0.0973   0.0894   0.0743
  3     0.0387   0.0743   0.1038   0.1250   0.1360   0.1360   0.1250   0.1038
  4     0.0466   0.0894   0.1250   0.1504   0.1637   0.1637   0.1504   0.1250
  5     0.0507   0.0973   0.1360   0.1637   0.1781   0.1781   0.1637   0.1360
  6     0.0507   0.0973   0.1360   0.1637   0.1781   0.1781   0.1637   0.1360
  7     0.0466   0.0894   0.1250   0.1504   0.1637   0.1637   0.1504   0.1250
  8     0.0387   0.0743   0.1038   0.1250   0.1360   0.1360   0.1250   0.1038
  9     0.0277   0.0531   0.0743   0.0894   0.0973   0.0973   0.0894   0.0743
 10     0.0144   0.0277   0.0387   0.0466   0.0507   0.0507   0.0466   0.0387

             9       10
  1     0.0277   0.0144
  2     0.0531   0.0277
  3     0.0743   0.0387
  4     0.0894   0.0466
  5     0.0973   0.0507
  6     0.0973   0.0507
  7     0.0894   0.0466
  8     0.0743   0.0387
  9     0.0531   0.0277
 10     0.0277   0.0144
```

Example 2

We approximate eigenvalues and eigenfunctions of the 1D Laplacian operator $-\frac{d^2u}{dx^2} = \lambda u$ on the unit interval, **[0,1]**. Equally spaced divided differences are used for the operator, which yields a tri-diagonal matrix. The eigenvalues and eigenfunctions are $\lambda_n = n^2\pi^2$, $u_n(x) = \sin(n\pi)$, n = 1,2,.... This example shows that using inverse iteration for approximating the largest *reciprocals* of eigenvalues is more efficient than directly computing the smallest *magnitude* eigenvalues by products of the operator. This requires the optional argument `CATEGORY=ARPACK_Shift_Invert`. The user function, `FCN`, requires the solution of a tri-diagonal system of linear equations applied to an input vector. The base class `ARPACKBASE` is extended to the user's type, `TYPE(ARPACKBASE_EXT)`, defined in the user module `ARPACK_SYMMETRIC_EX2_INT`. This extension includes the number of intervals, a total kept in `FCN` for noting the number of operations, and allocatable arrays used to store the *LU* factorization of the tri-diagonal matrix. When `FCN` is entered with `TASK=ARPACK_Prepare`, these arrays are allocated, defined, and the LU factorization of the shifted matrix $(A-\sigma I)$ is computed, here with $\sigma = 0$. When `FCN` is later entered with `TASK=ARPACK_inv_A_minus_Shift_x`, the *LU* factorization is available to efficiently compute $y = (A - \sigma I)^{-1}x = A^{-1}x$. The function `FCN` is also entered with `TASK=ARPACK_A_x`, to compute Ax.

(Example arpack_symmetric_ex2.f90)

```
      MODULE ARPACK_SYMMETRIC_EX2_INT
      USE ARPACK_INT
      USE LSLCR_INT
      USE N1RTY_INT
      IMPLICIT NONE

      TYPE, EXTENDS(ARPACKBASE) :: ARPACKBASE_EXT
         REAL(DKIND) :: HSQ=0._DKIND
         INTEGER ::     NX=0, NV=0
! This example extends the base type to
! information for solving tridiagonal systems.
         REAL(DKIND), ALLOCATABLE :: A(:), B(:), C(:)
         REAL(DKIND), ALLOCATABLE :: Y1(:), U(:)
         INTEGER, ALLOCATABLE :: IR(:), IS(:)
      END TYPE ARPACKBASE_EXT

      CONTAINS

      FUNCTION FCN(X, TASK, EX) RESULT(Y)
         CLASS (ARPACKBASE), INTENT(INOUT) :: EX
         REAL (DKIND), INTENT(INOUT) :: X(:)
         INTEGER, INTENT(IN) :: TASK
         REAL (DKIND) Y(size(X))
         INTEGER J, IERR, IJOB, NSIZE

         SELECT TYPE(EX)
            TYPE IS(ARPACKBASE_EXT)
            ASSOCIATE(N     =>    EX%NCOLS, &
                      NV    =>    EX%NV, &
                      HSQ   =>    EX%HSQ, &
                      SHIFT =>  EX%SHIFT)
            SELECT CASE(TASK)
               CASE(ARPACK_A_x)
                  Y(1) =  2._DKIND*X(1) - X(2)
```

```
                    DO J = 2,N-1
                       Y(J) = - X(J-1) + 2._DKIND*X(J) - X(J+1)
                    END DO

                    Y(N) = - X(N-1) + 2._DKIND*X(N)
                    Y=Y/HSQ
                    CASE(ARPACK_inv_A_minus_Shift_x)
! Compute Y=inv(A-*I)*x.  This is done with a solve
! step, using the LU factorization.  Note that the data
! for the factorization is stored in the user's extended
! data type.
                       EX%Y1(1:N) = X
                       IJOB = 2
                       CALL LSLCR (EX%C, EX%A, EX%B, EX%Y1, EX%U, &
                                    EX%IR, EX%IS, N=N, IJOB=IJOB)
                       Y(1:N) = EX%Y1(1:N)
                       IERR= N1RTY(1)
                       IF (IERR==4 .OR. IERR==5)  STOP 'IMSl_FATAL_ERROR_SOLVING'
! Total number of solve steps.
                       NV=NV+1
                    CASE(ARPACK_Prepare)
! Set up storage areas for factored tridiagonal matrix.
                       IF (ALLOCATED(EX%A)) DEALLOCATE(EX%A)
                       IF (ALLOCATED(EX%B)) DEALLOCATE(EX%B)
                       IF (ALLOCATED(EX%C)) DEALLOCATE(EX%C)
                       IF (ALLOCATED(EX%Y1)) DEALLOCATE(EX%Y1)
                       IF (ALLOCATED(EX%U)) DEALLOCATE(EX%U)
                       IF (ALLOCATED(EX%IR)) DEALLOCATE(EX%IR)
                       IF (ALLOCATED(EX%IS)) DEALLOCATE(EX%IS)
                       NSIZE = (log(dble(N))/log(2.0)) + 5
                       ALLOCATE(EX%A(2*N), EX%B(2*N), EX%C(2*N), EX%Y1(2*N), &
                                 EX%U(2*N), EX%IR(NSIZE),                &
                                 EX%IS(NSIZE),   STAT=IERR)
                       IF (IERR /= 0) STOP 'IMSL_ERROR_ALLOCATING_WORKSPACE'
! Define matrix values.
                       HSQ=1._DKIND/REAL((N+1)**2,DKIND)
                       EX%B(1:N) = -1._DKIND/HSQ
                       EX%A(1:N) = 2._DKIND/HSQ - SHIFT
                       EX%C(1:N) = EX%B(1:N)
                       EX%Y1(:) = 0.0_DKIND
! Factor the matrix with LU and partial pivoting.
                       IJOB = 3
                       CALL LSLCR (EX%C, EX%A, EX%B, EX%Y1, EX%U, &
                                    EX%IR, EX%IS, N=N, IJOB=IJOB)
                       IERR = N1RTY(1)
                       IF(IERR == 4 .or. IERR == 5) STOP 'IMSL FATAL ERROR'
! Give output some values to satisfy compiler.
                       Y=0._DKIND
                       NV=0
                    CASE DEFAULT
                       STOP 'IMSL_ERROR_WRONG_OPERATION'
                    END SELECT
              END ASSOCIATE
           END SELECT
        END FUNCTION
        END MODULE

        USE ARPACK_SYMMETRIC_EX2_INT
        USE UMACH_INT
        USE WRRRN_INT
        IMPLICIT NONE
! Compute the smallest eigenvalues of a discrete Laplacian,
! based on second order divided differences.
```

```
! The matrix is the 1 dimensional discrete Laplacian on
! the interval 0,1 with zero Dirichlet boundary condition.

      INTEGER, PARAMETER ::  NEV=4, N=100
      REAL(DKIND) :: VALUES(NEV), RES(N)
      REAL(DKIND), ALLOCATABLE :: VECTORS(:,:)
      REAL(DKIND) NORM
      LOGICAL SMALL, SOLVED
      INTEGER J, NOUT
      TYPE(ARPACKBASE_EXT) EX

      ASSOCIATE(NX  => EX%NX, &
                NV  => EX%NV, &
              SIGMA => EX%SHIFT)

      CALL UMACH(2, NOUT)
! Note that VECTORS(:,:) does not need to be allocated
! in the calling program.  That happens within the
! routine ARPACK_SYMMETRIC().  It is OK to do this but
! the sizes (N,NCV) are determined in ARPACK_SYMMETRIC.
      SIGMA=0._DKIND
      CALL ARPACK_SYMMETRIC(N, FCN, VALUES,&
         CATEGORY=ARPACK_Shift_Invert, EXTYPE=EX, VECTORS=VECTORS)

      WRITE(NOUT,*) 'Number of Matrix-Vector Products Required, EX-2'
      WRITE(NOUT,*) '-----------------------------------------------'
      WRITE(NOUT, '(5X, I4)') NV
      CALL WRRRN('Largest Laplacian Eigenvalues Near Zero Shift', &
                 VALUES)
! Check residuals, A*vectors = values*vectors:
      DO J=1,NEV
         RES=FCN(VECTORS(:,J),ARPACK_A_x,EX)-VALUES(J)*VECTORS(:,J)
         NORM=maxval(abs(RES))
            SMALL=(NORM <= ABS(VALUES(J))*SQRT(EPSILON(NORM)))
         IF(J==1) SOLVED=SMALL
            SOLVED=SOLVED .and. SMALL
      END DO

      IF(SOLVED) THEN
          WRITE(nout,'(A///)') &
               'All Ritz Values and Vectors have small residuals.'
      ELSE
          WRITE(nout,'(A///)') &
               'Some Ritz Values and Vectors have large residuals.'
      ENDIF
      END ASSOCIATE
      END
```

Output

```
 Number of Matrix-Vector Products Required, EX-2
 -----------------------------------------------
       24

 Largest Laplacian Eigenvalues Near Zero Shift
                   1      9.9
                   2     39.5
                   3     88.8
                   4    157.7
All Ritz Values and Vectors have small residuals.
```

Example 3

We compute the solution of a generalized problem. This comes from using equally spaced linear finite element test functions to solve eigenvalues and eigenfunctions of the 1D Laplacian operator $-\frac{d^2u}{dx^2} = \lambda u$ on the unit interval, **[0,1]**. This is *Example 2* but solved using finite elements. With matrix notation, we have the matrix problem $Ax = \lambda Bx$. Both A and B are tri-diagonal and symmetric. The matrix B is non-singular. We compute the smallest *magnitude* eigenvalues. This requires the optional arguments `TYPE = ARPACK_Generalized`, `CATEGORY = ARPACK_Regular_Inverse`, and `PLACE = ARPACK_Smallest_Magnitude`. The user function, `FCN`, requires the solution of a tri-diagonal system of linear equations applied to an input vector, $y = B^{-1}x$. The base class `ARPACKBASE` is extended to the user's type, `TYPE(ARPACKBASE_EXT)`, defined in the user module `ARPACK_SYMMETRIC_EX3_INT`. This extension includes the number of intervals, a total kept in `FCN` for noting the number of operations, *and* allocatable arrays used to store the *LU* factorization of *B*. When `FCN` is entered with `TASK=ARPACK_Prepare`, these arrays are allocated, defined, and the *LU* factorization of the matrix *B* is computed. The function `FCN` is entered with the three values `TASK=ARPACK_A_x`, for $y = Ax$; `TASK=ARPACK_B_x`, for $y = Bx$; and `TASK=ARPACK_inv_B_x`, for $y = B^{-1}x$.

Within the main program, the function interface for the external function `FCN` is specified with the declaration `PROCEDURE (DMV) FCN`.

(Example arpack_symmetric_ex3.f90)

```
      MODULE ARPACK_SYMMETRIC_EX3_INT
      USE ARPACK_INT
      USE LSLCR_INT
      USE N1RTY_INT
      IMPLICIT NONE

      TYPE, EXTENDS(ARPACKBASE) :: ARPACKBASE_EXT
         REAL(DKIND) :: H=0._DKIND
         INTEGER ::     NX=0, NV=0
! This example extends the base type to
! information for solving tridiagonal systems.
         REAL(DKIND), ALLOCATABLE ::  A(:), B(:), C(:)
         REAL(DKIND), ALLOCATABLE :: Y1(:), U(:)
         INTEGER, ALLOCATABLE :: IR(:), IS(:)

      END TYPE ARPACKBASE_EXT
      END MODULE



      PROGRAM  ARPACK_SYMMETRIC_EX3
      USE ARPACK_SYMMETRIC_EX3_INT
      USE UMACH_INT
      USE WRRRN_INT
      IMPLICIT NONE

!         We want to solve A*x = lambda*M*x in inverse mode,
!         where A and M are obtained by the finite element method
!         of the 1-dimensional discrete Laplacian
!                             d^2u / dx^2
!         on the interval 0,1, with zero Dirichlet boundary conditions,
```

```
!         using piecewise linear elements.

      INTEGER,PARAMETER ::  NEV=4, N=100
      REAL(DKIND) :: VALUES(NEV), RES(N)
      REAL(DKIND), ALLOCATABLE :: VECTORS(:,:)
      REAL(DKIND) NORM
      LOGICAL :: PRINTRESULTS = .FALSE.
      LOGICAL SMALL, SOLVED
      INTEGER J, NOUT
      PROCEDURE(DMV) FCN
      TYPE(ARPACKBASE_EXT) EX

      ASSOCIATE(NX  => EX%NX, &
                NV  => EX%NV)
              EX%FACTOR_MAXNCV=5._DKIND
      CALL UMACH(2, NOUT)
! Note that VECTORS(:,:) does not need to be allocated
! in the calling program.  That happens within the
! routine ARPACK_SYMMETRIC().  It is OK to do this but
! the sizes (N,NCV) are determined in ARPACK_SYMMETRIC.
      CALL ARPACK_SYMMETRIC(N, FCN, VALUES, &
         TYPE=ARPACK_Generalized, &
         CATEGORY=ARPACK_Regular_Inverse, &
         PLACE=ARPACK_Smallest_Magnitude, EXTYPE=EX, VECTORS=VECTORS)

      WRITE(NOUT,*) 'Number of Matrix-Vector Products Required, EX-3'
      WRITE(NOUT,*) '-----------------------------------------------'
      WRITE(NOUT, '(5X, I4)') NV
      CALL WRRRN('Largest Laplacian Eigenvalues', VALUES)

! Check residuals, A*vectors = values*B*vectors:
      DO J=1,NEV
         RES=FCN(VECTORS(:,J),ARPACK_A_x,EX)-&
            VALUES(J)*FCN(VECTORS(:,J),ARPACK_B_x,EX)
         NORM=maxval(abs(RES))
         SMALL=(NORM <= ABS(VALUES(J))*SQRT(EPSILON(NORM)))
         IF(J==1) SOLVED=SMALL
         SOLVED=SOLVED .and. SMALL
      END DO

      IF(SOLVED) THEN
          WRITE(nout,'(A///)') &
               'All Ritz Values and Vectors have small residuals.'
      ELSE
          WRITE(nout,'(A///)') &
               'Some Ritz Values and Vectors have large residuals.'
      ENDIF
      END ASSOCIATE
      END PROGRAM

      FUNCTION FCN(X, TASK, EX) RESULT(Y)
         USE ARPACK_SYMMETRIC_EX3_INT
         CLASS (ARPACKBASE), INTENT(INOUT) :: EX
         REAL (DKIND), INTENT(INOUT) :: X(:)
         INTEGER, INTENT(IN) :: TASK
         REAL (DKIND) Y(SIZE(X)), PI
         INTEGER J, IERR, IJOB, NSIZE

         SELECT TYPE(EX)
            TYPE IS(ARPACKBASE_EXT)
            ASSOCIATE(N   =>    EX%NCOLS, &
                      NV  =>    EX%NV, &
                      H   =>    EX%H)

            SELECT CASE(TASK)
               CASE(ARPACK_A_x)
```

```
                    Y(1) =  2._DKIND*X(1) - X(2)

                    DO J = 2,N-1
                       Y(J) = - X(J-1) + 2._DKIND*X(J) - X(J+1)
                    END DO

                    Y(N) = - X(N-1) + 2._DKIND*X(N)
                    Y=Y/H
                 CASE(ARPACK_B_x)
                    Y(1) = 4._DKIND*X(1) + X(2)

                    DO J = 2,N-1
                       Y(J) = X(J-1) + 4._DKIND*X(J) + X(J+1)
                    END DO

                    Y(N) = X(N-1) + 4._DKIND*X(N)
                    Y=Y*(H/6._DKIND)
                 CASE(ARPACK_inv_B_x)
! Compute Y=inv(A-*I)*x.  This is done with a solve
! step, using the LU factorization.  Note that the data
! for the factorization is stored in the user's extended
! data type.
                    EX%Y1(1:N) = X
                    IJOB = 2
                    CALL LSLCR (EX%C, EX%A, EX%B, EX%Y1, EX%U, &
                                EX%IR, EX%IS, N=N, IJOB=IJOB)
                    Y(1:N) = EX%Y1(1:N)
                    IERR= N1RTY(1)
                    IF (IERR==4 .OR. IERR==5)  STOP 'IMSl_FATAL_ERROR_SOLVING'
! Total number of solve steps.
                    NV=NV+1
                 CASE(ARPACK_Prepare)
! Set up storage areas for factored tridiagonal matrix.

                       IF (ALLOCATED(EX%A)) DEALLOCATE(EX%A)
                       IF (ALLOCATED(EX%B)) DEALLOCATE(EX%B)
                       IF (ALLOCATED(EX%C)) DEALLOCATE(EX%C)
                       IF (ALLOCATED(EX%Y1)) DEALLOCATE(EX%Y1)
                       IF (ALLOCATED(EX%U)) DEALLOCATE(EX%U)
                       IF (ALLOCATED(EX%IR)) DEALLOCATE(EX%IR)
                       IF (ALLOCATED(EX%IS)) DEALLOCATE(EX%IS)
                       NSIZE = (log(dble(N))/log(2.0d0)) + 5
                       ALLOCATE(EX%A(2*N), EX%B(2*N), EX%C(2*N), EX%Y1(2*N), &
                                 EX%U(2*N), EX%IR(NSIZE),                &
                                 EX%IS(NSIZE),    STAT=IERR)
                       IF (IERR /= 0) STOP 'IMSL_ERROR_ALLOCATING_WORKSPACE'

! Define matrix values.
                    PI=ATAN(1._DKIND)*4._DKIND
                    H=PI/REAL(N+1,DKIND)
                    EX%B(1:N) =  (1._DKIND/6._DKIND)*H
                    EX%A(1:N) =  (2._DKIND/3._DKIND)*H
                    EX%C(1:N) = EX%B(1:N)
                    EX%Y1(:) = 0.0_DKIND

! Factor the matrix with LU and partial pivoting.

                    IJOB = 3
                    CALL LSLCR (EX%C, EX%A, EX%B, EX%Y1, EX%U, &
                                EX%IR, EX%IS, N=N, IJOB=IJOB)
                    IERR = N1RTY(1)
                    IF(IERR == 4 .or. IERR == 5) STOP 'IMSL FATAL ERROR'
! Give output some values to satisfy compiler.
                    Y=0._DKIND
                    NV=0
                 CASE DEFAULT
```

```
                    write(*,*)TASK
                    STOP 'IMSL_ERROR_WRONG_OPERATION'
                 END SELECT
              END ASSOCIATE
           END SELECT
        END FUNCTION
```

Output

```
   Number of Matrix-Vector Products Required, EX-3
   -----------------------------------------------
       1126

   Largest Laplacian Eigenvalues
             1    1.00
             2    4.00
             3    9.01
             4   16.02
  All Ritz Values and Vectors have small residuals.
```

ARPACK_SVD

Computes some singular values and left and right singular vectors of a real rectangular matrix $A_{MxN} = USV^T$. There is no restriction on the relative sizes, *M* and *N*. This routine calls ARPACK_SYMMETRIC.

Required Arguments

M — The number of matrix rows. (Input)

N — The number of matrix columns. (Input)

F — User-supplied FUNCTION to return matrix-vector operations. This user function is written corresponding to the *abstract interface* for the function SVDMV (…) .The operations provided as code in the function F will be made based on the two matrix operations $y = Ax$ and $y = A^Tx \equiv x^TA$. The usage is F (X, TASK, EXTYPE), where

Function Return Value

F — An array of length N containing matrix-vector operations or linear equations solutions. Operations provided as code in the function F will be made depending upon the value of argument TASK.

Required Arguments

X — An array of length N containing the vector to which the operator will be applied. (Input)

TASK — An enumerated type which specifies the operation to be performed. (Input) TASK is an enumerated integer value, use-associated from the module ARPACK_INT. It will be one of the following:

Value	Description
ARPACK_Prepare	Take initial steps to prepare for the operations that follow. These steps can include defining the data for the matrices, factorizations for upcoming linear system solves, or recording the vectors used in the operations.
ARPACK_A_x	$y = Ax$
ARPACK_xt_A	$y = x^TA$

EXTYPE — A derived type of the extensible class ARPACKBASE, which may be used to pass additional information to/from the user-supplied function. (Input/Output)
The user must include a USE ARPACK_INT statement in the calling program to define this derived type. If EXTYPE is not included as an argument to ARPACK_SVD it should be ignored in the user-function, F.

The function F must be written according to the abstract interface for SVDMV. If F is not use-associated nor contained in the calling program, declare it with PROCEDURE(SVDMV) F.

SVALUES — A rank-1 array of singular values. (Output)
The value NEV = size(SVALUES) defines the number of singular values to be computed. The calling program declares or allocates the array SVALUES(1:NEV).

Optional Arguments

PLACE — Indicates the placement in the spectrum for required singular values. (Input)
PLACE can be one of the following enumerated integers as defined in ARPACK_INT:

Value
ARPACK_Largest_Algebraic
ARPACK_Smallest_Magnitude

Default: PLACE = ARPACK_Largest_Algebraic.

ITERATION_TYPE — Indicates the method for obtaining the required singular values. (Input)
ITERATION_TYPE can be one of the following enumerated integers as defined in ARPACK_INT:

Value
ARPACK_Normal
ARPACK_Expanded

For values $M \geq N$, ARPACK_Normal specifies computing singular values based on eigenvalues and eigenvectors of the *normal* symmetric matrix A^TA; for values $M < N$ this will be the alternate symmetric matrix AA^T.

For all values of M,N, ARPACK_Expanded specifies computing singular values based on the symmetric matrix eigenvalue problem for the matrices

$$\begin{bmatrix} 0 & A \\ A^T & 0 \end{bmatrix} \text{ or } \begin{bmatrix} 0 & A^T \\ A & 0 \end{bmatrix}$$

Default: ITERATION_TYPE = ARPACK_Normal.

EXTYPE — A derived type of the extensible class ARPACKBASE, which may be used to pass additional information to/from the user-supplied function. (Input/Output)
The user must include a USE ARPACK_INT statement in the calling program to define this derived type. If EXTYPE is not included as an argument to ARPACK_SVD it must still be supplied as an argument to user-function, F, but is not used.

U_VECTORS — An allocatable array of orthogonal left singular vectors. (Output)
It is not necessary to allocate U_VECTORS(:,:). If this argument is present, the allocation occurs within the routine ARPACK_SVD The output sizes are UVECTORS(1:M,1:NCV). The second dimension value is NCV=min(M, max(FACTOR_MAXNCV*NEV,NEV+1)), where the value FACTOR_MAXNCV is a component of the base class, ARPACKBASE. The first NEV columns of U_VECTORS(:,:) are the left singular vectors.

V_VECTORS — An allocatable array of orthogonal right singular vectors. (Output)
It is not necessary to allocate V_VECTORS(:,:). If this argument is present, the allocation occurs within the routine ARPACK_SVD. The output sizes are V_VECTORS(1:N,1:NCV). The second dimension value is NCV=min(M, max(FACTOR_MAXNCV*NEV,NEV+1)), where the value FACTOR_MAXNCV is a component of the base class, ARPACKBASE. The first NEV columns of V_VECTORS(:,:) are the right singular vectors.

FORTRAN 2003 Interface

Generic: ARPACK_SVD (M, N, F,SVALUES [,…])

Specific: The specific interface name is D_ARPACK_SVD.

FORTRAN 90 Interface

A Fortran 90 compiler version is not available for this routine.

Description

Routine ARPACK_SVD calls ARPACK_SYMMETRIC to compute partial singular value decompositions for rectangular real matrices. There is no restriction on the relative sizes of the number of rows and columns. A function internal to ARPACK_SVD is used in the call to ARPACK_SYMMETRIC. The internal function calls the user function, F, which provides matrix-vector products of the matrix and an internally generated vector. By including the class object EXTYPE as an argument to this function, user data and procedure pointers are available for the evaluations. A user code must extend the base class EXTYPE to include the extra data and procedure pointers.

Comments

The user function supplies requests for the matrix operations. Those cases that follow from the settings of `PLACE` and `ITERATION_TYPE` need to be provided in the user code. The enumerated `TASK` constants, `ARPACK_A_x` and `ARPACK_xt_A` are available by use-association from the module `ARPACK_INT`. The sizes of the inputs and outputs,*x*,*y*, switch between the values *n*, *m*. The values *n*, *m* are alternated in the base class components `EXTYPE%NCOLS` and `EXTYPE%MROWS`.

The value of `Iteration_Type` may impact the number of iterations required. Generally one expects `Iteration_Type=ARPACK_Normal` (the default) to result in the fewest iterations, and `Iteration_Type=ARPACK_Expanded` to result in singular values with the greatest accuracy.

The output arrays `U_VECTORS(:,:)`, `SVALUES(:)`, and `V_VECTORS(:,:)` allow for reconstruction of an approximation to the matrix *A*. This approximation is $B = USV^T$. The matrices *U*, *S* and *V* are available in these respective routine arguments. The terms U_{MxNSV} and V_{MxNSV} have orthogonal columns, $U^TU = I_{NSV} = V^TV$. The diagonal matrix $S_{NSVxNSV}$ has its entries in `SVALUES(:)`, ordered from largest to smallest. Use the value *NSV* = min(*size*(*SVALUES*), *NACC*), where *NACC* is the number of accurate singular values computed by `ARPACK_SYMMETRIC`. This is the component `EXTYPE%NACC` of the base class `EXTYPE`.

After computing the singular values and right singular vectors by iteration with the normal matrix A^TA, *U* is computed from the relation *AV* = *US*. The result is then processed with the modified Gram-Schmidt algorithm to assure that *U* is orthogonal. When iterating with AA^T we first compute the left singular vectors *U* and then obtain *V* by the Gram-Schmidt algorithm. If we use `Iteration_Type=ARPACK_Expanded`, *U* and *V* are computed simultaneously, and both are orthogonal.

Example

We define the $M \times N$ matrix $A = \{a_{i,j}\}$ with entries $a_{i,j} = i + j$. This matrix has two non-zero singular values. With the pair of values (*M*,*N*) = (512,265) and (*M*,*N*) = (265,512) we obtain the singular decomposition for these rectangular matrices. With each pair we compute the decomposition using the input `Iteration_Type=ARPACK_Normal` and `Iteration_Type=ARPACK_Expanded`. The latter value requires the larger number of iterations. The matrix *A* has its storage requirements changed from *M*,*N* to the value $2(M + N + 1)$. The resulting product $B = USV^T$, when rounded to the nearest integer, satisfies *B* = *A*.

The base class `ARPACKBASE` is extended to include an allocatable array, `EXTYPE%A(:,:)`. This is allocated and defined and stores the matrix *A*. The matrix operations $y = Ax$ and $y = A^Tx \equiv x^TA$ are computed with `DGEMV`.

(Example arpack_svd_ex1.f90)

```
MODULE ARPACK_SVD_EX1_INT
USE ARPACK_INT
```

```
      IMPLICIT NONE

      TYPE, EXTENDS(ARPACKBASE) :: ARPACKBASE_EXT
          REAL(DKIND), ALLOCATABLE :: A(:,:)
          INTEGER :: NV = 0
          INTEGER :: MM = 0
          INTEGER :: NN = 0
      END TYPE ARPACKBASE_EXT
      CONTAINS

      FUNCTION FCN(X, TASK, EXTYPE) RESULT(Y)
         USE UMACH_INT
         CLASS (ARPACKBASE), INTENT(INOUT) :: EXTYPE
         REAL (DKIND), INTENT(INOUT) :: X(EXTYPE % NCOLS)
         INTEGER, INTENT(IN) :: TASK
         REAL (DKIND) Y(EXTYPE % MROWS)
         INTEGER I, J, NOUT

         CALL UMACH(2, NOUT)
         SELECT TYPE(EXTYPE)
            TYPE IS(ARPACKBASE_EXT)
            ASSOCIATE(M => EXTYPE % MM,&
                      N => EXTYPE % NN,&
                      A => EXTYPE % A)
            SELECT CASE(TASK)
            CASE(ARPACK_A_x)
!     Computes y <-- A*x
               CALL DGEMV('N',M,N,1._DKIND,A,M,X,1,0._DKIND,Y,1)
               EXTYPE % NV = EXTYPE % NV + 1
            CASE(ARPACK_xt_A)

!     Computes y <-- A^T*x = x^T * A
               CALL DGEMV('T',M,N,1._DKIND,A,M,X,1,0._DKIND,Y,1)
               EXTYPE % NV = EXTYPE % NV + 1

            CASE(ARPACK_Prepare)
               EXTYPE % NV = 0
               IF(ALLOCATED(EXTYPE % A)) DEALLOCATE(EXTYPE % A)
               ALLOCATE(EXTYPE % A(M,N))

               DO J=1,N
                  DO I=1,M
                     EXTYPE % A (I,J) = I + J
                  END DO
               END DO
            CASE DEFAULT
               WRITE(NOUT,*) TASK, ': INVALID TASK REQUESTED'
               STOP 'IMSL_ERROR_WRONG_OPERATION'
            END SELECT

            END ASSOCIATE
         END SELECT
      END FUNCTION
      END MODULE

      USE ARPACK_SVD_EX1_INT
      USE UMACH_INT
      USE WRRRN_INT
! Compute the largest and smallest singular values of a
! patterned matrix.
      INTEGER, PARAMETER :: NSV=2
      INTEGER ::  COUNT, I, J, N, M, nout
      REAL(DKIND)   :: SVALUESMax(NSV)
      REAL(DKIND), ALLOCATABLE :: SVALUEsMin(:)
      REAL(DKIND), ALLOCATABLE :: VECTORS(:,:), B(:,:)
      REAL(DKIND), ALLOCATABLE :: U_VECTORS(:,:), V_VECTORS(:,:)
```

```
      REAL(DKIND) NORM
      LOGICAL SMALL, SOLVED
      TYPE(ARPACKBASE_EXT) EX

      ASSOCIATE(M=>EX % MM,&
                N=>EX % NN,&
                NACC=>EX % NACC,&
                TOL =>EX % TOL,&
                MAXMV => EX % MAXMV)
      SOLVED = .true.
      CALL UMACH(2, NOUT)
! Define size of matrix problem.
      N=800
      M=600
      DO COUNT =1,2
! Some values will not be accurately determined for rank
! deficient problems.  This next value drops the number
! requested after every sequence of iterations of this size.
         MAXMV=500
         CALL ARPACK_SVD(M, N, FCN, SVALUESMax, &
                PLACE=ARPACK_Largest_Algebraic, & !Default
                Iteration_TYPE=ARPACK_Normal,   & !Default
                EXTYPE=EX, U_VECTORS=U_VECTORS,   &
                V_VECTORS=V_VECTORS)
         CALL WRRRN( 'Largest Singular values, Normal Method', &
                     SVALUESMax)
         WRITE(NOUT, *) 'Number of matrix-vector products'
         WRITE(NOUT, *) '--------------------------------'
         WRITE(NOUT, '(5X, I4)') EX % NV
         IF(ALLOCATED(B))DEALLOCATE(B)
         ALLOCATE(B(M,N))
! Reconstruct an approximation to A, B = U * S * V ^T.
! Use only the singular values accurately determined.

         DO I=1,NACC
            U_VECTORS(:,I)=U_VECTORS(:,I)*SVALUESMax(I)
         END DO
         B=matmul(U_VECTORS(:,1:NACC),transpose(V_VECTORS(:,1:NACC)))
! Truncate the approximation to nearest integers.
! Subtract known integer matrix and check agreement with
! the approximation.
         DO I=1,M
            DO J=1,N
               B(I,J)=REAL(NINT(B(I,J)),DKIND)
               B(I,J)=B(I,J)-EX % A(I,J)
            END DO
         END DO
         WRITE(NOUT,'(/A,I6)')&
         'Number of singular values, S and columns of U,V =', NACC
         WRITE(NOUT,'(/A,F6.2)')&
               'Integer units of error with U,V and S =', maxval(B)
         if (maxval(B) > 0.0d0) then
            solved = .false.
         else
            solved = solved .and. .true.
         end if
         SVALUESMax=0._DKIND
! Do same SVD with the Expanded form of the symmetric matrix.
         CALL ARPACK_SVD(M, N, FCN, SVALUESMax,&
                         PLACE=ARPACK_Largest_Algebraic, & !Default
                         Iteration_TYPE=ARPACK_Expanded, &
                         EXTYPE=EX, U_VECTORS=U_VECTORS,    &
                         V_VECTORS=V_VECTORS)

         CALL WRRRN('Largest Singular values, Expanded Method', SVALUESMax)
         WRITE(NOUT, *) 'Number of matrix-vector products'
```

```
          WRITE(NOUT, *) '--------------------------------'
          WRITE(NOUT, '(5X,I4)') EX % NV
! Reconstruct an approximation to A, B = U * S * V ^T.
! Use only the singular values accurately determined.
          DO I=1,NACC
             U_VECTORS(:,I)=U_VECTORS(:,I)*SVALUESMax(I)
          END DO
          B=matmul(U_VECTORS(:,1:NACC),transpose(V_VECTORS(:,1:NACC)))
! Truncate the approximation to nearest integers.
! Subtract known integer matrix and check agreement with
! the approximation.
          DO I=1,M
             DO J=1,N
                B(I,J)=REAL(NINT(B(I,J)),DKIND)
                B(I,J)=B(I,J)-EX % A(I,J)
             END DO
          END DO
          WRITE(NOUT,'(A,I6)')&
               'Number of singular values, S and columns of U,V =', NACC
          WRITE(NOUT,'(A,F6.2)')&
                'Integer units of error with U,V and S =', maxval(B)
          if (maxval(B) > 0.0d0) then
             solved = .false.
          else
             solved = solved .and. .true.
          end if

          M=800
          N=600
          DEALLOCATE(U_VECTORS, V_VECTORS)
       END DO

       END ASSOCIATE
       END
```

Output

```
 Largest Singular values, Normal Method
              1   523955.7
              2    36644.2
 Number of matrix-vector products
 --------------------------------
       12

Number of singular values, S and columns of U,V =     2

Integer units of error with U,V and S =  0.00

 Largest Singular values, Expanded Method
               1   523955.7
               2    36644.2
 Number of matrix-vector products
 --------------------------------
       22
Number of singular values, S and columns of U,V =     2
Integer units of error with U,V and S =  0.00

 Largest Singular values, Normal Method
              1   523955.7
              2    36644.2
 Number of matrix-vector products
 --------------------------------
       12

Number of singular values, S and columns of U,V =     2
```

```
 Integer units of error with U,V and S =  0.00

  Largest Singular values, Expanded Method
                1   523955.7
                2    36644.2
  Number of matrix-vector products
  --------------------------------
        18
 Number of singular values, S and columns of U,V =     2
 Integer units of error with U,V and S =  0.00
```

ARPACK_NONSYMMETRIC

Compute some eigenvalues and eigenvectors of the generalized eigenvalue problem $Ax = \lambda Bx$. This can be used for the case $B = I$. The values for A,B are real, but eigenvalues may be complex and occur in conjugate pairs.

Required Arguments

N — The dimension of the problem. (Input)

F — User-supplied `FUNCTION` to return matrix-vector operations or linear solutions. This user function is written corresponding to the abstract interface for the function `DMV`(…). The usage is `F` (`X`, `TASK`, `EXTYPE`), where

Function Return Value

`F` — An array of length `N` containing matrix-vector operations or linear equations solutions. Operations provided as code in the function `F` will be made depending upon the value of argument `TASK`.

Required Arguments

`X` — An array of length `N` containing the vector to which the operator will be applied. (Input)

`TASK` — An enumerated type which specifies the operation to be performed. (Input) `TASK` is an enumerated integer value, use-associated from the module `ARPACK_INT`. It will be one of the following:

Value	**Description**
`ARPACK_Prepare`	Take initial steps to prepare for the operations that follow. These steps can include defining the data for the matrices, factorizations for upcoming linear system solves, or recording the vectors used in the operations.
`ARPACK_A_x`	$y = Ax$
`ARPACK_B_x`	$y = Bx$
`ARPACK_inv_A_minus_Shift_x`	$y = (A - \sigma I)^{-1}x$
`ARPACK_inv_B_x`	$y = B^{-1}x$
`ARPACK_inv_A_minus_Shift_B_x`	$y = (A - \sigma B)^{-1}x$

EXTYPE — A derived type of the extensible class ARPACKBASE, which may be used to pass additional information to/from the user-supplied function. (Input/Output)
The user must include a USE ARPACK_INT statement in the calling program to define this derived type. If EXTYPE is not included as an argument to ARPACK_NONSYMMETRIC it should be ignored in the user-function, F.

The function F must be written according to the abstract interface for DMV. If F is not use-associated nor contained in the calling program, declare it with PROCEDURE(DMV) F.

ZVALUES — A complex array of eigenvalues. (Output)
The value NEV=size(ZVALUES) defines the number of eigenvalues to be computed. The calling program declares or allocates the array ZVALUES(1:NEV). The size value NEV should account for pairs of complex conjugates. The number of eigenvalues computed accurately is optionally available as the component EXTYPE%NACC of the base class EXTYPE.

Optional Arguments

***PLACE* —** Defines the placement in the spectrum for required eigenvalues. (Input)
PLACE can be one of the following enumerated integers as defined in ARPACK_INT:

Value
ARPACK_Largest_Magnitude
ARPACK_Smallest_Magnitude
ARPACK_Largest_Real_Parts
ARPACK_Smallest_Real_Parts
ARPACK_Largest_Imag_Parts
ARPACK_Smallest_Imag_Parts

Default: ARPACK_Largest_Magnitude.

***TYPE* —** Defines the eigenvalue problem as either a standard or generalized eigenvalue problem. (Input)
TYPE can be one of the following enumerated integers as defined in ARPACK_INT:

Value	Description
ARPACK_Standard	$Ax = \lambda x$
ARPACK_Generalized	$Ax = \lambda Bx$

Default: TYPE = ARPACK_Standard.

***CATEGORY* —** CATEGORY and TYPE define the operation sequence provided in the user-written function. (Input)

CATEGORY can be one of the following enumerated integers as defined in ARPACK_INT:

Value	Description
ARPACK_Regular	$Ax = \lambda x$
ARPACK_Regular_Inverse	$y = Ax, y = Bx, y = B^{-1}x$
ARPACK_Shift_Invert	$y = Ax, y = (A - \sigma I)^{-1}x, y = (A - \sigma B)^{-1}x$
ARPACK_Complex_Part_Shift_Invert	$y = Ax, y = (A - \sigma I)^{-1}x, y = (A - \sigma B)^{-1}x$ $y = Ax, y = Bx, y = \mathrm{Im}\{(A - \sigma B)^{-1}x\}$ $y = Ax, y = Bx, y = \mathrm{Re}\{(A - \sigma B)^{-1}x\}$

Default: CATEGORY = ARPACK_Regular.

EXTYPE — A derived type of the extensible class ARPACKBASE, which may be used to pass additional information to/from the user-supplied function. (Input/Output)
The user must include a USE ARPACK_INT statement in the calling program to define this derived type. If EXTYPE is not included as an argument to ARPACK_NONSYMMETRIC it must still be supplied as an argument to user-function, F, but is not used.

VECTORS — An allocatable array of approximate eigenvectors. (Output)
It is not necessary to allocate VECTORS(:,:). If this argument is used the allocation occurs within the routine ARPACK_NONSYMMETRIC. The output sizes are VECTORS(1:N,1:NCV). The second dimension value is NCV=min(N, max(FACTOR_MAXNCV*NEV,NEV+1)), where the value FACTOR_MAXNCV is a component of the base class, ARPACKBASE. The first NEV columns of VECTORS(:,:) represent the eigenvectors (see *Comments*).

FORTRAN 2003 Interface

Generic: ARPACK_NONSYMMETRIC (N, F,ZVALUES [,…])

Specific: The specific interface name is D_ARPACK_NONSYMMETRIC.

Fortran 90 Interface

A Fortran 90 compiler version is not available for this routine.

Description

Routine ARPACK_NONSYMMETRIC calls ARPACK subroutines to compute partial eigenvalue-eigenvector decompositions for real matrices. The ARPACK routines are dnaupd and dneupd (see *ARPACK Users' Guide*, SIAM Publications, (1998)), which use "reverse communication" to obtain the required matrix-vector operations for this approximation. Responses to these requests are made by calling the user-written function F. By including the class object EXTYPE as an argument to this function, user data and procedure pointers are available for the evaluations. A user code must extend the base class EXTYPE to include the extra data and procedure pointers.

Comments

The non-symmetric problem may have complex eigenvalues that occur in conjugate pairs, and the eigenvectors are returned in the REAL(DKIND) array VECTORS(:,:) but with a compact representation: If the eigenvalue λ_j has an imaginary part with a negative value, construct the complex eigenvector from the relation $w_j = v_j + iv_{j+1}$. The real vectors v_j, v_{j+1} are consecutive columns of the array VECTORS (:,:). The eigenvalue-eigenvector relationship is $Aw_j = \lambda_j w_j$. Since A is real, λ is also an eigenvalue; thus the conjugate relationship $A\overline{w}_j = \overline{\lambda}_j\overline{w}_j$ will hold. For purposes of checking results the complex residual $r_j = Aw_j - \lambda_j w_j$ should be small in norm relative to the norm of A. If that is true, there is no need to check the alternate relationship. This compact representation of the eigenvectors can be expanded to require twice the storage requirements, but that is not done here in the interest of saving large blocks of storage.

For the generalized eigenvalue problem $Ax = \lambda Bx$ the eigenvalues are optionally computed based on the Raleigh Quotient. Because of the shifts used, only the eigenvectors may be computed. The eigenvalues are returned by solving $Aw_j = \lambda Bw_j$ for λ: $\lambda_j = \left(w_j^H A w_j\right) / \left(w_j^H B w_j\right)$. λ_j is valid if the denominator is non-zero. If λ_j has a non-zero imaginary part, then the complex conjugate $\overline{\lambda}_j$ is also an eigenvalue. The Raleigh Quotient for eigenvalues of generalized problems is used when vectors are requested and the user has requested it be used with the base class component EXTYPE%RALEIGH_QUOTIENT == .TRUE. This is the component's default value.

Example

We solve the generalized eigenvalue problem $Ax = \lambda Bx$ using the shift-invert category. The matrix A is tri-diagonal with the values 2 on the diagonal, -2 on the sub-diagonal, and 3 on the super-diagonal. The matrix B is tri-diagonal with the values 4 on the diagonal and 1 on the off-diagonals. We use the complex shift $\sigma = 0.4 + 0.6i$ and increase the factor for the number of Ritz vectors from 2.5 to 5. Two strategies of shift-invert are illustrated, $y = \mathrm{Re}(A - \sigma B)^{-1}Bx$ and $y = \mathrm{Im}(A - \sigma B)^{-1}Bx$. In each case NEV=6 eigenvalues are obtained, each with 3 pairs of complex conjugate values.

(Example arpack_nonsymmetric_ex1.f90)

```
      MODULE ARPACK_NONSYMMETRIC_EX1_INT
      USE ARPACK_INT
      USE LSLCQ_INT
      USE N1RTY_INT
      IMPLICIT NONE

      TYPE, EXTENDS(ARPACKBASE) :: ARPACKBASE_EXT
         INTEGER ::     NX=0
         INTEGER ::     NV=0
! This example extends the base type to
! information for solving complex tridiagonal systems.
         COMPLEX(DKIND), ALLOCATABLE :: A(:), B(:), C(:)
         INTEGER, ALLOCATABLE ::  IR(:), IS(:)
! This controls the type of shifting.  When
! the value is 1, use real part of inv(A-*M)*x.
! If value is 2, use imaginary part of same.
         INTEGER :: SHIFT_STRATEGY=1
      END TYPE ARPACKBASE_EXT

      CONTAINS
      FUNCTION FCN(X, TASK, EX) RESULT(Y)
         USE UMACH_INT

         CLASS (ARPACKBASE), INTENT(INOUT) :: EX
         REAL (DKIND), INTENT(INOUT) :: X(:)
         INTEGER, INTENT(IN) :: TASK
         INTEGER, PARAMETER :: NSIZE=12
         REAL(DKIND) Y(size(X))
         REAL(DKIND) DL, DD, DU
         COMPLEX(DKIND) Z(2*size(X))
         REAL(DKIND) U(2*size(X))
         INTEGER J, IERR, NOUT, IJOB
         CALL UMACH(2, NOUT)
         SELECT TYPE(EX)
            TYPE IS(ARPACKBASE_EXT)
            ASSOCIATE(N    =>    EX % NCOLS,&
                      NV   =>    EX % NV, &
                      SHIFT =>   EX % SHIFT)

            SELECT CASE(TASK)

               CASE(ARPACK_A_x)
                  DL =  -2._DKIND
                  DD =   2._DKIND
                  DU =   3._DKIND
                  Y(1) =  DD*X(1) + DU*X(2)
                  DO J = 2,N-1
                     Y(J) = DL*X(J-1) + DD*X(J) + DU*X(J+1)
                  END DO
                  Y(N) =  DL*X(N-1) + DD*X(N)
                  NV=NV+1

               CASE(ARPACK_B_x)
                  Y(1) = 4._DKIND*X(1) + X(2)
                  DO J = 2,N-1
                     Y(J) = X(J-1) + 4._DKIND*X(J) + X(J+1)
                  END DO
                  Y(N) = X(N-1) + 4._DKIND*X(N)
                  NV=NV+1

               CASE(ARPACK_inv_A_minus_Shift_B_x)
! Compute Y=REAL/AIMAG(inv(A-*B)*x).  This is done with a solve
! step, using the LU factorization.  Note that the data
```

```
! for the factorization is stored in the user's extended
! data type.
                  Z=CMPLX(X,0._DKIND,DKIND)
                  IJOB = 2
                  CALL LSLCQ (EX%C, EX%A, EX%B, Z, U, &
                              EX%IR, EX%IS, N=N, IJOB=IJOB)
                  IERR= N1RTY(1)
                  IF (IERR==4 .OR. IERR==5)  &
                      STOP 'IMSl_FATAL_ERROR_SOLVING'


                  IF(EX % SHIFT_STRATEGY == 1) THEN
                     Y(1:N)=REAL( Z(1:N),DKIND)
                  ELSE IF (EX % SHIFT_STRATEGY == 2)THEN
                     Y(1:N)=AIMAG(Z(1:N))
                  END IF

! Total number of solve steps.
                  NV=NV+1

               CASE(ARPACK_Prepare)
! Set up storage areas for factored tridiagonal matrix.

                  IF (ALLOCATED(EX%A)) DEALLOCATE(EX%A)
                  IF (ALLOCATED(EX%B)) DEALLOCATE(EX%B)
                  IF (ALLOCATED(EX%C)) DEALLOCATE(EX%C)
                  IF (ALLOCATED(EX%IR)) DEALLOCATE(EX%IR)
                  IF (ALLOCATED(EX%IS)) DEALLOCATE(EX%IS)
                  ALLOCATE(EX%A(2*N), EX%B(2*N), EX%C(2*N), &
                           EX%IR(NSIZE), EX%IS(NSIZE), STAT=IERR)
                  IF (IERR /= 0) STOP 'IMSL_ERROR_ALLOCATING_WORKSPACE'

! Define matrix, A-SHIFT*B.
                  EX % B(1:N) =  -2._DKIND-SHIFT
                  EX % A(1:N) =  2._DKIND-4._DKIND*SHIFT
                  EX % C(1:N) =  3._DKIND-SHIFT
! Factor the matrix with LU and partial pivoting.
                  IJOB = 3
                  CALL LSLCQ (EX%C, EX%A, EX%B, Z, U, &
                              EX%IR, EX%IS, N=N, IJOB=IJOB)
                  IERR = N1RTY(1)
                  IF(IERR == 4 .or. IERR == 5) STOP 'IMSL FATAL ERROR'

! Give output some ZVALUES to satisfy compiler.
                  Y=0._DKIND
                  NV=0

               CASE DEFAULT
                  WRITE(NOUT,*) TASK, ': INVALID OPERATION REQUESTED'
                  STOP 'IMSL_ERROR_WRONG_OPERATION'
               END SELECT
            END ASSOCIATE
            END SELECT
      END FUNCTION
      END MODULE


!         Suppose we want to solve A*x = lambda*B*x in -invert mode
!         The matrix A is the tridiagonal matrix with 2 on the diagonal,
!         -2 on the subdiagonal and 3 on the superdiagonal.  The matrix
!         is the tridiagonal matrix with 4 on the diagonal and 1 on the
!         off-diagonals.
!         The  sigma is a complex number (sigmar, sigmai).
!         OP = Real_Part{invA-(SIGMAR,SIGMAI)*B*B.

      USE ARPACK_NONSYMMETRIC_EX1_INT
```

```
      USE UMACH_INT
      USE WRCRN_INT

      INTEGER, PARAMETER ::  NEV=6, N=100
      COMPLEX(DKIND)  :: ZVALUES(NEV), RES(N),U(N),V(N),W(N)
      REAL(DKIND), ALLOCATABLE :: VECTORS(:,:)
      REAL(DKIND) NORM
      LOGICAL SKIP, SMALL, SOLVED
      INTEGER J, STRATEGY, NOUT
      CHARACTER(LEN=12) TAG
      CHARACTER(LEN=60) TITLE
      TYPE(ARPACKBASE_EXT) EX

      ASSOCIATE(NX  => EX % NX, &
                NV  => EX % NV, &
                SHIFT  => EX % SHIFT,&
                FACTOR => EX % FACTOR_MAXNCV,&
                NACC   => EX % NACC)
! Note that VECTORS(:,:) does not need to be allocated
! in the calling program.  That happens within the
! routine ARPACK_NONSYMMETRIC().  It is OK to do this but
! the sizes (N,NCV) are determined in ARPACK_NONSYMMETRIC.

      CALL UMACH(2, NOUT)
      SOLVED=.TRUE.
      DO STRATEGY=1,2
         SHIFT=CMPLX(0.4_DKIND,0.6_DKIND,DKIND)
         FACTOR=5._DKIND
         EX % SHIFT_STRATEGY=STRATEGY

         CALL ARPACK_NONSYMMETRIC(N, FCN, ZVALUES,         &
                 TYPE=ARPACK_Generalized,                  &
                 CATEGORY=ARPACK_Complex_Part_Shift_Invert, &
                 EXTYPE=EX, VECTORS=VECTORS)

         WRITE(NOUT, *) &
             'Number of Matrix-Vector Products Required, NS Ex-1'
         WRITE(NOUT, *) &
             '---------------------------------------------------'
         WRITE(NOUT, '(5X,I4)') NV
         WRITE(NOUT, *) 'Number of accurate values determined'
         WRITE(NOUT, *) '------------------------------------'
         WRITE(NOUT, '(5X, I4)') NACC
! Check residuals, A*vectors = ZVALUES*M*vectors:

         SKIP=.FALSE.
         DO J=1,NACC
            IF(SKIP) THEN
               SKIP=.FALSE.
               CYCLE
            END IF
! The eigenvalue is complex and the pair of vectors
! for the complex eigenvector is returned.
            IF(AIMAG(ZVALUES(J)) /= 0._DKIND)THEN
! Make calls for real and imaginary parts of eigenvectors
! applied to the operators A, M
               U=CMPLX(FCN(VECTORS(:,J),ARPACK_A_x,EX),&
                       FCN(VECTORS(:,J+1),ARPACK_A_x,EX),DKIND)
               V=CMPLX(FCN(VECTORS(:,J),ARPACK_B_x,EX),&
                       FCN(VECTORS(:,J+1),ARPACK_B_x,EX),DKIND)
! Since the matrix is real, there is an additional conjugate:
               RES=U-ZVALUES(J)*V
               SKIP=.TRUE.
            ELSE
! The eigenvalue is real and the real eigenvector is returned.
```

```
                RES=FCN(VECTORS(:,J),ARPACK_A_x,EX)-ZVALUES(J)*&
                    FCN(VECTORS(:,J),ARPACK_B_x,EX)
             END IF
             NORM=maxval(abs(RES))
             SMALL=(NORM <= ABS(ZVALUES(J))*SQRT(EPSILON(NORM)))
             SOLVED=SOLVED .and. SMALL
          END DO
          IF(STRATEGY==1) TAG='REAL SHIFT'
          IF(STRATEGY==2) TAG='IMAG SHIFT'

          TITLE = 'Largest Raleigh Quotient Eigenvalues,'//TAG
          CALL WRCRN(TITLE, ZVALUES)

          IF(SOLVED) THEN
              WRITE(NOUT,'(A///)') &
                   'All Ritz Values and Vectors have small residuals.'
          ELSE
              WRITE(NOUT,'(A///)') &
                   'Some Ritz Values and Vectors have large residuals.'
          END IF
       END DO ! Shift strategy
       END ASSOCIATE

       END
```

Output

```
   Number of Matrix-Vector Products Required, NS Ex-1
   --------------------------------------------------
        280
   Number of accurate values determined
   ------------------------------------
          6

   Largest Raleigh Quotient Eigenvalues,REAL SHIFT
                 1  ( 0.5000,-0.5958)
                 2  ( 0.5000, 0.5958)
                 3  ( 0.5000,-0.6331)
                 4  ( 0.5000, 0.6331)
                 5  ( 0.5000, 0.5583)
                 6  ( 0.5000,-0.5583)
  All Ritz Values and Vectors have small residuals.



   Number of Matrix-Vector Products Required, NS Ex-1
   --------------------------------------------------
        248
   Number of accurate values determined
   ------------------------------------
          6

   Largest Raleigh Quotient Eigenvalues,IMAG SHIFT
                 1  ( 0.5000,-0.5958)
                 2  ( 0.5000, 0.5958)
                 3  ( 0.5000,-0.5583)
                 4  ( 0.5000, 0.5583)
                 5  ( 0.5000,-0.6331)
                 6  ( 0.5000, 0.6331)
  All Ritz Values and Vectors have small residuals.
```

ARPACK_COMPLEX

Compute some eigenvalues and eigenvectors of the generalized eigenvalue problem $Ax = \lambda Bx$. This can be used for the case $B = I$. The values for A,B are real or complex. When the values are complex the eigenvalues may be complex and are not expected to occur in complex conjugate pairs.

Required Arguments

N — The dimension of the problem. (Input)

F — User-supplied FUNCTION to return matrix-vector operations or linear solutions. This user function is written corresponding to the *abstract interface* for the function ZMV(…). The usage is F(X, TASK, EXTYPE), where

Function Return Value

F — An array of length N containing matrix-vector operations or linear equations solutions. Operations provided as code in the function F will be made depending upon the value of argument TASK.

Required Arguments

X — An array of length N containing the vector to which the operator will be applied. (Input)

TASK — An enumerated type which specifies the operation to be performed. (Input) TASK is an enumerated integer value, use-associated from the module ARPACK_INT. It will be one of the following:

Value	Description
ARPACK_Prepare	Take initial steps to prepare for the operations that follow. These steps can include defining the data for the matrices, factorizations for upcoming linear system solves, or recording the vectors used in the operations.
ARPACK_A_x	$y = Ax$
ARPACK_B_x	$y = Bx$

EXTYPE — A derived type of the extensible class ARPACKBASE, which may be used to pass additional information to/from the user-supplied function. (Input/Output) The user must include a USE ARPACK_INT statement in the calling program to define this derived type. If EXTYPE is not included as an argument to ARPACK_COMPLEX it should be ignored in the user-function, F.

The function F must be written according to the abstract interface for ZMV. If F is not use-associated nor contained in the calling program, declare it with PROCEDURE(ZMV) F.

ZVALUES — A complex array of eigenvalues. (Output)
The value NEV=size(ZVALUES) defines the number of eigenvalues to be computed. The calling program declares or allocates the array ZVALUES(1:NEV). The number of eigenvalues computed accurately is optionally available as the component EXTYPE%NACC of the base class EXTYPE.

Optional Arguments

PLACE **—** Defines the output content of VALUES. (Input)
PLACE specifies the placement within the spectrum for the required eigenvalues. PLACE can be one of the following enumerated integers as defined in ARPACK_INT:

Value
ARPACK_Largest_Magnitude
ARPACK_Smallest_Magnitude
ARPACK_Largest_Real_Parts
ARPACK_Smallest_Real_Parts
ARPACK_Largest_Imag_Parts
ARPACK_Smallest_Imag_Parts

Default: PLACE = ARPACK_Largest_Magnitude.

TYPE **—** Defines the eigenvalue problem as either a standard or generalized eigenvalue problem. (Input)
TYPE can be one of the following enumerated integers as defined in ARPACK_INT:

Value	Description
ARPACK_Standard	$Ax = \lambda x$
ARPACK_Generalized	$Ax = \lambda Bx$

Default: TYPE = ARPACK_Standard.

CATEGORY **—** CATEGORY and TYPE define the operation sequence provided in the user-written function. (Input)

CATEGORY can be one of the following enumerated integers as defined in ARPACK_INT:

Value	Description
ARPACK_Regular	$y = Ax$
ARPACK_Regular_Inverse	$y = Ax, y = Bx, y = B^{-1}x$
ARPACK_Shift_Invert	$y = Ax, y = (A - \sigma I)^{-1}x, y = (A - \sigma B)^{-1}x$
ARPACK_Complex_Part_Shift_Invert	$y = Ax, y = Bx$, $y = \mathrm{Re}\{(A - \sigma B)^{-1}x\}$ $y = Ax, y = Bx$, $y = \mathrm{Im}\{(A - \sigma B)^{-1}x\}$

Default: CATEGORY = ARPACK_Regular.

EXTYPE — A derived type of the extensible class ARPACKBASE, which may be used to pass additional information to/from the user-supplied function. (Input/Output)
The user must include a USE ARPACK_INT statement in the calling program to define this derived type. If EXTYPE is not included as an argument to ARPACK_COMPLEX it must still be supplied as an argument to user-function, F, but is not used.

VECTORS — An allocatable array of approximate eigenvectors. (Output)
It is not necessary to allocate VECTORS(:,:). If this argument is used the allocation occurs within the routine ARPACK_NONSYMMETRIC. The output sizes are VECTORS(1:N,1:NCV). The second dimension value is NCV=min(N, max(FACTOR_MAXNCV*NEV,NEV+1)), where the value FACTOR_MAXNCV is a component of the base class, ARPACKBASE. The first NEV columns of VECTORS(:,:) represent the eigenvectors w_j (see *Comments*).

FORTRAN 2003 Interface

Generic: ARPACK_COMPLEX (N, F,ZVALUES [,…])

Specific: The specific interface name is Z_ARPACK_COMPLEX.

Fortran 90 Interface

A Fortran 90 compiler version is not available for this routine.

Description

Routine ARPACK_COMPLEX calls ARPACK subroutines to compute partial eigenvalue-eigenvector decompositions for complex matrices. The ARPACK routines are dzaupd and dzeupd (see *ARPACK Users' Guide*, SIAM Publications, (1998)), which use "reverse communication" to obtain the required matrix-vector operations for this approximation. Responses to these requests are made by calling the user-written function F. By including the class object EXTYPE as an argument to this function, user data and procedure pointers are available for the evaluations. A user code must extend the base class EXTYPE to include the extra data and procedure pointers.

Comments

For purposes of checking results the complex residual $r_j = Aw_j - \lambda_j w_j$ should be small in norm relative to the norm of A. For the generalized eigenvalue problem $Ax = \lambda Bx$ the eigenvalues are optionally computed based on the Raleigh Quotient. Because of the shifts used, only the eigenvectors may be computed. The eigenvalues are returned based on solving $Aw_j = \lambda Bw_j$ for λ_j,

where

$$\lambda_j = \left(w_j^H A w_j\right) / \left(w_j^H B w_j\right)$$

The eigenvalue λ_j is finite and valid if the denominator is non-zero. The Raleigh Quotient for eigenvalues of generalized problems is used only when vectors are requested and the user has requested it be used with the base class component EXTYPE%RALEIGH_QUOTIENT = .TRUE. This is the component's default value.

Example

This example is a variation of the first *example* for ARPACK_SYMMETRIC. We approximate eigenvalues and eigenfunctions of the Laplacian operator

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \equiv \Delta u, - \Delta u + \rho \frac{\partial u}{\partial x} = \lambda u$$

on the unit square, [0,1] × [0,1]. But now the parameter ρ is complex. Thus the eigenvalues and eigenfunctions are complex.

(Example arpack_complex_ex1.f90)

```
      MODULE ARPACK_COMPLEX_EX1_INT
      USE ARPACK_INT
      IMPLICIT NONE

      TYPE, EXTENDS(ARPACKBASE), PUBLIC :: ARPACKBASE_EXT
         REAL(DKIND) :: H   =0._DKIND
         REAL(DKIND) :: HSQ=0._DKIND
         COMPLEX(DKIND) :: RHO=(0._DKIND,0._DKIND)
         COMPLEX(DKIND) :: DL=(0._DKIND,0._DKIND)
         COMPLEX(DKIND) :: DD=(0._DKIND,0._DKIND)
         COMPLEX(DKIND) :: DU=(0._DKIND,0._DKIND)
         INTEGER :: NX=0
```

```
         INTEGER :: NV=0
      END TYPE ARPACKBASE_EXT
      CONTAINS
      FUNCTION FZ1(X, TASK, EXTYPE) RESULT(Y)
         USE UMACH_INT

         CLASS (ARPACKBASE), INTENT(INOUT) :: EXTYPE
         COMPLEX (DKIND), INTENT(INOUT) :: X(:)
         INTEGER, INTENT(IN) :: TASK
         COMPLEX (DKIND) Y(size(X))
         COMPLEX (DKIND) DT(3)
         REAL(DKIND) :: ONE=1._DKIND
         INTEGER J, NOUT

         CALL UMACH(2, NOUT)
         SELECT TYPE(EXTYPE)
            TYPE IS(ARPACKBASE_EXT)
            ASSOCIATE(NX  => EXTYPE % NX,&
                      H   => EXTYPE % H,&
                      HSQ => EXTYPE % HSQ,&
                      RHO => EXTYPE % RHO,&
                      DL  => EXTYPE % DL,&
                      DD  => EXTYPE % DD,&
                      DU  => EXTYPE % DU,&
                      NV  => EXTYPE % NV)

            SELECT CASE(TASK)
               CASE(ARPACK_A_x)
!     Computes y <-- A*x, where A is the N**2 by N**2 block
!     tridiagonal matrix deriving from (Laplacian u) + rho*(du/dx).

                  DT=(/DL,DD,DU/)
                  Y(1:NX)=T(NX,X(1:NX),DT) - X(NX+1:2*NX)/HSQ
                  DO J=NX+1,NX**2-NX,NX
                     Y(J:J+NX-1)=T(NX,X(J:J+NX-1),DT) &
                                 - (X(J-NX:J-1)+ X(J+NX:J+2*NX-1))/HSQ
                  END DO
                  Y((NX-1)*NX+1:NX**2)= - X((NX-1)*NX-NX+1:(NX-1)*NX) &
                                  / HSQ + T(NX,X((NX-1)*NX+1:NX**2),DT)
! Total the number of matrix-vector products.
                  NV=NV+1

               CASE(ARPACK_Prepare)
! Define 1/H**2, etc. so they are available in the evaluator.
                  H   = ONE/REAL(NX+1,DKIND)
                  HSQ = H**2
                  DD  = (4.0D+0, 0.0D+0)  / HSQ
                  DL  = -ONE/HSQ - (5.0D-1, 0.0D+0) *RHO/H
                  DU  = -ONE/HSQ + (5.0D-1, 0.0D+0) *RHO/H
                  NV = 0
               CASE DEFAULT
                  WRITE(nout,*) TASK, ': INVALID TASK REQUESTED'
                  STOP 'IMSL_ERROR_WRONG_OPERATION'
            END SELECT
            END ASSOCIATE
         END SELECT
      END FUNCTION

      FUNCTION T(NX, X, DT)RESULT(V)
         INTEGER, INTENT(IN) :: NX
         COMPLEX(DKIND), INTENT(IN) :: X(:), DT(3)
         COMPLEX(DKIND) :: V(NX)
         INTEGER J
         ASSOCIATE(DL => DT(1),&
                   DD => DT(2),&
                   DU => DT(3))
```

```
          V(1) =  DD*X(1) + DU*X(2)
          DO J = 2,NX-1
             V(J) = DL*X(J-1) + DD*X(J) + DU*X(J+1)
          END DO
          V(NX) =  DL*X(NX-1) + DD*X(NX)
          END ASSOCIATE
       END FUNCTION
       END MODULE

 ! Compute the largest magnitude eigenvalues of a discrete Laplacian,
 ! based on second order divided differences.

 !     The matrix used is obtained from the standard central difference
 !         discretization of the convection-diffusion operator
 !                 (Laplacian u) + rho*(du / dx)
 !         on the unit squre 0,1x0,1 with zero Dirichlet boundary
 !         conditions.
       USE ARPACK_COMPLEX_EX1_INT
       USE UMACH_INT
       USE WRCRN_INT

       INTEGER, PARAMETER :: NEV=6
       INTEGER ::  J, N, NOUT
       COMPLEX(DKIND) :: VALUES(NEV)
       COMPLEX(DKIND), ALLOCATABLE :: RES(:), EF(:,:)
       COMPLEX(DKIND), ALLOCATABLE :: VECTORS(:,:)
       REAL(DKIND) NORM
       LOGICAL SMALL, SOLVED
       TYPE(ARPACKBASE_EXT) EX

       ASSOCIATE(NX   => EX % NX, &
                 NV   => EX % NV, &
                 RHO  => EX % RHO,&
                 NACC => EX % NACC)

       CALL UMACH(2, NOUT)
       NX=10
       RHO=(100._DKIND,1._DKIND)

 ! Define size of matrix problem.
       N=NX**2
 ! Note that VECTORS(:,:) does not need to be allocated
 ! in the calling program.  That happens within the
 ! routine ARPACK_COMPLEX().  It is OK to do this but
 ! the sizes (N,NCV) are determined in ARPACK_COMPLEX.
       CALL ARPACK_COMPLEX(N, FZ1, VALUES, EXTYPE=EX, VECTORS=VECTORS)

       WRITE(NOUT, *) 'Number of eigenvalues requested, and accurate'
       WRITE(NOUT, *) '---------------------------------------------'
       WRITE(NOUT, '(5X, I4, 5X, I4)') NEV, NACC
       WRITE(NOUT, *) 'Number of Matrix-Vector Products Required, ZEX-1'
       WRITE(NOUT, *) '------------------------------------------------'
       WRITE(NOUT,  '(5X, I4)') NV
       CALL WRCRN ('Largest Magnitude Operator Eigenvalues', VALUES)
 ! Check residuals, A*vectors = values*vectors:
       ALLOCATE(RES(N))
       DO J=1,NACC
          RES=FZ1(VECTORS(:,J),ARPACK_A_x,EX)-VALUES(J)*VECTORS(:,J)
          NORM=maxval(abs(RES))
          SMALL=(NORM <= ABS(VALUES(J))*SQRT(EPSILON(NORM)))
          IF(J==1) SOLVED=SMALL
          SOLVED=SOLVED .and. SMALL
       END DO

       IF(SOLVED) THEN
          WRITE(NOUT,'(A///)') &
```

```
               'All Ritz Values and Vectors have small residuals.'
         ELSE
            WRITE(NOUT,'(A///)') &
               'Some Ritz Values and Vectors have large residuals.'
         END IF

         END ASSOCIATE
         END
```

Output

```
   Number of eigenvalues requested, and accurate
   ---------------------------------------------
          6        6
   Number of Matrix-Vector Products Required, ZEX-1
   ------------------------------------------------
        475

   Largest Magnitude Operator Eigenvalues
            1  (  727.0,-1029.6)
            2  (  705.4, 1029.6)
            3  (  698.4,-1029.6)
            4  (  676.8, 1029.6)
            5  (  653.3,-1029.6)
            6  (  631.7, 1029.6)
  All Ritz Values and Vectors have small residuals.
```

Interpolation and Approximation

Routines

3.10 Cubic Spline Smoothing

3.11 Rational L_∞ Approximation

Usage Notes

The majority of the routines in this chapter produce piecewise polynomial or spline functions that either interpolate or approximate given data, or are support routines for the evaluation, integration, and conversion from one representation to another. Two major subdivisions of routines are provided. The cubic spline routines begin with the letters "CS" and utilize the piecewise polynomial representation described below. The B-spline routines begin with the letters "BS" and utilize the B-spline representation described below. Most of the spline routines are based on routines in the book by de Boor (1978).

Piecewise Polynomials

A univariate piecewise polynomial (function) p is specified by giving its breakpoint sequence $\xi \in \mathbf{R}^n$, the order k (degree $k - 1$) of its polynomial pieces, and the $k \times (n - 1)$ matrix c of its local polynomial coefficients. In terms of this information, the piecewise polynomial (pp) function is given by

$$p(x) = \sum_{j=1}^{k} c_{ji} \frac{(x - \xi_i)^{j-1}}{(j-1)!} \quad \mathit{for} \quad \xi_i \le x < \xi_{i+1}$$

The breakpoint sequence ξ is assumed to be strictly increasing, and we extend the pp function to the entire real axis by extrapolation from the first and last intervals. The subroutines in this chapter will consistently make the following identifications for FORTRAN variables:

$$c = \text{PPCOEF}$$
$$\xi = \text{BREAK}$$
$$k = \text{KORDER}$$
$$N = \text{NBREAK}$$

This representation is redundant when the pp function is known to be smooth. For example, if p is known to be continuous, then we can compute $c_{1,i+1}$ from the c_{ji} as follows

$$c_{1,i+1} = p(\xi_{i+1}) = c_{1i} + c_{2i}\Delta\xi_i + \dots + c_{ki}\frac{(\Delta\xi_i)^{k-1}}{(k-1)!}$$

where $\Delta\xi_i := \xi_{i+1} - \xi_i$. For smooth pp, we prefer to use the irredundant representation in terms of the B-(for 'basis')-splines, at least when such a function is first to be determined. The above pp representation is employed for evaluation of the pp function at many points since it is more efficient.

Splines and B-splines

B-splines provide a particularly convenient and suitable basis for a given class of smooth pp functions. Such a class is specified by giving its breakpoint sequence, its order, and the required smoothness across each of the interior breakpoints. The corresponding B-spline basis is specified by giving its knot sequence $\mathbf{t} \in \mathbf{R}^M$. The specification rule is the following: If the class is to have all derivatives up to and including the j-th derivative continuous across the interior breakpoint ξ_i, then the number ξ_i should occur $k - j - 1$ times in the knot sequence. Assuming that ξ_1, and ξ_n are the endpoints of the interval of interest, one chooses the first k knots equal to ξ_1 and the last k knots equal to ξ_n. This can be done since the B-splines are defined to be right continuous near ξ_1 and left continuous near ξ_n.

When the above construction is completed, we will have generated a knot sequence $\boldsymbol{t}$ of length M; and there will be $m := M - k$ B-splines of order k, say $B_1, \ldots, B_m$ that span the pp functions on the interval with the indicated smoothness. That is, each pp function in this class has a unique representation

$$p = a_1 B_1 + a_2 B_2 + \ldots + a_m B_m$$

as a linear combination of B-splines. The B-spline routines will consistently make use of the following identifiers for FORTRAN variables:

$$a = \text{BSCOEF}$$
$$\mathbf{t} = \text{XKNOT}$$
$$m = \text{NCOEF}$$
$$M = \text{NKNOT}$$

A B-spline is a particularly compact pp function. B_i is a nonnegative function that is nonzero only on the interval $[t_i, t_{i+k}]$. More precisely, the support of the i-th B-spline is $[t_i, t_{i+k}]$. No pp function in the same class (other than the zero function) has smaller support (i.e., vanishes on more intervals) than a B-spline. This makes B-splines particularly attractive basis functions since the influence of any particular B-spline coefficient extends only over a few intervals. When it is necessary to emphasize the dependence of the B-spline on its parameters, we will use the notation

$$B_{i,k,t}$$

to denote the i-th B-spline of order k for the knot sequence $\mathbf{t}$.

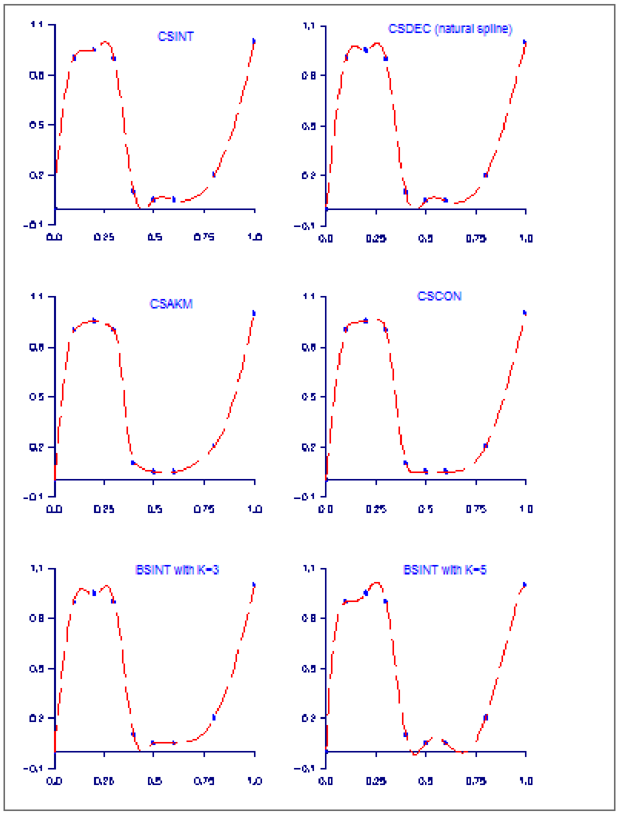


Figure 3, Spline Interpolants of the Same Data

Cubic Splines

Cubic splines are smooth (i.e., C^1 or C^2) fourth-order pp functions. For historical and other reasons, cubic splines are the most heavily used pp functions. Therefore, we provide special routines for their construction and evaluation. The routines for their determination use yet another representation (in terms of value and slope at all the breakpoints) but output the pp representation as described above for general pp functions.

We provide seven cubic spline interpolation routines: `CSIEZ`, `CSINT`, `CSDEC`, `CSHER`, `CSAKM`, `CSCON`, and `CSPER`. The first routine, `CSIEZ`, is an easy-to-use version of `CSINT` coupled with `CSVAL`. The routine `CSIEZ` will compute the value of the cubic spline interpolant (to given data using the 'not-a-knot' criterion) on a grid. The routine `CSDEC` allows the user to specify various endpoint conditions (such as the value of the first or second derivative at the right and left points). This means that the natural cubic spline can be obtained using this routine by setting the second derivative to zero at both endpoints. If function values and derivatives are available, then the Hermite cubic interpolant can be computed using `CSHER`. The two routines `CSAKM` and `CSCON` are designed so that the shape of the curve matches the shape of the data. In particular, `CSCON` preserves the convexity of the data while

CSAKM attempts to minimize oscillations. If the data is periodic, then CSPER will produce a periodic interpolant. The routine CONFT allows the user wide latitude in enforcing shapes. This routine returns the B-spline representation.

It is possible that the cubic spline interpolation routines will produce unsatisfactory results. The adventurous user should consider using the B-spline interpolation routine BSINT that allows one to choose the knots and order of the spline interpolant.

In *Figure 3*, we display six spline interpolants to the same data. This data can be found in Example 1 of the IMSL routine CSCON Notice the different characteristics of the interpolants. The interpolation routines CSAKM and CSCON are the only two that attempt to preserve the shape of the data. The other routines tend to have extraneous inflection points, with the piecewise quartic (k = 5) exhibiting the most oscillation.

Tensor Product Splines

The simplest method of obtaining multivariate interpolation and approximation routines is to take univariate methods and form a multivariate method via tensor products. In the case of two-dimensional spline interpolation, the development proceeds as follows: Let $\mathbf{t}_x$ be a knot sequence for splines of order k_x, and $\mathbf{t}_y$ be a knot sequence for splines of order k_y. Let $N_x + k_x$ be the length of $\mathbf{t}_x$, and $N_y + k_y$ be the length of $\mathbf{t}_y$. Then, the tensor product spline has the form

$$\sum_{m=1}^{N_y}\sum_{n=1}^{N_x} c_{nm} B_{n,k_x,\mathbf{t}_x}(x) B_{m,k_y,\mathbf{t}_y}(y)$$

Given two sets of points

$$\{x_i\}_{i=1}^{N_x} \text{ and } \{y_i\}_{i=1}^{N_y}$$

for which the corresponding univariate interpolation problem could be solved, the tensor product interpolation problem becomes: Find the coefficients c_{nm} so that

$$\sum_{m=1}^{N_y}\sum_{n=1}^{N_x} c_{nm} B_{n,k_x,\mathbf{t}_x}(x_i) B_{m,k_y,\mathbf{t}_y}(y_i) = f_{ij}$$

This problem can be solved efficiently by repeatedly solving univariate interpolation problems as described in de Boor (1978, page 347). Three-dimensional interpolation has analogous behavior. In this chapter, we provide routines that compute the two-dimensional tensor-product spline coefficients given two-dimensional interpolation data (BS2IN), compute the three-dimensional tensor-product spline coefficients given three-dimensional interpolation data (BS3IN) compute the two-dimensional tensor-product spline coefficients for a tensor-product least squares problem (BSLS2), and compute the three-dimensional tensor-product spline coefficients for a tensor-product least squares problem (BSLS3). In addition, we provide evaluation, differentiation, and integration routines for the two- and three-dimensional tensor-product spline functions. The relevant routines are BS2VL, BS3VL, BS2DR, BS3DR, BS2GD, BS3GD, BS2IG, and BS3IG.

Quadratic Interpolation

The routines that begin with the letters "QD" in this chapter are designed to interpolate a one-, two-, or three-dimensional (tensor product) table of values and return an approximation to the value of the underlying function or one of its derivatives at a given point. These routines are all based on quadratic polynomial interpolation.

Multi-dimensional Interpolation

We have one routine, SURF, that will return values of an interpolant to scattered data in the plane. This routine is based on work by Akima (1978), which utilizes C^1 piecewise quintics on a triangular mesh. SURFND computes a piecewise polynomial interpolant, of up to 15-th degree, to a function of up to 7 variables, defined on a multi-dimensional grid.

Least Squares

Routines are provided to smooth noisy data: regression using linear regression using arbitrary polynomials (RCURV), and regression using user-supplied functions (FNLSQ). Additional routines compute the least-squares fit using splines with fixed knots (BSLSQ) or free knots (BSVLS). These routines can produce cubic-spline least-squares fit simply by setting the order to 4. The routine CONFT computes a fixed-knot spline weighted least-squares fit subject to linear constraints. This routine is very general and is recommended if issues of shape are important. The two- and three-dimensional tensor-product spline regression routines are (BSLS2) and (BSLS3).

Smoothing by Cubic Splines

Two "smoothing spline" routines are provided. The routine CSSMH returns the cubic spline that smooths the data, given a smoothing parameter chosen by the user. Whereas, CSSCV estimates the smoothing parameter by cross-validation and then returns the cubic spline that smooths the data. In this sense, CSSCV is the easier of the two routines to use. The routine CSSED returns a smoothed data vector approximating the values of the underlying function when the data are contaminated by a few random spikes.

Rational Chebyshev Approximation

The routine RATCH computes a rational Chebyshev approximation to a user-supplied function. Since polynomials are rational functions, this routine can be used to compute best polynomial approximations.

Using the Univariate Spline Routines

An easy to use spline interpolation routine CSIEZ is provided. This routine computes an interpolant and returns the values of the interpolant on a user-supplied grid. A slightly more advanced routine SPLEZ computes (at the users discretion) one of several interpolants or least-squares fits and returns function values or derivatives on a user-supplied grid.

For more advanced uses of the interpolation (or least squares) spline routines, one first forms an interpolant from interpolation (or least-squares) data. Then it must be evaluated, differentiated, or integrated once the interpolant has been formed. One way to perform these tasks, using cubic splines with the 'not-a-knot' end condition, is to call CSINT to obtain the local coefficients of the piecewise cubic interpolant and then call CSVAL to evaluate the interpolant. A more complicated situation arises if one wants to compute a quadratic spline interpolant and then evaluate it (efficiently) many times. Typically, the sequence of routines called might be BSNAK (get the knots), BSINT (returns the B-spline coefficients of the interpolant), BSCPP (convert to pp form), and PPVAL (evaluate). The last two calls could be replaced by a call to the B-spline grid evaluator BS1GD, or the last call could be replaced with pp grid evaluator PP1GD. The interconnection of the spline routines is summarized in *Figure 4*.

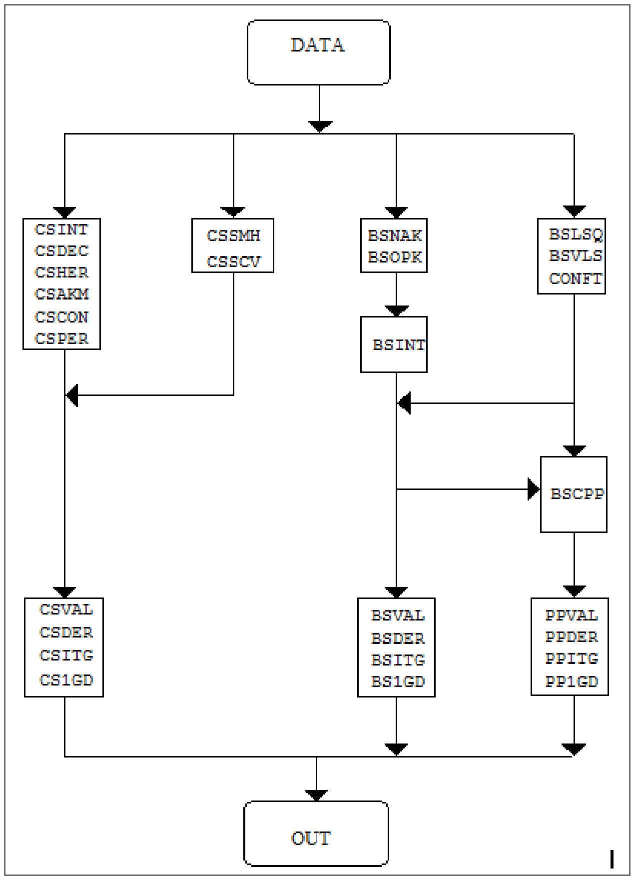


Figure 4, Interrelation of the Spline Routines

Choosing an Interpolation Routine

The choice of an interpolation routine depends both on the type of data and on the use of the interpolant. We provide 19 interpolation routines. These routines are depicted in a decision tree in Figure 3-3. This figure provides a guide for selecting an appropriate interpolation routine. For example, if periodic one-dimensional (univariate) data is available, then the path through *univariate* to *periodic* leads to the IMSL routine `CSPER`, which is the proper routine for this setting. The general-purpose univariate interpolation routines can be found in the box beginning with `CSINT`. Multidimensional tensor-product interpolation routines are also provided. For two-dimensional scattered data, the appropriate routine is `SURF`.

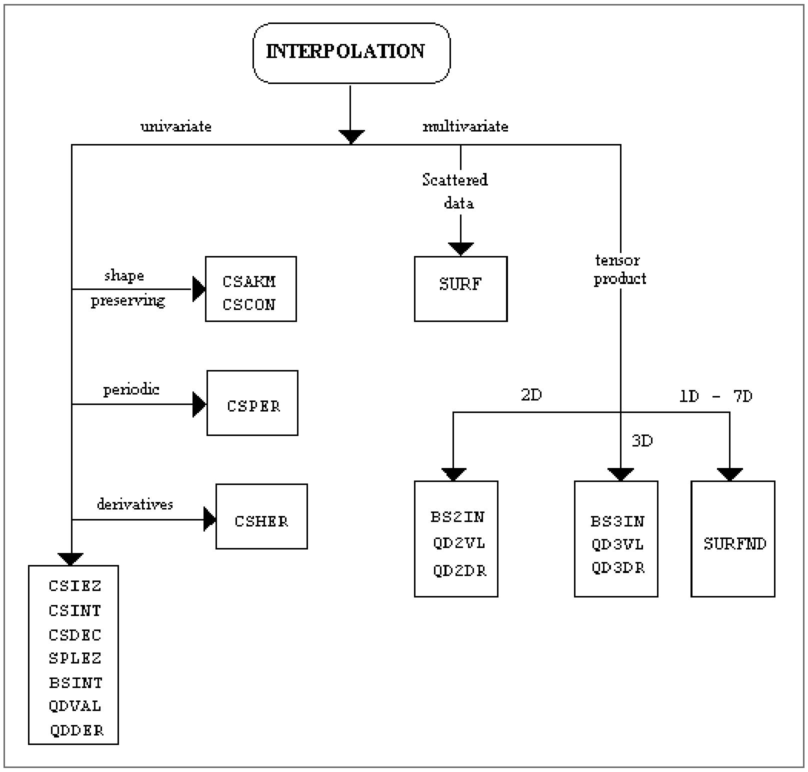


Figure 5, Choosing an Interpolation Routine

SPLINE_CONSTRAINTS

This function returns the derived type array result, `?_SPLINE_CONSTRAINTS`, given optional input. There are optional arguments for the derivative index, the value applied to the spline, and the periodic point for any periodic constraint.

The function is used, for entry number `j`,

```
?_SPLINE_CONSTRAINTS(J) = &
   SPLINE_CONSTRAINTS([DERIVATIVE=DERIVATIVE_INDEX,] &
   POINT = WHERE_APPLIED, [VALUE=VALUE_APPLIED,], &
   TYPE = CONSTRAINT_INDICATOR, &
   [PERIODIC_POINT = VALUE_APPLIED])
```

The square brackets enclose optional arguments. For each constraint either (but not both) the `'VALUE ='` or the `'PERIODIC_POINT ='` optional arguments must be present.

Required Arguments

POINT = `WHERE_APPLIED` (Input)
The point in the data interval where a constraint is to be applied.

TYPE = `CONSTRAINT_INDICATOR` (Input)
The indicator for the type of constraint the spline function or its derivatives is to satisfy at the point: `where_applied`. The choices are the character strings `'=='`, `'<='`, `'>='`, `'.=.'`, and `'.=-'`. They respectively indicate that the spline value or its derivatives will be equal to, not greater than, not less than, equal to the value of the spline at another point, or equal to the negative of the spline value at another point. These last two constraints are called *periodic* and *negative-periodic*, respectively. The alternate independent variable point is `value_applied` for either periodic constraint. There is a use of periodic constraints in .

Optional Arguments

DERIVATIVE = `DERIVATIVE_INDEX` (Input)
This is the number of the derivative for the spline to apply the constraint. The value 0 corresponds to the function, the value 1 to the first derivative, etc. If this argument is not present in the list, the value 0 is substituted automatically. Thus a constraint without the derivative listed applies to the spline function.

PERIODIC_POINT = `VALUE_APPLIED`

This optional argument improves readability by automatically identifying the second independent variable value for periodic constraints.

FORTRAN 90 Interface

Generic: `CALL SPLINE_CONSTRAINTS (POINT, TYPE [, …])`

Specific: The specific interface names are `S_SPLINE_CONSTRAINTS` and `D_SPLINE_CONSTRAINTS`.

SPLINE_VALUES

This rank-1 array function returns an array result, given an array of input. Use the optional argument for the covariance matrix when the square root of the variance function is required. The result will be a scalar value when the input variable is scalar.

Required Arguments

DERIVATIVE = `DERIVATIVE` (Input)
The index of the derivative evaluated. Use non-negative integer values. For the function itself use the value 0.

VARIABLES = `VARIABLES` (Input)
The independent variable values where the spline or its derivatives are evaluated. Either a rank-1 array or a scalar can be used as this argument.

KNOTS = `KNOTS` (Input)
The derived type `?_spline_knots`, defined as the array `COEFFS` was obtained with the function `SPLINE_FITTING`. This contains the polynomial spline degree and the number of knots and the knots themselves for this spline function.

COEFFS = `C` (Input)
The coefficients in the representation for the spline function,

$$f(x) = \sum_{j=1}^{N} c_j B_j(x)$$

These result from the fitting process or array assignment `C=SPLINE_FITTING(...)`, defined below. The value *N = size(C)* satisfies the identity *N – 1 + spline_degree = size* (*?_knots*), where the two right-most quantities refer to components of the argument `knots`.

Optional Arguments

COVARIANCE = `G` (Input)
This argument, when present, results in the evaluation of the square root of the variance function

$$e(x) = (b(x)^T G b(x))^{1/2}$$

where

$$b(x) = [B_1(x),\ldots,B_{\boldsymbol{N}}(x)]^{\boldsymbol{T}}$$

and *G* is the covariance matrix associated with the coefficients of the spline

$$c = [c_1,\ldots,c_{\boldsymbol{N}}]^{\boldsymbol{T}}$$

The argument `G` is an optional output parameter from the function `SPLINE_FITTING`, described below. When the square root of the variance function is computed, the arguments `DERIVATIVE` and `C` are not used.

IOPT = `IOPT` (Input)
This optional argument, of derived type `?_options`, is not used in this release.

FORTRAN 90 Interface

Generic: `CALL SPLINE_VALUES (DERIVATIVE, VARAIBLES, KNOTS, COEFFS [, …])`

Specific: The specific interface names are `S_SPLINE_VALUES` and `D_SPLINE_VALUES`.

SPLINE_FITTING

Weighted least-squares fitting by B-splines to discrete One-Dimensional data is performed. Constraints on the spline or its derivatives are optional. The spline function

$$f(x) = \sum_{j=1}^{N} c_j B_j(x)$$

its derivatives, or the square root of its variance function are evaluated after the fitting.

Required Arguments

DATA = DATA(1:3,:) (Input/Output)
An assumed-shape array with `size(data,1) = 3`. The data are placed in the array: `data(1,i)` = x_i, `data(2,i)` = y_i, and `data(3,i)` = σ_i, $i = 1,\ldots,ndata$. If the variances are not known but are proportional to an unknown value, users may set `data(3,i)` = 1, $i = 1,\ldots,ndata$.

KNOTS = KNOTS (Input)
A derived type, `?_spline_knots`, that defines the degree of the spline and the breakpoints for the data fitting interval.

Optional Arguments

CONSTRAINTS = SPLINE_CONSTRAINTS (Input)
A rank-1 array of derived type `?_spline_constraints` that give constraints the output spline is to satisfy.

COVARIANCE = G (Output)
An assumed-shape rank-2 array of the same precision as the data. This output is the covariance matrix of the coefficients. It is optionally used to evaluate the square root of the variance function.

IOPT = IOPT(:) (Input/Output)
Derived type array with the same precision as the input array; used for passing optional data to `SPLINE_FITTING`. The options are as follows:

Packaged Options for **SPLINE_FITTING**		
Prefix = None	Option Name	Option Value

Packaged Options for SPLINE_FITTING		
	SPLINE_FITTING_TOL_EQUAL	1
	SPLINE_FITTING_TOL_LEAST	2

IOPT(IO) = ?_OPTIONS(SPLINE_FITTING_TOL_EQUAL, ?_VALUE)

This resets the value for determining that equality constraint equations are rank-deficient. The default is ?_value = 10^{-4}.

IOPT(IO) = ?_OPTIONS(SPLINE_FITTING_TOL_LEAST, ?_VALUE)

This resets the value for determining that least-squares equations are rank-deficient. The default is ?_value = 10^{-4}.

FORTRAN 90 Interface

Generic: CALL SPLINE_FITTING (DATA, KNOTS [, …])

Specific: The specific interface names are S_SPLINE_FITTING and D_SPLINE_FITTING.

Description

This routine has similar scope to CONFT found in IMSL (2003, pp 734-743). We provide the square root of the variance function, but we do not provide for constraints on the integral of the spline. The least-squares matrix problem for the coefficients is banded, with band-width equal to the spline order. This fact is used to obtain an efficient solution algorithm when there are no constraints. When constraints are present the routine solves a linear-least squares problem with equality and inequality constraints. The processed least-squares equations result in a banded and upper triangular matrix, following accumulation of the spline fitting equations. The algorithm used for solving the constrained least-squares system will handle rank-deficient problems. A set of reference are available in Hanson (1995) and Lawson and Hanson (1995). The CONFT routine uses QPROG (*loc cit*., p. 959), which requires that the least-squares equations be of full rank.

Fatal and Terminal Error Messages

See the *messages.gls* file for error messages for SPLINE_FITTING. These error messages are numbered 1340–1367.

Examples

Example 1: Natural Cubic Spline Interpolation to Data

The function

$$g(x) = \exp\left(-x^2/2\right)$$

is interpolated by cubic splines on the grid of points

$$x_i = (i-1)\Delta x, i = 1, \ldots ndata$$

Those natural conditions are

$$f(x_i) = g(x_i), i = 0, \ldots ndata; \frac{d^2 f}{dx^2}(x_i) = \frac{d^2 g}{dx^2}(x_i), i = 0 \text{ and } ndata$$

Our program checks the term *const.* appearing in the maximum truncation error term

$$error \approx const. \times \Delta x^4$$

at a finer grid.

```
      USE spline_fitting_int
      USE show_int
      USE norm_int

      implicit none

! This is Example 1 for SPLINE_FITTING, Natural Spline
! Interpolation using cubic splines.  Use the function
! exp(-x**2/2) to generate samples.

      integer :: i
      integer, parameter :: ndata=24, nord=4, ndegree=nord-1, &
        nbkpt=ndata+2*ndegree, ncoeff=nbkpt-nord, nvalues=2*ndata
      real(kind(1e0)), parameter :: zero=0e0, one=1e0, half=5e-1
      real(kind(1e0)), parameter :: delta_x=0.15, delta_xv=0.4*delta_x
      real(kind(1e0)), target :: xdata(ndata), ydata(ndata), &
            spline_data (3, ndata), bkpt(nbkpt), &
            ycheck(nvalues), coeff(ncoeff), &
            xvalues(nvalues), yvalues(nvalues), diffs

      real(kind(1e0)), pointer :: pointer_bkpt(:)
      type (s_spline_knots) break_points
      type (s_spline_constraints) constraints(2)

      xdata = (/((i-1)*delta_x, i=1,ndata)/)
      ydata = exp(-half*xdata**2)
      xvalues =(/(0.03+(i-1)*delta_xv,i=1,nvalues)/)
      ycheck= exp(-half*xvalues**2)
      spline_data(1,:)=xdata
      spline_data(2,:)=ydata
      spline_data(3,:)=one
```

```
! Define the knots for the interpolation problem.
         bkpt(1:ndegree) = (/(i*delta_x, i=-ndegree,-1)/)
         bkpt(nord:nbkpt-ndegree) = xdata
         bkpt(nbkpt-ndegree+1:nbkpt) =  &
         (/(xdata(ndata)+i*delta_x, i=1,ndegree)/)

! Assign the degree of the polynomial and the knots.
      pointer_bkpt => bkpt
      break_points=s_spline_knots(ndegree, pointer_bkpt)

! These are the natural conditions for interpolating cubic
! splines.  The derivatives match those of the interpolating
! function at the ends.
      constraints(1)=spline_constraints &
         (derivative=2, point=bkpt(nord), type='==', value=-one)
      constraints(2)=spline_constraints &
         (derivative=2,point=bkpt(nbkpt-ndegree), type= '==', &
         value=(-one+xdata(ndata)**2)*ydata(ndata))

      coeff = spline_fitting(data=spline_data, knots=break_points,&
              constraints=constraints)
      yvalues=spline_values(0, xvalues, break_points, coeff)

      diffs=norm(yvalues-ycheck,huge(1))/delta_x**nord

      if (diffs <= one) then
        write(*,*) 'Example 1 for SPLINE_FITTING is correct.'
      end if
      end
```

Output

```
Example 1 for SPLINE_FITTING is correct.
```

Example 2: Shaping a Curve and its Derivatives

The function

$$g(x) = \exp\left(-x^2/2\right)\left(1 + noise\right)$$

is fit by cubic splines on the grid of equally spaced points

$$x_i = \left(i - 1\right)\Delta x, i = 1, \ldots ndata$$

The term *noise* is uniform random numbers from the normalized interval [$-\tau$, τ] where τ = 0.01. The spline curve is constrained to be convex down for $0 \le x \le 1$ convex upward for $1 < x \le 4$, and have the second derivative exactly equal to the value zero at $x = 1$. The first derivative is constrained with the value zero at $x = 0$ and is non-negative at the right and of the interval, $x = 4$. A sample table of independent variables, second derivatives and square root of variance function values is printed.

```
      use spline_fitting_int
      use show_int
      use rand_int
      use norm_int

      implicit none
```

```
! This is Example 2 for SPLINE_FITTING. Use 1st and 2nd derivative
! constraints to shape the splines.

      integer :: i, icurv
      integer, parameter :: nbkptin=13, nord=4, ndegree=nord-1, &
             nbkpt=nbkptin+2*ndegree, ndata=21, ncoeff=nbkpt-nord
      real(kind(1e0)), parameter :: zero=0e0, one=1e0, half=5e-1
      real(kind(1e0)), parameter :: range=4.0, ratio=0.02, tol=ratio*half
      real(kind(1e0)), parameter :: delta_x=range/(ndata-1), &
      delta_b=range/(nbkptin-1)
      real(kind(1e0)), target :: xdata(ndata), ydata(ndata), ynoise(ndata),&
            sddata(ndata), spline_data (3, ndata), bkpt(nbkpt), &
            values(ndata), derivat1(ndata), derivat2(ndata), &
            coeff(ncoeff), root_variance(ndata), diffs
      real(kind(1e0)), dimension(ncoeff,ncoeff) :: sigma_squared

      real(kind(1e0)), pointer :: pointer_bkpt(:)
      type (s_spline_knots) break_points
      type (s_spline_constraints) constraints(nbkptin+2)

      xdata = (/((i-1)*delta_x, i=1,ndata)/)
      ydata = exp(-half*xdata**2)
      ynoise = ratio*ydata*(rand(ynoise)-half)
      ydata = ydata+ynoise
      sddata = ynoise
      spline_data(1,:)=xdata
      spline_data(2,:)=ydata
      spline_data(3,:)=sddata

      bkpt=(/((i-nord)*delta_b, i=1,nbkpt)/)

! Assign the degree of the polynomial and the knots.
      pointer_bkpt => bkpt
      break_points=s_spline_knots(ndegree, pointer_bkpt)

      icurv=int(one/delta_b)+1

! At first shape the curve to be convex down.
      do i=1,icurv-1
        constraints(i)=spline_constraints &
 (derivative=2, point=bkpt(i+ndegree), type='<=', value=zero)
      end do

! Force a curvature change.
      constraints(icurv)=spline_constraints &
 (derivative=2, point=bkpt(icurv+ndegree), type='==', value=zero)

! Finally, shape the curve to be convex up.
      do i=icurv+1,nbkptin
        constraints(i)=spline_constraints &
 (derivative=2, point=bkpt(i+ndegree), type='>=', value=zero)
      end do

! Make the slope zero and value non-negative at right.
      constraints(nbkptin+1)=spline_constraints &
 (derivative=1, point=bkpt(nord), type='==', value=zero)
      constraints(nbkptin+2)=spline_constraints &
 (derivative=0, point=bkpt(nbkptin+ndegree), type='>=', value=zero)

      coeff = spline_fitting(data=spline_data, knots=break_points, &
              constraints=constraints, covariance=sigma_squared)

!     Compute value, first two derivatives and the variance.
      values=spline_values(0, xdata, break_points, coeff)
      root_variance=spline_values(0, xdata, break_points, coeff, &
                               covariance=sigma_squared)
```

```
      derivat1=spline_values(1, xdata, break_points, coeff)
      derivat2=spline_values(2, xdata, break_points, coeff)

      call show(reshape((/xdata, derivat2, root_variance/),(/ndata,3/)),&
"The x values, 2-nd derivatives, and square root of variance.")

! See that differences are relatively small and the curve has
! the right shape and signs.
      diffs=norm(values-ydata)/norm(ydata)
      if (all(values > zero) .and. all(derivat1 < epsilon(zero))&
         .and. diffs <= tol) then
        write(*,*) 'Example 2 for SPLINE_FITTING is correct.'
      end if

      end
```

Output

```
Example 2 for SPLINE_FITTING is correct.
```

Example 3: Splines Model a Random Number Generator

The function

$$g(x) = \begin{cases} \exp\left(-x^2/2\right), & -1 < x < 1 \\ 0, & |\,x\,| \geq 1 \end{cases}$$

is an unnormalized probability distribution. This function is similar to the standard Normal distribution, with specific choices for the mean and variance, except that it is truncated. Our algorithm interpolates $g(x)$ with a natural cubic spline, $f(x)$. The cumulative distribution is approximated by precise evaluation of the function

$$q(x) = \int_{-1}^{x} f(t)\,dt$$

Gauss-Legendre quadrature formulas, IMSL (1994, pp. 621-626), of order two are used on each polynomial piece of $f(t)$ to evaluate $q(x)$ cheaply. After normalizing the cubic spline so that $q(1) = 1$, we may then generate random numbers according to the distribution $f(x \cong g(x$. The values of x are evaluated by solving $q(x) = u$, $-1 < x < 1$. Here u is a *uniform* random sample. Newton's method, for a vector of unknowns, is used for the solution algorithm. Recalling the relation

$$\frac{d}{dx}\left(q(x) - u\right) = f(x), -1 < x < 1$$

we believe this illustrates a method for generating a vector of random numbers according to a continuous distribution function having finite support.

```
      use spline_fitting_int
      use linear_operators
      use Numerical_Libraries

      implicit none
```

```
! This is Example 3 for SPLINE_FITTING.  Use splines to
! generate random (almost normal) numbers.  The normal distribution
! function has support (-1,+1), and is zero outside this interval.
! The variance is 0.5.

       integer i, niterat
        integer, parameter :: iweight=1, nfix=0, nord=4, ndata=50
        integer, parameter :: nquad=(nord+1)/2, ndegree=nord-1
        integer, parameter :: nbkpt=ndata+2*ndegree, ncoeff=nbkpt-nord
        integer, parameter :: last=nbkpt-ndegree, n_samples=1000
        integer, parameter :: limit=10
       real(kind(1e0)), dimension(n_samples) :: fn, rn, x, alpha_x, beta_x
        INTEGER LEFT_OF(n_samples)
       real(kind(1e0)), parameter :: one=1e0, half=5e-1, zero=0e0, two=2e0
       real(kind(1e0)), parameter :: delta_x=two/(ndata-1)
        real(kind(1e0)), parameter :: qalpha=zero, qbeta=zero, domain=two
        real(kind(1e0)) qx(nquad), qxi(nquad), qw(nquad), qxfix(nquad)
        real(kind(1e0)) alpha_, beta_, quad(0:ndata-1)
        real(kind(1e0)), target :: xdata(ndata), ydata(ndata),&
        coeff(ncoeff), spline_data(3, ndata), bkpt(nbkpt)

        real(kind(1e0)), pointer :: pointer_bkpt(:)
        type (s_spline_knots) break_points
        type (s_spline_constraints) constraints(2)

! Approximate the probability density function by splines.
        xdata = (/(-one+(i-1)*delta_x, i=1,ndata)/)
        ydata = exp(-half*xdata**2)

        spline_data(1,:)=xdata
        spline_data(2,:)=ydata
        spline_data(3,:)=one

        bkpt=(/(-one+(i-nord)*delta_x, i=1,nbkpt)/)

! Assign the degree of the polynomial and the knots.
      pointer_bkpt => bkpt
      break_points=s_spline_knots(ndegree, pointer_bkpt)

! Define the natural derivatives constraints:
        constraints(1)=spline_constraints &
          (derivative=2, point=bkpt(nord), type='==', &
          value=(-one+xdata(1)**2)*ydata(1))
        constraints(2)=spline_constraints &
          (derivative=2, point=bkpt(last), type='==', &
          value=(-one+xdata(ndata)**2)*ydata(ndata))

! Obtain the spline coefficients.
        coeff=spline_fitting(data=spline_data, knots=break_points,&
        constraints=constraints)

! Compute the evaluation points 'qx(*)' and weights 'qw(*)' for
! the Gauss-Legendre quadrature.  This will give a precise
! quadrature for polynomials of degree <= nquad*2.
        call gqrul(nquad, iweight, qalpha, qbeta, nfix, qxfix, qx, qw)

! Compute pieces of the accumulated distribution function:
        quad(0)=zero
       do i=1, ndata-1
          alpha_= (bkpt(nord+i)-bkpt(ndegree+i))*half
          beta_ = (bkpt(nord+i)+bkpt(ndegree+i))*half

! Normalized abscissas are stretched to each spline interval.
! Each polynomial piece is integrated and accumulated.
          qxi = alpha_*qx+beta_
          quad(i) = sum(qw*spline_values(0, qxi, break_points,&
```

```
       coeff))*alpha_&
                  + quad(i-1)
        end do

  ! Normalize the coefficients and partial integrals so that the
  ! total integral has the value one.
         coeff=coeff/quad(ndata-1); quad=quad/quad(ndata-1)
         rn=rand(rn)
         x=zero; niterat=0

        solve_equation: do

  ! Find the intervals where the x values are located.
           LEFT_OF=NDEGREE; I=NDEGREE
             do
                I=I+1; if(I >= LAST) EXIT
                WHERE(x >= BKPT(I))LEFT_OF = LEFT_OF+1
             end do

  ! Use Newton's method to solve the nonlinear equation:
  ! accumulated_distribution_function - random_number = 0.
             alpha_x = (x-bkpt(LEFT_OF))*half
             beta_x  = (x+bkpt(LEFT_OF))*half
             FN=QUAD(LEFT_OF-NORD)-RN
             DO I=1,NQUAD
                FN=FN+QW(I)*spline_values(0, alpha_x*QX(I)+beta_x,&
                      break_points, coeff)*alpha_x
             END DO

  ! This is the Newton method update step:
             x=x-fn/spline_values(0, x, break_points, coeff)
             niterat=niterat+1

  ! Constrain the values so they fall back into the interval.
  ! Newton's method may give approximates outside the interval.
             where(x <= -one .or. x >= one) x=zero

             if(norm(fn,1) <= sqrt(epsilon(one))*norm(x,1))&
               exit solve_equation
         end do solve_equation

  ! Check that Newton's method converges.

         if (niterat <= limit) then
           write (*,*) 'Example 3 for SPLINE_FITTING is correct.'
         end if

       end
```

Output

```
Example 3 for SPLINE_FITTING is correct.
```

Example 4: Represent a Periodic Curve

The curve tracing the edge of a rectangular box, traversed in a counter-clockwise direction, is parameterized with a spline representation for each coordinate function, $(x(t), y(t))$. The functions are constrained to be periodic at the ends of the parameter interval. Since the perimeter arcs are piece-wise linear functions, the degree of the splines is the value one. Some breakpoints are chosen so they correspond to corners of the box, where the derivatives of the coordinate functions are discontinuous. The value of this representation is that for each t the splines representing ($x(t)$, $y(t)$) are points on the perimeter of the box. This “eases” the complexity of evaluating the edge of the box. This example illustrates a method for representing the edge of a domain in two dimensions, bounded by a periodic curve.

```
      use spline_fitting_int
      use norm_int

      implicit none

! This is Example 4 for SPLINE_FITTING. Use piecewise-linear
! splines to represent the perimeter of a rectangular box.

      integer i, j
      integer, parameter :: nbkpt=9, nord=2, ndegree=nord-1, &
               ncoeff=nbkpt-nord, ndata=7, ngrid=100, &
               nvalues=(ndata-1)*ngrid
      real(kind(1e0)), parameter :: zero=0e0, one=1e0
      real(kind(1e0)), parameter ::  delta_t=one, delta_b=one, delta_v=0.01
      real(kind(1e0)) delta_x, delta_y
      real(kind(1e0)), dimension(ndata) ::  sddata=one,  &
! These are redundant coordinates on the edge of the box.
             xdata=(/0.0, 1.0, 2.0, 2.0, 1.0, 0.0, 0.0/), &
             ydata=(/0.0, 0.0, 0.0, 1.0, 1.0, 1.0, 0.0/)
      real(kind(1e0)) tdata(ndata), xspline_data(3, ndata), &
            yspline_data(3, ndata), tvalues(nvalues), &
            xvalues(nvalues), yvalues(nvalues), xcoeff(ncoeff), &
            ycoeff(ncoeff), xcheck(nvalues), ycheck(nvalues), diffs
      real(kind(1e0)), target :: bkpt(nbkpt)
      real(kind(1e0)), pointer :: pointer_bkpt(:)
      type (s_spline_knots) break_points
      type (s_spline_constraints) constraints(1)

      tdata = (/((i-1)*delta_t, i=1,ndata)/)
      xspline_data(1,:)=tdata; yspline_data(1,:)=tdata
      xspline_data(2,:)=xdata; yspline_data(2,:)=ydata
      xspline_data(3,:)=sddata; yspline_data(3,:)=sddata

      bkpt(nord:nbkpt-ndegree)=(/((i-nord)*delta_b,  &
                            i=nord, nbkpt-ndegree)/)
! Collapse the outside knots.
      bkpt(1:ndegree)=bkpt(nord)
      bkpt(nbkpt-ndegree+1:nbkpt)=bkpt(nbkpt-ndegree)

! Assign the degree of the polynomial and the knots.
      pointer_bkpt => bkpt
      break_points=s_spline_knots(ndegree, pointer_bkpt)

! Make the two parametric curves also periodic.
      constraints(1)=spline_constraints &
        (derivative=0, point=bkpt(nord), type='.=.', &
        value=bkpt(nbkpt-ndegree))

      xcoeff = spline_fitting(data=xspline_data, knots=break_points, &
                        constraints=constraints)
      ycoeff = spline_fitting(data=yspline_data, knots=break_points, &
                        constraints=constraints)

! Use the splines to compute the coordinates of points along the perimeter.
! Compare them with the coordinates of the edge points.
      tvalues= (/((i-1)*delta_v, i=1,nvalues)/)
      xvalues=spline_values(0, tvalues, break_points, xcoeff)
      yvalues=spline_values(0, tvalues, break_points, ycoeff)
      do i=1, nvalues
        j=(i-1)/ngrid+1
```

```
          delta_x=(xdata(j+1)-xdata(j))/ngrid
         delta_y=(ydata(j+1)-ydata(j))/ngrid
          xcheck(i)=xdata(j)+mod(i+ngrid-1,ngrid)*delta_x
          ycheck(i)=ydata(j)+mod(i+ngrid-1,ngrid)*delta_y
        end do

        diffs=norm(xvalues-xcheck,1)/norm(xcheck,1)+&
             norm(yvalues-ycheck,1)/norm(ycheck,1)
        if (diffs <= sqrt(epsilon(one))) then
          write(*,*) 'Example 4 for SPLINE_FITTING is correct.'
        end if

        end
```

Output

```
Example 4 for SPLINE_FITTING is correct.
```

SURFACE_CONSTRAINTS

To further shape a surface defined by a tensor product of B-splines, the routine SURFACE_FITTING will least squares fit data with equality, inequality and periodic constraints. These can apply to the surface function or its partial derivatives. Each constraint is packaged in the derived type ?_SURFACE_CONSTRAINTS. This function uses the data consisting of: the place where the constraint is to hold, the partial derivative indices, and the type of the constraint. This object is returned as the derived type function result ?_SURFACE_CONSTRAINTS. The function itself has two required and two optional arguments. In a list of constraints, the *j-th* item will be:

```
?_SURFACE_CONSTRAINTS(j) = &
SURFACE_CONSTRAINTS&
   ([DERIVATIVE=DERIVATIVE_INDEX(1:2),] &
   POINT = WHERE_APPLIED(1:2),[VALUE=VALUE_APPLIED,],&
   TYPE = CONSTRAINT_INDICATOR, &
   [PERIODIC_POINT = PERIODIC_POINT(1:2)])
```

The square brackets enclose optional arguments. For each constraint the arguments 'value =' and 'PERIODIC_POINT =' are not used at the same time.

Required Arguments

POINT = WHERE_APPLIED (Input)
The point in the data domain where a constraint is to be applied. Each point has an ***x*** and ***y*** coordinate, in that order.

TYPE = CONSTRAINT_INDICATOR (Input)
The indicator for the type of constraint the tensor product spline function or its partial derivatives is to satisfy at the point: where_applied. The choices are the character strings '==', '<=', '>=', '.=.', and '.=-'. They respectively indicate that the spline value or its derivatives will be equal to, not greater than, not less than, equal to the value of the spline at another point, or equal to the negative of the spline value at another point. These last two constraints are called *periodic* and *negative-periodic*, respectively.

Optional Arguments

DERIVATIVE = DERIVATIVE_INDEX(1:2) (Input)
These are the number of the partial derivatives for the tensor product spline to apply the constraint. The array (/0,0/) corresponds to the function, the value (/1,0/) to the first partial derivative with respect to *x*, etc. If this argument is not present in the list, the value (/0,0/) is substituted automatically. Thus a constraint without the derivatives listed applies to the tensor product spline function.

PERIODIC = PERIODIC_POINT(1:2)

This optional argument improves readability by identifying the second pair of independent variable values for periodic constraints.

FORTRAN 90 Interface

Generic: CALL SURFACE_CONSTRAINTS (POINT, TYPE [, …])

Specific: The specific interface names are S_SURFACE_CONSTRAINTS and D_SURFACE_CONSTRAINTS.

SURFACE_VALUES

This rank-2 array function returns a tensor product array result, given two arrays of independent variable values. Use the optional input argument for the covariance matrix when the square root of the variance function is evaluated. The result will be a scalar value when the input independent variable is scalar.

Required Arguments

DERIVATIVE = `DERIVATIVE(1:2)` (Input)
The indices of the partial derivative evaluated. Use non-negative integer values. For the function itself use the array `(/0,0/)`.

VARIABLESX = `VARIABLESX` (Input)
The independent variable values in the first or *x* dimension where the spline or its derivatives are evaluated. Either a rank-1 array or a scalar can be used as this argument.

VARIABLESY = `VARIABLESY` (Input)
The independent variable values in the second or *y* dimension where the spline or its derivatives are evaluated. Either a rank-1 array or a scalar can be used as this argument.

KNOTSX = `KNOTSX` (Input)
The derived type `?_spline_knots`, used when the array `coeffs(:,:)` was obtained with the function `SURFACE_FITTING`. This contains the polynomial spline degree and the number of knots and the knots themselves, in the ***x*** dimension.

KNOTSY = `KNOTSY` (Input)
The derived type `?_spline_knots`, used when the array `coeffs(:,:)` was obtained with the function `SURFACE_FITTING`. This contains the polynomial spline degree and the number of knots and the knots themselves, in the *y* dimension.

COEFFS = `C` (Input)
The coefficients in the representation for the spline function,

$$f(x,y) = \sum_{j=1}^{N} \sum_{i=1}^{M} c_{ij} B_i(y) B_j(x)$$

These result from the fitting process or array assignment `C=SURFACE_FITTING(...)`, defined below.

The values $M = size\,(C,1)$ and $N = size\,(C,2)$ satisfies the respective identities $N - 1 + spline\_degree = size\,(?\_knotsx)$, and $M - 1 + spline\_degree = size\,(?\_knotsy)$, where the two rightmost quantities in both equations refer to components of the arguments knotsx and knotsy. The same value of *spline_degree* must be used for both *knotsx* and *knotsy*.

Optional Arguments

COVARIANCE = G (Input)

This argument, when present, results in the evaluation of the square root of the variance function

$$e(x,y) = (b(x,y)^{T} G b(x,y))^{1/2}$$

where

$$b(x,y) = [B_1(x)B_1(y),\ldots,B_N(x)B_N(y),\ldots]^{T}$$

and G is the covariance matrix associated with the coefficients of the spline

$$c = [c_{11},\ldots,c_{N1},\ldots]^{T}$$

The argument G is an optional output from SURFACE_FITTING, described below. When the square root of the variance function is computed, the arguments DERIVATIVE and C are not used.

IOPT = IOPT (Input)

This optional argument, of derived type ?_options, is not used in this release.

FORTRAN 90 Interface

Generic: CALL SURFACE_VALUES (DERIVATIVE, VARIABLESX, VARIABLESY, KNOTSX, KNOTSY, COEFFS [, …])

Specific: The specific interface names are S_SURFACE_VALUES and D_SURFACE_VALUES.

SURFACE_FITTING

Weighted least-squares fitting by tensor product B-splines to discrete two-dimensional data is performed. Constraints on the spline or its partial derivatives are optional. The spline function

$$f(x,y) = \sum_{j=1}^{N} \sum_{i=1}^{M} c_{ij} B_i(y) B_j(x)$$

its derivatives, or the square root of its variance function are evaluated after the fitting.

Required Arguments

DATA = `DATA(1:4,:)` (Input/Output)

An assumed-shape array with `size(data,1) = 4`. The data are placed in the array:

`data(1,i)` = x_i,

`data(2,i)` = y_i,

`data(3,i)` = z_i,

`data(4,i)` = σ_i, $i = 1,\ldots ndata$.

If the variances are not known, but are proportional to an unknown value, use

`data(4,i)` = 1,$i = 1,\ldots ndata$.

KNOTSX = `KNOTSX` (Input)

A derived type, `?_SPLINE_KNOTS`, that defines the degree of the spline and the breakpoints for the data fitting domain, in the first dimension.

KNOTSY = `KNOTSY` (Input)

A derived type, `?_SPLINE_KNOTS`, that defines the degree of the spline and the breakpoints for the data fitting domain, in the second dimension.

Optional Arguments

CONSTRAINTS = `SURFACE_CONSTRAINTS` (Input)

A rank-1 array of derived type `?_SURFACE_CONSTRAINTS` that defines constraints the tensor product spline is to satisfy.

COVARIANCE = G (Output)

An assumed-shape rank-2 array of the same precision as the data. This output is the covariance matrix of the coefficients. It is optionally used to evaluate the square root of the variance function.

IOPT = IOPT(:) (Input/Output)

Derived type array with the same precision as the input array; used for passing optional data to SURFACE_FITTING. The options are as follows:

Packaged Options for SURFACE_FITTING		
Prefix = None	Option Name	Option Value
	SURFACE_FITTING_SMALLNESS	1
	SURFACE_FITTING_FLATNESS	2
	SURFACE_FITTING_TOL_EQUAL	3
	SURFACE_FITTING_TOL_LEAST	4
	SURFACE_FITTING_RESIDUALS	5
	SURFACE_FITTING_PRINT	6
	SURFACE_FITTING_THINNESS	7

IOPT(IO) = ?_OPTIONS&

(surface_fitting_smallnes, ?_value)

This resets the square root of the regularizing parameter multiplying the squared integral of the unknown function. The argument ?_value is replaced by the default value. The default is ?_value = 0.

IOPT(IO) = ?_OPTIONS&

(SURFACE_FITTING_FLATNESS, ?_VALUE)

This resets the square root of the regularizing parameter multiplying the squared integral of the partial derivatives of the unknown function. The argument ?_VALUE is replaced by the default value.

The default is ?_VALUE = SQRT(EPSILON(?_VALUE))*SIZE, where

$$size = \sum |data(3,:)/data(4,:)| / (ndata+1)$$

IOPT(IO) = ?_OPTIONS&

(SURFACE_FITTING_TOL_EQUAL, ?_VALUE)

This resets the value for determining that equality constraint equations are rank-deficient. The default is ?_VALUE = 10^{-4}.

IOPT(IO) = ?_OPTIONS&

`(SURFACE_FITTING_TOL_LEAST, ?_VALUE)`
This resets the value for determining that least-squares equations are rank-deficient. The default is `?_VALUE` = 10^{-4}.

IOPT(IO) = `?_OPTIONS&`

`(SURFACE_FITTING_RESIDUALS, DUMMY)`
This option returns the *residuals* = *surface* - *data*, in `data(4,:)`. That row of the array is overwritten by the residuals. The data is returned in the order of cell processing order, or left-to-right in *x* and then increasing in *y*. The allocation of a temporary for `data(1:4,:)` is avoided, which may be desirable for problems with large amounts of data. The default is to not evaluate the residuals and to leave `data(1:4,:)` as input.

IOPT(IO) = `?_OPTIONS&`

`(SURFACE_FITTING_PRINT, DUMMY)`
This option prints the knots or breakpoints for *x* and *y*, and the count of data points in cell processing order. The default is to not print these arrays.

IOPT(IO) = `?_OPTIONS&`

`(SURFACE_FITTING_THINNESS, ?_VALUE)`
This resets the square root of the regularizing parameter multiplying the squared integral of the second partial derivatives of the unknown function. The argument `?_VALUE` is replaced by the default value. The default is `?_VALUE` = 10^{-3} × `SIZE`, where

$$size = \sum |data(3,:) / data(4,:)| / (ndata + 1)$$

FORTRAN 90 Interface

Generic: `CALL SURFACE_FITTING (DATA, KNOTSX, KNOTSX, KNOTSY [, …])`

Specific: The specific interface names are `S_SURFACE_FITTING` and `D_SURFACE_FITTING`.

Description

The coefficients are obtained by solving a least-squares system of linear algebraic equations, subject to linear equality and inequality constraints. The system is the result of the weighted data equations and regularization. If there are no constraints, the solution is computed using a banded least-squares solver. Details are found in Hanson (1995).

Fatal and Terminal Error Messages

See the *messages.gls* file for error messages for `SURFACE_FITTING`. These error messages are numbered 1151-1152, 1161-1162, 1370-1393.

Examples

Example 1: Tensor Product Spline Fitting of Data

The function

$$g(x,y) = \exp\left(-x^2 - y^2\right)$$

is least-squares fit by a tensor product of cubic splines on the square

$$\left[0,2\right] \otimes \left[0,2\right]$$

There are *ndata* random pairs of values for the independent variables. Each datum is given unit uncertainty. The grid of knots in both *x* and *y* dimensions are equally spaced, in the interior cells, and identical to each other. After the coefficients are computed a check is made that the surface approximately agrees with *g*(*x*,*y*) at a tensor product grid of equally spaced values.

```
      USE surface_fitting_int
      USE rand_int
      USE norm_int

      implicit none

! This is Example 1 for SURFACE_FITTING, tensor product
! B-splines approximation.  Use the function
! exp(-x**2-y**2) on the square (0, 2) x (0, 2) for samples.
! The spline order is "nord" and the number of cells is
! "(ngrid-1)**2".  There are "ndata" data values in the square.

      integer :: i
      integer, parameter :: ngrid=9, nord=4, ndegree=nord-1, &
        nbkpt=ngrid+2*ndegree, ndata = 2000, nvalues=100
      real(kind(1d0)), parameter :: zero=0d0, one=1d0, two=2d0
      real(kind(1d0)), parameter :: TOLERANCE=1d-3
      real(kind(1d0)), target :: spline_data (4, ndata), bkpt(nbkpt), &
              coeff(ngrid+ndegree-1,ngrid+ndegree-1), delta, sizev, &
              x(nvalues), y(nvalues), values(nvalues, nvalues)

      real(kind(1d0)), pointer :: pointer_bkpt(:)
      type (d_spline_knots) knotsx, knotsy

! Generate random (x,y) pairs and evaluate the
! example exponential function at these values.
      spline_data(1:2,:)=two*rand(spline_data(1:2,:))
      spline_data(3,:)=exp(-sum(spline_data(1:2,:)**2,dim=1))
      spline_data(4,:)=one

! Define the knots for the tensor product data fitting problem.
```

```
          delta = two/(ngrid-1)
          bkpt(1:ndegree) = zero
          bkpt(nbkpt-ndegree+1:nbkpt) =  two
          bkpt(nord:nbkpt-ndegree)=(/(i*delta,i=0,ngrid-1)/)

! Assign the degree of the polynomial and the knots.
      pointer_bkpt => bkpt
      knotsx=d_spline_knots(ndegree, pointer_bkpt)
      knotsy=knotsx

! Fit the data and obtain the coefficients.
      coeff = surface_fitting(spline_data, knotsx, knotsy)

! Evaluate the residual = spline - function
! at a grid of points inside the square.
      delta=two/(nvalues+1)
      x=(/(i*delta,i=1,nvalues)/); y=x

      values=exp(-spread(x**2,1,nvalues)-spread(y**2,2,nvalues))
      values=surface_values((/0,0/), x, y, knotsx, knotsy, coeff)-&
             values

! Compute the R.M.S. error:
      sizev=norm(pack(values, (values == values)))/nvalues

      if (sizev <= TOLERANCE) then
        write(*,*) 'Example 1 for SURFACE_FITTING is correct.'
      end if
      end
```

Output

```
Example 1 for SURFACE_FITTING is correct.
```

Example 2: Parametric Representation of a Sphere

From Struik (1961), the parametric representation of points (*x,y,z*) on the surface of a sphere of radius $a > 0$ is expressed in terms of *spherical coordinates*,

$$x(u,v) = a\cos(u)\cos(v), -\pi \le 2u \le \pi$$
$$y(u,v) = a\cos(u)\sin(v), -\pi \le v \le \pi$$
$$z(u,v) = a\sin(u)$$

The parameters are radians of *latitude* (u) and *longitude* (v). The example program fits the same $ndata$ random pairs of latitude and longitude in each coordinate. We have covered the sphere twice by allowing:

$$-\pi \le u \le \pi$$

for latitude. We solve three data fitting problems, one for each coordinate function. Periodic constraints on the value of the spline are used for both u and v. We could reduce the computational effort by fitting a spline function in one variable for the z coordinate. To illustrate the representation of more general surfaces than spheres, we did not do this. When the surface is evaluated we compute latitude, moving from the South Pole to the North Pole,

$$-\pi \le 2u \le \pi$$

Our surface will approximately satisfy the equality

$$x^2 + y^2 + z^2 = a^2$$

These residuals are checked at a rectangular mesh of latitude and longitude pairs. To illustrate the use of some options, we have reset the three regularization parameters to the value zero, the least-squares system tolerance to a smaller value than the default, and obtained the residuals for each parametric coordinate function at the data points.

```
      USE surface_fitting_int
      USE rand_int
      USE norm_int
      USE Numerical_Libraries

      implicit none

! This is Example 2 for SURFACE_FITTING, tensor product
! B-splines approximation.  Fit x, y, z parametric functions
! for points on the surface of a sphere of radius "A".
! Random values of latitude and longitude are used to generate
! data.  The functions are evaluated at a rectangular grid
! in latitude and longitude and checked to lie on the surface
! of the sphere.

      integer :: i, j
      integer, parameter :: ngrid=6, nord=6, ndegree=nord-1, &
        nbkpt=ngrid+2*ndegree, ndata =1000, nvalues=50, NOPT=5
      real(kind(1d0)), parameter :: zero=0d0, one=1d0, two=2d0
      real(kind(1d0)), parameter :: TOLERANCE=1d-2
      real(kind(1d0)), target :: spline_data (4, ndata, 3), bkpt(nbkpt), &
              coeff(ngrid+ndegree-1,ngrid+ndegree-1, 3), delta, sizev, &
              pi, A, x(nvalues), y(nvalues), values(nvalues, nvalues), &
              data(4,ndata)

      real(kind(1d0)), pointer :: pointer_bkpt(:)
      type (d_spline_knots) knotsx, knotsy
      type (d_options) OPTIONS(NOPT)

! Get the constant "pi" and a random radius, > 1.
      pi = DCONST("pi"); A=one+rand(A)

! Generate random (latitude, longitude) pairs and evaluate the
! surface parameters at these points.
      spline_data(1:2,:,1)=pi*(two*rand(spline_data(1:2,:,1))-one)
      spline_data(1:2,:,2)=spline_data(1:2,:,1)
      spline_data(1:2,:,3)=spline_data(1:2,:,1)

! Evaluate x, y, z parametric points.
      spline_data(3,:,1)=A*cos(spline_data(1,:,1))*cos(spline_data(2,:,1))
      spline_data(3,:,2)=A*cos(spline_data(1,:,2))*sin(spline_data(2,:,2))
      spline_data(3,:,3)=A*sin(spline_data(1,:,3))

! The values are equally uncertain.
      spline_data(4,:,:)=one

! Define the knots for the tensor product data fitting problem.
      delta = two*pi/(ngrid-1)
      bkpt(1:ndegree) = -pi
      bkpt(nbkpt-ndegree+1:nbkpt) =  pi
      bkpt(nord:nbkpt-ndegree)=(/(-pi+i*delta,i=0,ngrid-1)/)
```

```
! Assign the degree of the polynomial and the knots.
      pointer_bkpt => bkpt
      knotsx=d_spline_knots(ndegree, pointer_bkpt)
      knotsy=knotsx

! Fit a data surface for each coordinate.
! Set default regularization parameters to zero and compute
! residuals of the individual points. These are returned
! in DATA(4,:).
      do j=1,3
        data=spline_data(:,:,j)
      OPTIONS(1)=d_options(surface_fitting_thinness,zero)
      OPTIONS(2)=d_options(surface_fitting_flatness,zero)
      OPTIONS(3)=d_options(surface_fitting_smallness,zero)
      OPTIONS(4)=d_options(surface_fitting_tol_least,1d-5)
      OPTIONS(5)=surface_fitting_residuals
      coeff(:,:,j) = surface_fitting(data, knotsx, knotsy,&
           IOPT=OPTIONS)
      end do

! Evaluate the function at a grid of points inside the rectangle of
! latitude and longitude covering the sphere just once.  Add the
! sum of squares. They should equal "A**2" but will not due to
! truncation and rounding errors.
      delta=pi/(nvalues+1)
      x=(/(-pi/two+i*delta,i=1,nvalues)/); y=two*x
      values=zero
      do j=1,3
        values=values+&
        surface_values((/0,0/), x, y, knotsx, knotsy, coeff(:,:,j))**2
      end do
      values=values-A**2
! Compute the R.M.S. error:

      sizev=norm(pack(values, (values == values)))/nvalues

      if (sizev <= TOLERANCE) then
        write(*,*) "Example 2 for SURFACE_FITTING is correct."
      end if
      end
```

Output

```
Example 2 for SURFACE_FITTING is correct.
```

Example 3: Constraining Some Points using a Spline Surface

This example illustrates the use of discrete constraints to shape the surface. The data fitting problem of Example 1 is modified by requiring that the surface interpolate the value one at $x = y = 0$. The shape is constrained so first partial derivatives in both x and y are zero at $x = y = 0$. These constraints mimic some properties of the function $g(x,y)$. The size of the residuals at a grid of points and the residuals of the constraints are checked.

```
      USE surface_fitting_int
      USE rand_int
      USE norm_int

      implicit none

! This is Example 3 for SURFACE_FITTING, tensor product
! B-splines approximation, f(x,y).  Use the function
```

```
! exp(-x**2-y**2) on the square (0, 2) x (0, 2) for samples.
! The spline order is "nord" and the number of cells is
! "(ngrid-1)**2".  There are "ndata" data values in the square.
! Constraints are put on the surface at (0,0).  Namely
! f(0,0) = 1, f_x(0,0) = 0, f_y(0,0) = 0.

      integer :: i
      integer, parameter :: ngrid=9, nord=4, ndegree=nord-1, &
        nbkpt=ngrid+2*ndegree, ndata = 2000, nvalues=100, NC = 3
      real(kind(1d0)), parameter :: zero=0d0, one=1d0, two=2d0
      real(kind(1d0)), parameter :: TOLERANCE=1d-3
      real(kind(1d0)), target :: spline_data (4, ndata), bkpt(nbkpt), &
             coeff(ngrid+ndegree-1,ngrid+ndegree-1), delta, sizev, &
             x(nvalues), y(nvalues), values(nvalues, nvalues), &
             f_00, f_x00, f_y00

      real(kind(1d0)), pointer :: pointer_bkpt(:)
      type (d_spline_knots) knotsx, knotsy
      type (d_surface_constraints) C(NC)
      LOGICAL PASS

! Generate random (x,y) pairs and evaluate the
! example exponential function at these values.
      spline_data(1:2,:)=two*rand(spline_data(1:2,:))
      spline_data(3,:)=exp(-sum(spline_data(1:2,:)**2,dim=1))
      spline_data(4,:)=one

! Define the knots for the tensor product data fitting problem.
         delta = two/(ngrid-1)
         bkpt(1:ndegree) = zero
         bkpt(nbkpt-ndegree+1:nbkpt) =  two
         bkpt(nord:nbkpt-ndegree)=(/(i*delta,i=0,ngrid-1)/)

! Assign the degree of the polynomial and the knots.
      pointer_bkpt => bkpt
      knotsx=d_spline_knots(ndegree, pointer_bkpt)
      knotsy=knotsx

! Define the constraints for the fitted surface.
     C(1)=surface_constraints(point=(/zero,zero/),type='==',value=one)
     C(2)=surface_constraints(derivative=(/1,0/),&
          point=(/zero,zero/),type='==',value=zero)
     C(3)=surface_constraints(derivative=(/0,1/),&
          point=(/zero,zero/),type='==',value=zero)

! Fit the data and obtain the coefficients.

      coeff = surface_fitting(spline_data, knotsx, knotsy,&
              CONSTRAINTS=C)

! Evaluate the residual = spline - function
! at a grid of points inside the square.
      delta=two/(nvalues+1)
      x=(/(i*delta,i=1,nvalues)/); y=x

      values=exp(-spread(x**2,1,nvalues)-spread(y**2,2,nvalues))
      values=surface_values((/0,0/), x, y, knotsx, knotsy, coeff)-&
             values
      f_00 = surface_values((/0,0/), zero, zero,  knotsx, knotsy, coeff)
      f_x00= surface_values((/1,0/), zero, zero,  knotsx, knotsy, coeff)
      f_y00= surface_values((/0,1/), zero, zero,  knotsx, knotsy, coeff)

! Compute the R.M.S. error:
      sizev=norm(pack(values, (values == values)))/nvalues
      PASS = sizev <= TOLERANCE
      PASS = abs (f_00 - one) <= sqrt(epsilon(one)) .and. PASS
```

```
       PASS = f_x00 <= sqrt(epsilon(one)) .and. PASS
       PASS = f_y00 <= sqrt(epsilon(one)) .and. PASS

       if (PASS) then
         write(*,*) 'Example 3 for SURFACE_FITTING is correct.'
       end if
       end
```

Output

```
 Example 3 for SURFACE_FITTING is correct.
```

Example 4: Constraining a Spline Surface to be non-Negative

The review of interpolating methods by Franke (1982) uses a test data set originally due to James Ferguson. We use this data set of 25 points, with unit uncertainty for each dependent variable. Our algorithm does not interpolate the data values but approximately fits them in the least-squares sense. We reset the regularization parameter values of *flatness* and *thinness*, Hanson (1995). Then the surface is fit to the data and evaluated at a grid of points. Although the surface appears smooth and fits the data, the values are negative near one corner. Our scenario for the application assumes that the surface be non-negative at all points of the rectangle containing the independent variable data pairs. Our algorithm for constraining the surface is simple but effective in this case. The data fitting is repeated one more time but with positive constraints at the grid of points where it was previously negative.

```
       USE surface_fitting_int
       USE rand_int
       USE surface_fitting_int
       USE rand_int
       USE norm_int

       implicit none

 ! This is Example 4 for SURFACE_FITTING, tensor product
 ! B-splines approximation, f(x,y).  Use the data set from
 ! Franke, due to Ferguson.  Without constraints the function
 ! becomes negative in a corner.  Constrain the surface
 ! at a grid of values so it is non-negative.

       integer :: i, j, q
       integer, parameter :: ngrid=9, nord=4, ndegree=nord-1, &
         nbkpt=ngrid+2*ndegree, ndata = 25, nvalues=50
       real(kind(1d0)), parameter :: zero=0d0, one=1d0
       real(kind(1d0)), parameter :: TOLERANCE=1d-3
       real(kind(1d0)), target :: spline_data (4, ndata), bkptx(nbkpt), &
              bkpty(nbkpt),coeff(ngrid+ndegree-1,ngrid+ndegree-1), &
              x(nvalues), y(nvalues), values(nvalues, nvalues), &
              delta
       real(kind(1d0)), pointer :: pointer_bkpt(:)
       type (d_spline_knots) knotsx, knotsy
       type (d_surface_constraints), allocatable :: C(:)

       real(kind(1e0)) :: data (3*ndata) = & ! This is Ferguson's data:
 (/2.0   ,  15.0  ,    2.5 ,      2.49 ,     7.647,     3.2,&
   2.981 ,   0.291,    3.4 ,      3.471,    -7.062,     3.5,&
   3.961 , -14.418,    3.5 ,      7.45 ,    12.003,     2.5,&
   7.35  ,   6.012,    3.5 ,      7.251,     0.018,     3.0,&
   7.151 ,  -5.973,    2.0 ,      7.051,   -11.967,     2.5,&
   10.901,   9.015,    2.0 ,     10.751,     4.536,     1.925,&
```

```
   10.602,   0.06 ,    1.85,     10.453,    -4.419,    1.576,&
   10.304,  -8.895,    1.7 ,     14.055,    10.509,    1.5,&
   14.194,   6.783,    1.3 ,     14.331,     3.054,    1.7,&
   14.469,  -0.672,    2.1 ,     14.607,    -4.398,    1.75,&
   15.0  ,  12.0  ,    0.5 ,     15.729,     8.067,    0.5,&
   16.457,   4.134,    0.7 ,     17.185,     0.198,    1.1,&
   17.914,  -3.735,    1.7/)

       spline_data(1:3,:)=reshape(data,(/3,ndata/)); spline_data(4,:)=one

 ! Define the knots for the tensor product data fitting problem.
 ! Use the data limits to  the knot sequences.
          bkptx(1:ndegree) = minval(spline_data(1,:))
          bkptx(nbkpt-ndegree+1:nbkpt) =  maxval(spline_data(1,:))
          delta=(bkptx(nbkpt)-bkptx(ndegree))/(ngrid-1)
          bkptx(nord:nbkpt-ndegree)=(/(bkptx(1)+i*delta,i=0,ngrid-1)/)

 ! Assign the degree of the polynomial and the knots for x.
       pointer_bkpt => bkptx
       knotsx=d_spline_knots(ndegree, pointer_bkpt)
          bkpty(1:ndegree) = minval(spline_data(2,:))
          bkpty(nbkpt-ndegree+1:nbkpt) =  maxval(spline_data(2,:))
          delta=(bkpty(nbkpt)-bkpty(ndegree))/(ngrid-1)
          bkpty(nord:nbkpt-ndegree)=(/(bkpty(1)+i*delta,i=0,ngrid-1)/)

 ! Assign the degree of the polynomial and the knots for y.
       pointer_bkpt => bkpty
       knotsy=d_spline_knots(ndegree, pointer_bkpt)

 ! Fit the data and obtain the coefficients.
       coeff = surface_fitting(spline_data, knotsx, knotsy)

       delta=(bkptx(nbkpt)-bkptx(1))/(nvalues+1)
       x=(/(bkptx(1)+i*delta,i=1,nvalues)/)
       delta=(bkpty(nbkpt)-bkpty(1))/(nvalues+1)
       y=(/(bkpty(1)+i*delta,i=1,nvalues)/)

 ! Evaluate the function at a rectangular grid.
 ! Use non-positive values to  a constraint.
       values=surface_values((/0,0/), x, y, knotsx, knotsy, coeff)

 ! Count the number of values <= zero.  Then constrain the spline
 ! so that it is >= TOLERANCE at those points where it was <= zero.
       q=count(values <= zero)
       allocate (C(q))
       DO I=1,nvalues
          DO J=1,nvalues
            IF(values(I,J) <= zero) THEN
              C(q)=surface_constraints(point=(/x(i),y(j)/), type='>=',&
                   value=TOLERANCE)
              q=q-1
            END IF
          END DO
       END DO

 ! Fit the data with constraints and obtain the coefficients.
       coeff = surface_fitting(spline_data, knotsx, knotsy,&
               CONSTRAINTS=C)
       deallocate(C)

 ! Evaluate the surface at a grid and check, once again, for
 ! non-positive values.  All values should now be positive.
       values=surface_values((/0,0/), x, y, knotsx, knotsy, coeff)
 if (count(values <= zero) == 0) then
         write(*,*) 'Example 4 for SURFACE_FITTING is correct.'
       end if
```

```
        end
```

Output

```
Example 4 for SURFACE_FITTING is correct.
```

CSIEZ

Computes the cubic spline interpolant with the 'not-a-knot' condition and return values of the interpolant at specified points.

Required Arguments

XDATA — Array of length NDATA containing the data point abscissas. (Input)
The data point abscissas must be distinct.

FDATA — Array of length NDATA containing the data point ordinates. (Input)

XVEC — Array of length N containing the points at which the spline is to be evaluated. (Input)

VALUE — Array of length N containing the values of the spline at the points in XVEC. (Output)

Optional Arguments

NDATA — Number of data points. (Input)
NDATA must be at least 2.
Default: NDATA = size (XDATA,1).

N — Length of vector XVEC. (Input)
Default: N = size (XVEC,1).

FORTRAN 90 Interface

Generic: CALL CSIEZ (XDATA, FDATA, XVEC, VALUE [, …])

Specific: The specific interface names are S_CSIEZ and D_CSIEZ.

FORTRAN 77 Interface

Single: CALL CSIEZ (NDATA, XDATA, FDATA, N, XVEC, VALUE)

Double: The double precision name is DCSIEZ.

Description

This routine is designed to let the user easily compute the values of a cubic spline interpolant. The routine CSIEZ computes a spline interpolant to a set of data points (x_i, f_i) for $i = 1, \ldots,$ NDATA. The output for this routine consists of a vector of values of the computed cubic spline. Specifically, let $n = N$, v = XVEC, and y = VALUE, then if s is the computed spline we set

$$y_j = s(v_j) \quad j = 1, \ldots, n$$

Additional documentation can be found by referring to the IMSL routines CSINT or SPLEZ.

Comments

Workspace may be explicitly provided, if desired, by use of C2IEZ/DC2IEZ. The reference is:

CALL C2IEZ (NDATA, XDATA, FDATA, N, XVEC, VALUE, IWK, WK1, WK2)

The additional arguments are as follows:

IWK — Integer work array of length MAX0(N, NDATA) + N.

WK1 — Real work array of length 5 * NDATA.

WK2 — Real work array of length 2 * N.

Example

In this example, a cubic spline interpolant to a function *F* is computed. The values of this spline are then compared with the exact function values.

```
      USE CSIEZ_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    NDATA
      PARAMETER  (NDATA=11)
!
      INTEGER    I, NOUT
      REAL       F, FDATA(NDATA), FLOAT, SIN, VALUE(2*NDATA-1), X,&
                 XDATA(NDATA), XVEC(2*NDATA-1)
      INTRINSIC  FLOAT, SIN
!                                  Define function
      F(X) = SIN(15.0*X)
!                                  Set up a grid
      DO 10  I=1, NDATA
         XDATA(I) = FLOAT(I-1)/FLOAT(NDATA-1)
         FDATA(I) = F(XDATA(I))
   10 CONTINUE
      DO 20  I=1, 2*NDATA - 1
         XVEC(I) = FLOAT(I-1)/FLOAT(2*NDATA-2)
   20 CONTINUE
!                                  Compute cubic spline interpolant
      CALL CSIEZ (XDATA, FDATA, XVEC, VALUE)
!                                  Get output unit number
```

```
      CALL UMACH (2, NOUT)
!                                  Write heading
      WRITE (NOUT,99998)
99998 FORMAT (13X, 'X', 9X, 'INTERPOLANT', 5X, 'ERROR')
!                                  Print the interpolant and the error
!                                  on a finer grid
      DO 30  I=1, 2*NDATA - 1
         WRITE (NOUT,99999) XVEC(I), VALUE(I), F(XVEC(I)) - VALUE(I)
   30 CONTINUE
99999 FORMAT(' ', 2F15.3, F15.6)
      END
```

Output

```
  X         INTERPOLANT     ERROR
0.000          0.000       0.000000
0.050          0.809      -0.127025
0.100          0.997       0.000000
0.150          0.723       0.055214
0.200          0.141       0.000000
0.250         -0.549      -0.022789
0.300         -0.978       0.000000
0.350         -0.843      -0.016246
0.400         -0.279       0.000000
0.450          0.441       0.009348
0.500          0.938       0.000000
0.550          0.903       0.019947
0.600          0.412       0.000000
0.650         -0.315      -0.004895
0.700         -0.880       0.000000
0.750         -0.938      -0.029541
0.800         -0.537       0.000000
0.850          0.148       0.034693
0.900          0.804       0.000000
0.950          1.086      -0.092559
1.000          0.650       0.000000
```

CSINT

Computes the cubic spline interpolant with the 'not-a-knot' condition.

Required Arguments

XDATA — Array of length NDATA containing the data point abscissas. (Input)
The data point abscissas must be distinct.

FDATA — Array of length NDATA containing the data point ordinates. (Input)

BREAK — Array of length NDATA containing the breakpoints for the piecewise cubic representation. (Output)

CSCOEF — Matrix of size 4 by NDATA containing the local coefficients of the cubic pieces. (Output)

Optional Arguments

NDATA — Number of data points. (Input)
NDATA must be at least 2.
Default: NDATA = size (XDATA,1).

FORTRAN 90 Interface

Generic:	CALL CSINT (XDATA, FDATA, BREAK, CSCOEF [, …])
Specific:	The specific interface names are S_CSINT and D_CSINT.

FORTRAN 77 Interface

Single:	CALL CSINT (NDATA, XDATA, FDATA, BREAK, CSCOEF)
Double:	The double precision name is DCSINT.

Description

The routine CSINT computes a C^2 cubic spline interpolant to a set of data points (x_i, f_i) for $i = 1, \ldots,$ NDATA = N. The breakpoints of the spline are the abscissas. Endpoint conditions are automatically determined by the program. These conditions correspond to the "not-a-knot" condition (see de Boor 1978), which requires that the third derivative of the spline be continuous at the second and next-to-last breakpoint. If N is 2 or 3, then the linear or quadratic interpolating polynomial is computed, respectively.

If the data points arise from the values of a smooth (say C^4) function f, i.e. $f_i = f(x_i)$, then the error will behave in a predictable fashion. Let ξ be the breakpoint vector for the above spline interpolant. Then, the maximum absolute error satisfies

$$\left\| f - s \right\|_{[\xi_1, \xi_N]} \le C \left\| f^{(4)} \right\|_{[\xi_1, \xi_N]} |\xi|^4$$

where

$$|\xi| := \max_{i = 2, \ldots, N} |\xi_i - \xi_{i-1}|$$

For more details, see de Boor (1978, pages 55– 56).

Comments

1. Workspace may be explicitly provided, if desired, by use of C2INT/DC2INT. The reference is:

   CALL C2INT (NDATA, XDATA, FDATA, BREAK, CSCOEF, IWK)

   The additional argument is

   IWK — Work array of length NDATA.

2. The cubic spline can be evaluated using CSVAL; its derivative can be evaluated using CSDER.

3. Note that column NDATA of CSCOEF is used as workspace.

Example

In this example, a cubic spline interpolant to a function F is computed. The values of this spline are then compared with the exact function values.

```
      USE CSINT_INT
      USE UMACH_INT
      USE CSVAL_INT

      IMPLICIT   NONE
```

```
!                                  Specifications
      INTEGER    NDATA
      PARAMETER  (NDATA=11)
!
      INTEGER    I, NINTV, NOUT
      REAL       BREAK(NDATA), CSCOEF(4,NDATA), F,&
                 FDATA(NDATA), FLOAT, SIN, X, XDATA(NDATA)
      INTRINSIC  FLOAT, SIN
!                                  Define function
      F(X) = SIN(15.0*X)
!                                  Set up a grid
      DO 10  I=1, NDATA
         XDATA(I) = FLOAT(I-1)/FLOAT(NDATA-1)
         FDATA(I) = F(XDATA(I))
   10 CONTINUE
!                                  Compute cubic spline interpolant
      CALL CSINT (XDATA, FDATA, BREAK, CSCOEF)
!                                  Get output unit number.
      CALL UMACH (2, NOUT)
!                                  Write heading
      WRITE (NOUT,99999)
99999 FORMAT (13X, 'X', 9X, 'Interpolant', 5X, 'Error')
      NINTV = NDATA - 1
!                                  Print the interpolant and the error
!                                  on a finer grid
      DO 20  I=1, 2*NDATA - 1
         X = FLOAT(I-1)/FLOAT(2*NDATA-2)
         WRITE (NOUT,'(2F15.3,F15.6)') X, CSVAL(X,BREAK,CSCOEF),&
                                      F(X) - CSVAL(X,BREAK,&
                                      CSCOEF)
   20 CONTINUE
      END
```

Output

```
   X          Interpolant     Error
0.000           0.000       0.000000
0.050           0.809      -0.127025
0.100           0.997       0.000000
0.150           0.723       0.055214
0.200           0.141       0.000000
0.250          -0.549      -0.022789
0.300          -0.978       0.000000
0.350          -0.843      -0.016246
0.400          -0.279       0.000000
0.450           0.441       0.009348
0.500           0.938       0.000000
0.550           0.903       0.019947
0.600           0.412       0.000000
0.650          -0.315      -0.004895
0.700          -0.880       0.000000
0.750          -0.938      -0.029541
0.800          -0.537       0.000000
0.850           0.148       0.034693
0.900           0.804       0.000000
0.950           1.086      -0.092559
1.000           0.650       0.000000
```

CSDEC

Computes the cubic spline interpolant with specified derivative endpoint conditions.

Required Arguments

XDATA — Array of length NDATA containing the data point abscissas. (Input) The data point abscissas must be distinct.

FDATA — Array of length NDATA containing the data point ordinates. (Input)

ILEFT — Type of end condition at the left endpoint. (Input)

ILEFT	Condition
0	"Not-a-knot" condition
1	First derivative specified by DLEFT
2	Second derivative specified by DLEFT

DLEFT — Derivative at left endpoint if ILEFT is equal to 1 or 2. (Input)
If ILEFT = 0, then DLEFT is ignored.

IRIGHT — Type of end condition at the right endpoint. (Input)

IRIGHT	Condition
0	"Not-a-knot" condition
1	First derivative specified by DRIGHT
2	Second derivative specified by DRIGHT

DRIGHT — Derivative at right endpoint if IRIGHT is equal to 1 or 2. (Input) If IRIGHT = 0 then DRIGHT is ignored.

BREAK — Array of length NDATA containing the breakpoints for the piecewise cubic representation. (Output)

CSCOEF — Matrix of size 4 by NDATA containing the local coefficients of the cubic pieces. (Output)

Optional Arguments

NDATA — Number of data points. (Input)
Default: `NDATA` = size (`XDATA`,1).

FORTRAN 90 Interface

Generic: `CALL CSDEC (XDATA, FDATA, ILEFT, DLEFT, IRIGHT, DRIGHT, BREAK, CSCOEF [, …])`

Specific: The specific interface names are `S_CSDEC` and `D_CSDEC`.

FORTRAN 77 Interface

Single: `CALL CSDEC (NDATA, XDATA, FDATA, ILEFT, DLEFT, IRIGHT, DRIGHT, BREAK, CSCOEF)`

Double: The double precision name is `DCSDEC`.

Description

The routine `CSDEC` computes a C^2 cubic spline interpolant to a set of data points (x_i, f_i) for $i = 1, \ldots,$ `NDATA` $= N$. The breakpoints of the spline are the abscissas. Endpoint conditions are to be selected by the user. The user may specify not-a-knot, first derivative, or second derivative at each endpoint (see de Boor 1978, Chapter 4).

If the data (including the endpoint conditions) arise from the values of a smooth (say C^4) function f, i.e. $f_i = f(x_i)$, then the error will behave in a predictable fashion. Let ξ be the breakpoint vector for the above spline interpolant. Then, the maximum absolute error satisfies

$$\|f - s\|_{[\xi_1, \xi_N]} \le C \left\| f^{(4)} \right\|_{[\xi_1, \xi_N]} |\xi|^4$$

where

$$|\xi| := \max_{i = 2, \ldots, N} |\xi_i - \xi_{i-1}|$$

For more details, see de Boor (1978, Chapter 4 and 5).

Comments

1. Workspace may be explicitly provided, if desired, by use of `C2DEC`/`DC2DEC`. The reference is:

```
CALL C2DEC (NDATA, XDATA, FDATA, ILEFT, DLEFT, IRIGHT,
   DRIGHT, BREAK, CSCOEF, IWK)
```

The additional argument is:

IWK — Work array of length `NDATA`.

2. The cubic spline can be evaluated using `CSVAL`; its derivative can be evaluated using `CSDER`.

3. Note that column `NDATA` of `CSCOEF` is used as workspace.

Examples

Example 1

In Example 1, a cubic spline interpolant to a function *f* is computed. The value of the derivative at the left end-point and the value of the second derivative at the right endpoint are specified. The values of this spline are then compared with the exact function values.

```
      USE CSDEC_INT
      USE UMACH_INT
      USE CSVAL_INT

      IMPLICIT   NONE
      INTEGER    ILEFT, IRIGHT, NDATA
      PARAMETER  (ILEFT=1, IRIGHT=2, NDATA=11)
!
      INTEGER    I, NINTV, NOUT
      REAL       BREAK(NDATA), COS, CSCOEF(4,NDATA), DLEFT,&
                 DRIGHT, F, FDATA(NDATA), FLOAT, SIN, X, XDATA(NDATA)
      INTRINSIC  COS, FLOAT, SIN
!                                  Define function
      F(X) = SIN(15.0*X)
!                                  Initialize DLEFT and DRIGHT
      DLEFT  = 15.0*COS(15.0*0.0)
      DRIGHT = -15.0*15.0*SIN(15.0*1.0)
!                                  Set up a grid
      DO 10  I=1, NDATA
         XDATA(I) = FLOAT(I-1)/FLOAT(NDATA-1)
         FDATA(I) = F(XDATA(I))
   10 CONTINUE
!                                  Compute cubic spline interpolant
      CALL CSDEC (XDATA, FDATA, ILEFT, DLEFT, IRIGHT, &
                  DRIGHT, BREAK, CSCOEF)
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Write heading
      WRITE (NOUT,99999)
99999 FORMAT (13X, 'X', 9X, 'Interpolant', 5X, 'Error')
      NINTV = NDATA - 1
!                                  Print the interpolant on a finer grid
      DO 20  I=1, 2*NDATA - 1
         X = FLOAT(I-1)/FLOAT(2*NDATA-2)
         WRITE (NOUT,'(2F15.3,F15.6)') X, CSVAL(X,BREAK,CSCOEF),&
                                    F(X) - CSVAL(X,BREAK,&
                                    CSCOEF)
   20 CONTINUE
      END
```

Output

```
   X         Interpolant     Error
0.000          0.000       0.000000
0.050          0.675       0.006332
0.100          0.997       0.000000
0.150          0.759       0.019485
0.200          0.141       0.000000
0.250         -0.558      -0.013227
0.300         -0.978       0.000000
0.350         -0.840      -0.018765
0.400         -0.279       0.000000
0.450          0.440       0.009859
0.500          0.938       0.000000
0.550          0.902       0.020420
0.600          0.412       0.000000
0.650         -0.312      -0.007301
0.700         -0.880       0.000000
0.750         -0.947      -0.020391
0.800         -0.537       0.000000
0.850          0.182       0.000497
0.900          0.804       0.000000
0.950          0.959       0.035074
1.000          0.650       0.000000
```

Example 2

In Example 2, we compute the *natural* cubic spline interpolant to a function *f* by forcing the second derivative of the interpolant to be zero at both endpoints. As in the previous example, we compare the exact function values with the values of the spline.

```
      USE CSDEC_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    ILEFT, IRIGHT, NDATA, NOUT
      PARAMETER  (ILEFT=2, IRIGHT=2, NDATA=11)
!
      INTEGER    I, NINTV
      REAL       BREAK(NDATA), CSCOEF(4,NDATA), DLEFT, DRIGHT,&
                 F, FDATA(NDATA), FLOAT, SIN, X, XDATA(NDATA), CSVAL
      INTRINSIC  FLOAT, SIN
!                                  Initialize DLEFT and DRIGHT
      DATA DLEFT/0./, DRIGHT/0./
!                                  Define function
      F(X) = SIN(15.0*X)
!                                  Set up a grid
      DO 10  I=1, NDATA
         XDATA(I) = FLOAT(I-1)/FLOAT(NDATA-1)
         FDATA(I) = F(XDATA(I))
   10 CONTINUE
!                                  Compute cubic spline interpolant
      CALL CSDEC (XDATA, FDATA, ILEFT, DLEFT, IRIGHT, DRIGHT,&
                  BREAK, CSCOEF)
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Write heading
      WRITE (NOUT,99999)
99999 FORMAT (13X, 'X', 9X, 'Interpolant', 5X, 'Error')
      NINTV = NDATA - 1
!                                  Print the interpolant on a finer grid
      DO 20  I=1, 2*NDATA - 1
```

```
         X = FLOAT(I-1)/FLOAT(2*NDATA-2)
         WRITE (NOUT,'(2F15.3,F15.6)') X, CSVAL(X,BREAK,CSCOEF),&
                                       F(X) - CSVAL(X,BREAK,&
                                       CSCOEF)
   20 CONTINUE
      END
```

Output

```
     X          Interpolant      Error
  0.000           0.000       0.000000
  0.050           0.667       0.015027
  0.100           0.997       0.000000
  0.150           0.761       0.017156
  0.200           0.141       0.000000
  0.250          -0.559      -0.012609
  0.300          -0.978       0.000000
  0.350          -0.840      -0.018907
  0.400          -0.279       0.000000
  0.450           0.440       0.009812
  0.500           0.938       0.000000
  0.550           0.902       0.020753
  0.600           0.412       0.000000
  0.650          -0.311      -0.008586
  0.700          -0.880       0.000000
  0.750          -0.952      -0.015585
  0.800          -0.537       0.000000
```

CSHER

Computes the Hermite cubic spline interpolant.

Required Arguments

XDATA — Array of length NDATA containing the data point abscissas. (Input)
The data point abscissas must be distinct.

FDATA — Array of length NDATA containing the data point ordinates. (Input)

DFDATA — Array of length NDATA containing the values of the derivative. (Input)

BREAK — Array of length NDATA containing the breakpoints for the piecewise cubic representation. (Output)

CSCOEF — Matrix of size 4 by NDATA containing the local coefficients of the cubic pieces. (Output)

Optional Arguments

NDATA — Number of data points. (Input)
Default: NDATA = size (XDATA,1).

FORTRAN 90 Interface

Generic: CALL CSHER (XDATA, FDATA, DFDATA, BREAK, CSCOEF [, …])

Specific: The specific interface names are S_CSHER and D_CSHER.

FORTRAN 77 Interface

Single: CALL CSHER (NDATA, XDATA, FDATA, BREAK, CSCOEF)

Double: The double precision name is DCSHER.

Description

The routine CSHER computes a C^1 cubic spline interpolant to the set of data points

$$\left(x_{\mathrm{i}}, f_{\mathrm{i}}\right) \text{ and } \left(x_{\mathrm{i}}, f'_{\mathrm{i}}\right)$$

for i = 1, …, NDATA = N. The breakpoints of the spline are the abscissas.

If the data points arise from the values of a smooth (say C^4) function f, i.e.,

$$f_{\mathrm{i}} = f\left(x_{\mathrm{i}}\right) \text{ and } f'_{\mathrm{i}} = f'\left(x_{\mathrm{i}}\right)$$

then the error will behave in a predictable fashion. Let ξ be the breakpoint vector for the above spline interpolant. Then, the maximum absolute error satisfies

$$\|f - s\|_{\left[\xi_1, \xi_N\right]} \le C \left\| f^{(4)} \right\|_{\left[\xi_1, \xi_N\right]} |\xi|^4$$

where

$$|\xi| := \max_{i = 2, \ldots, N} |\xi_i - \xi_{i-1}|$$

For more details, see de Boor (1978, page 51).

Comments

1. Workspace may be explicitly provided, if desired, by use of C2HER/DC2HER. The reference is:

   ```
   CALL C2HER (NDATA, XDATA, FDATA, DFDATA, BREAK, CSCOEF, IWK)
   ```

   The additional argument is:

   IWK — Work array of length NDATA.

2. Informational error

Type	Code	Description
4	2	The XDATA values must be distinct.

3. The cubic spline can be evaluated using CSVAL; its derivative can be evaluated using CSDER.

4. Note that column NDATA of CSCOEF is used as workspace.

Example

In this example, a cubic spline interpolant to a function *f* is computed. The value of the function *f* and its derivative *f'* are computed on the interpolation nodes and passed to CSHER. The values of this spline are then compared with the exact function values.

```
      USE CSHER_INT
      USE UMACH_INT
      USE CSVAL_INT

      IMPLICIT   NONE
      INTEGER    NDATA
      PARAMETER  (NDATA=11)
!
      INTEGER    I, NINTV, NOUT
      REAL       BREAK(NDATA), COS, CSCOEF(4,NDATA), DF,&
                 DFDATA(NDATA), F, FDATA(NDATA), FLOAT, SIN, X,&
                 XDATA(NDATA)
      INTRINSIC  COS, FLOAT, SIN
!                                  Define function and derivative
      F(X)  = SIN(15.0*X)
      DF(X) = 15.0*COS(15.0*X)
!                                  Set up a grid
      DO 10  I=1, NDATA
         XDATA(I)  = FLOAT(I-1)/FLOAT(NDATA-1)
         FDATA(I)  = F(XDATA(I))
         DFDATA(I) = DF(XDATA(I))
   10 CONTINUE
!                                  Compute cubic spline interpolant
      CALL CSHER (XDATA, FDATA, DFDATA, BREAK, CSCOEF)
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Write heading
      WRITE (NOUT,99999)
99999 FORMAT (13X, 'X', 9X, 'Interpolant', 5X, 'Error')
      NINTV = NDATA - 1
!                                  Print the interpolant on a finer grid
      DO 20  I=1, 2*NDATA - 1
         X = FLOAT(I-1)/FLOAT(2*NDATA-2)
         WRITE (NOUT,'(2F15.3, F15.6)') X, CSVAL(X,BREAK,CSCOEF)&
                                      , F(X) - CSVAL(X,BREAK,&
                                      CSCOEF)

   20 CONTINUE
      END
```

Output

```
   X         Interpolant     Error
0.000           0.000       0.000000
0.050           0.673       0.008654
0.100           0.997       0.000000
0.150           0.768       0.009879
0.200           0.141       0.000000
0.250          -0.564      -0.007257
0.300          -0.978       0.000000
0.350          -0.848      -0.010906
0.400          -0.279       0.000000
0.450           0.444       0.005714
0.500           0.938       0.000000
0.550           0.911       0.011714
0.600           0.412       0.000000
```

```
 0.650         -0.315      -0.004057
 0.700         -0.880       0.000000
 0.750         -0.956      -0.012288
 0.800         -0.537       0.000000
 0.850          0.180       0.002318
 0.900          0.804       0.000000
 0.950          0.981       0.012616
 1.000          0.650       0.000000
```

CSAKM

Computes the Akima cubic spline interpolant.

Required Arguments

XDATA — Array of length `NDATA` containing the data point abscissas. (Input)
The data point abscissas must be distinct.

FDATA — Array of length `NDATA` containing the data point ordinates. (Input)

BREAK — Array of length `NDATA` containing the breakpoints for the piecewise cubic representation. (Output)

CSCOEF — Matrix of size 4 by `NDATA` containing the local coefficients of the cubic pieces. (Output)

Optional Arguments

NDATA — Number of data points. (Input)
Default: `NDATA` = size (`XDATA`,1).

FORTRAN 90 Interface

Generic: `CALL CSAKM (XDATA, FDATA, BREAK, CSCOEF [, …])`

Specific: The specific interface names are `S_CSAKM` and `D_CSAKM`.

FORTRAN 77 Interface

Single: `CALL CSAKM (NDATA, XDATA, FDATA, BREAK, CSCOEF)`

Double: The double precision name is `DCSAKM`.

Description

The routine `CSAKM` computes a C^1 cubic spline interpolant to a set of data points (x_i, f_i) for $i = 1, \ldots,$ `NDATA` $= N$. The breakpoints of the spline are the abscissas. Endpoint conditions are automatically determined by the program; see Akima (1970) or de Boor (1978).

If the data points arise from the values of a smooth (say C^4) function f, i.e. $f_i = f(x_i)$, then the error will behave in a predictable fashion. Let ξ be the breakpoint vector for the above spline interpolant. Then, the maximum absolute error satisfies

$$\|f - s\|_{[\xi_1,\xi_N]} \le C\left\|f^{(2)}\right\|_{[\xi_1,\xi_N]}|\xi|^2$$

where

$$|\xi| := \max_{i = 2, \ldots, N}|\xi_i - \xi_{i-1}|$$

The routine CSAKM is based on a method by Akima (1970) to combat wiggles in the interpolant. The method is nonlinear; and although the interpolant is a piecewise cubic, cubic polynomials are not reproduced. (However, linear polynomials are reproduced.)

Comments

1. Workspace may be explicitly provided, if desired, by use of C2AKMD/C2AKM. The reference is:

   CALL C2AKM (NDATA, XDATA, FDATA, BREAK, CSCOEF, IWK)

   The additional argument is:

   IWK — Work array of length NDATA.

2. The cubic spline can be evaluated using CSVAL; its derivative can be evaluated using CSDER.

3. Note that column NDATA of CSCOEF is used as workspace.

Example

In this example, a cubic spline interpolant to a function f is computed. The values of this spline are then compared with the exact function values.

```
      USE CSAKM_INT
      USE UMACH_INT
      USE CSVAL_INT

      IMPLICIT   NONE
      INTEGER    NDATA
      PARAMETER  (NDATA=11)
!
      INTEGER    I, NINTV, NOUT
      REAL       BREAK(NDATA), CSCOEF(4,NDATA), F,&
                 FDATA(NDATA), FLOAT, SIN, X, XDATA(NDATA)
      INTRINSIC  FLOAT, SIN
!                                  Define function
      F(X) = SIN(15.0*X)
!                                  Set up a grid
```

```
      DO 10  I=1, NDATA
         XDATA(I) = FLOAT(I-1)/FLOAT(NDATA-1)
         FDATA(I) = F(XDATA(I))
   10 CONTINUE
!                                   Compute cubic spline interpolant
      CALL CSAKM (XDATA, FDATA, BREAK, CSCOEF)
!                                   Get output unit number
      CALL UMACH (2, NOUT)
!                                   Write heading
      WRITE (NOUT,99999)
99999 FORMAT (13X, 'X', 9X, 'Interpolant', 5X, 'Error')
      NINTV = NDATA - 1
!                                   Print the interpolant on a finer grid
      DO 20  I=1, 2*NDATA - 1
         X = FLOAT(I-1)/FLOAT(2*NDATA-2)
         WRITE (NOUT,'(2F15.3,F15.6)') X, CSVAL(X,BREAK,CSCOEF),&
                                     F(X) - CSVAL(X,BREAK,&
                                     CSCOEF)
   20 CONTINUE
      END
```

Output

```
   X         Interpolant     Error
0.000           0.000       0.000000
0.050           0.818      -0.135988
0.100           0.997       0.000000
0.150           0.615       0.163487
0.200           0.141       0.000000
0.250          -0.478      -0.093376
0.300          -0.978       0.000000
0.350          -0.812      -0.046447
0.400          -0.279       0.000000
0.450           0.386       0.064491
0.500           0.938       0.000000
0.550           0.854       0.068274
0.600           0.412       0.000000
0.650          -0.276      -0.043288
0.700          -0.880       0.000000
0.750          -0.889      -0.078947
0.800          -0.537       0.000000
0.850           0.149       0.033757
0.900           0.804       0.000000
0.950           0.932       0.061260
1.000           0.650       0.000000
```

CSCON

Computes a cubic spline interpolant that is consistent with the concavity of the data.

Required Arguments

XDATA — Array of length NDATA containing the data point abscissas. (Input)
The data point abscissas must be distinct.

FDATA — Array of length NDATA containing the data point ordinates. (Input)

IBREAK — The number of breakpoints. (Output)
It will be less than 2 * NDATA.

BREAK — Array of length IBREAK containing the breakpoints for the piecewise cubic representation in its first IBREAK positions. (Output)
The dimension of BREAK must be at least 2 * NDATA.

CSCOEF — Matrix of size 4 by N where N is the dimension of BREAK. (Output)
The first IBREAK − 1 columns of CSCOEF contain the local coefficients of the cubic pieces.

Optional Arguments

NDATA — Number of data points. (Input)
NDATA must be at least 3.
Default: NDATA = size (XDATA,1).

FORTRAN 90 Interface

Generic: CALL CSCON (XDATA, FDATA, IBREAK, BREAK, CSCOEF [, …])

Specific: The specific interface names are S_CSCON and D_CSCON.

FORTRAN 77 Interface

Single: CALL CSCON (NDATA, XDATA, FDATA, IBREAK, BREAK, CSCOEF)

Double: The double precision name is DCSCON.

Description

The routine CSCON computes a cubic spline interpolant to n = NDATA data points $\{x_i, f_i\}$ for $i = 1, \ldots, n$. For ease of explanation, we will assume that $x_i < x_{i+1}$, although it is not necessary for the user to sort these data values. If the data are strictly convex, then the computed spline is convex, C^2, and minimizes the expression

$$\int_{x_1}^{x_n} (g'')^2$$

over all convex C^1 functions that interpolate the data. In the general case when the data have both convex and concave regions, the convexity of the spline is consistent with the data and the above integral is minimized under the appropriate constraints. For more information on this interpolation scheme, we refer the reader to Micchelli et al. (1985) and Irvine et al. (1986).

One important feature of the splines produced by this subroutine is that it is not possible, a priori, to predict the number of breakpoints of the resulting interpolant. In most cases, there will be breakpoints at places other than data locations. The method is nonlinear; and although the interpolant is a piecewise cubic, cubic polynomials are not reproduced. (However, linear polynomials are reproduced.) This routine should be used when it is important to preserve the convex and concave regions implied by the data.

Comments

1. Workspace may be explicitly provided, if desired, by use of C2CON/DC2CON. The reference is:

```
CALL C2CON (NDATA, XDATA, FDATA, IBREAK, BREAK, CSCOEF,
   ITMAX, XSRT, FSRT, A, Y, DIVD, ID, WK)
```

   The additional arguments are as follows:

   ITMAX — Maximum number of iterations of Newton's method. (Input)

   XSRT — Work array of length NDATA to hold the sorted XDATA values.

   FSRT — Work array of length NDATA to hold the sorted FDATA values.

   A — Work array of length NDATA.

   Y — Work array of length NDATA − 2.

   DIVD — Work array of length NDATA − 2.

   ID — Integer work array of length NDATA.

   WK — Work array of length 5 * (NDATA − 2).

2. Informational errors

Type	Code	Description
3	16	Maximum number of iterations exceeded, call C2CON/DC2CON to set a larger number for ITMAX.
4	3	The XDATA values must be distinct.

3. The cubic spline can be evaluated using CSVAL; its derivative can be evaluated using CSDER.

4. The default value for ITMAX is 25. This can be reset by calling C2CON/DC2CON directly.

Example

We first compute the shape-preserving interpolant using CSCON, and display the coefficients and breakpoints. Second, we interpolate the same data using CSINT in a program not shown and overlay the two results. The graph of the result from CSINT is represented by the dashed line. Notice the extra inflection points in the curve produced by CSINT.

```
      USE CSCON_INT
      USE UMACH_INT
      USE WRRRL_INT

      IMPLICIT   NONE
!                                  Specifications
      INTEGER    NDATA
      PARAMETER  (NDATA=9)
!
      INTEGER    IBREAK, NOUT
      REAL       BREAK(2*NDATA), CSCOEF(4,2*NDATA), FDATA(NDATA),&
                 XDATA(NDATA)
      CHARACTER  CLABEL(14)*2, RLABEL(4)*2
!
      DATA XDATA/0.0, .1, .2, .3, .4, .5, .6, .8, 1./
      DATA FDATA/0.0, .9, .95, .9, .1, .05, .05, .2, 1./
      DATA RLABEL/' 1', ' 2', ' 3', ' 4'/
      DATA CLABEL/'  ', ' 1', ' 2', ' 3', ' 4', ' 5', ' 6',&
           ' 7', ' 8', ' 9', '10', '11', '12', '13'/
!                                  Compute cubic spline interpolant
      CALL CSCON (XDATA, FDATA, IBREAK, BREAK, CSCOEF)
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Print the BREAK points and the
!                                  coefficients (CSCOEF) for
!                                  checking purposes.
      WRITE (NOUT,'(1X,A,I2)') 'IBREAK = ', IBREAK
      CALL WRRRL ('BREAK', BREAK, RLABEL, CLABEL, 1, IBREAK, 1, &
                  FMT='(F9.3)')
      CALL WRRRL ('CSCOEF', CSCOEF, RLABEL, CLABEL, 4, IBREAK, 4, &
                  FMT='(F9.3)')
      END
```

Output

```
IBREAK = 13
                               BREAK
```

```
             1           2           3           4           5           6
 1       0.000       0.100       0.136       0.200       0.259       0.300

             7           8           9          10          11          12
 1       0.400       0.436       0.500       0.600       0.609       0.800

            13
 1       1.000

                                   CSCOEF
             1           2           3           4           5           6
 1       0.000       0.900       0.942       0.950       0.958       0.900
 2      11.886       3.228       0.131       0.131       0.131      -4.434
 3       0.000    -173.170       0.000       0.000       0.000     220.218
 4   -1731.699    4841.604       0.000       0.000   -5312.082    4466.875

             7           8           9          10          11          12
 1       0.100       0.050       0.050       0.050       0.050       0.200
 2      -4.121       0.000       0.000       0.000       0.000       2.356
 3     226.470       0.000       0.000       0.000       0.000      24.664
 4   -6222.348       0.000       0.000       0.000     129.115     123.321

            13
 1       1.000
 2       0.000
 3       0.000
 4       0.000
```

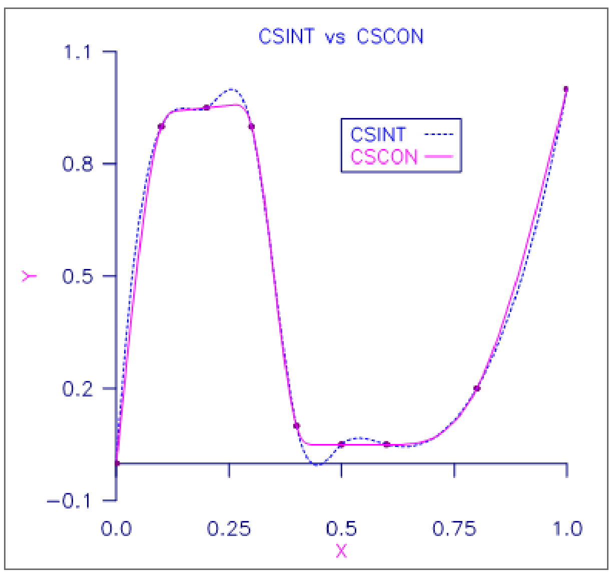


Figure 6, *CSCON* vs. *CSINT*

CSPER

Computes the cubic spline interpolant with periodic boundary conditions.

Required Arguments

XDATA — Array of length NDATA containing the data point abscissas. (Input)
The data point abscissas must be distinct.

FDATA — Array of length NDATA containing the data point ordinates. (Input)

BREAK — Array of length NDATA containing the breakpoints for the piecewise cubic representation. (Output)

CSCOEF — Matrix of size 4 by NDATA containing the local coefficients of the cubic pieces. (Output)

Optional Arguments

NDATA — Number of data points. (Input)
NDATA must be at least 4.
Default: NDATA = size (XDATA,1).

FORTRAN 90 Interface

Generic: CALL CSPER (XDATA, FDATA, BREAK, CSCOEF [, …])

Specific: The specific interface names are S_CSPER and D_CSPER.

FORTRAN 77 Interface

Single: CALL CSPER (NDATA, XDATA, FDATA, BREAK, CSCOEF)

Double: The double precision name is DCSPER.

Description

The routine CSPER computes a C^2 cubic spline interpolant to a set of data points (x_i, f_i) for $i = 1, \ldots,$ NDATA $= N$. The breakpoints of the spline are the abscissas. The program enforces periodic endpoint conditions. This means that the spline s satisfies $s(a) = s(b)$, $s'(a) = s'(b)$, and $s''(a) = s''(b)$, where a is the leftmost abscissa and b is the rightmost abscissa. If the ordinate values corresponding to a and b are not equal, then a warning message is issued. The ordinate value at b is set equal to the ordinate value at a and the interpolant is computed.

If the data points arise from the values of a smooth (say C^4) periodic function f, i.e. $f_i = f(x_i)$, then the error will behave in a predictable fashion. Let ξ be the breakpoint vector for the above spline interpolant. Then, the maximum absolute error satisfies

$$\|f - s\|_{[\xi_1, \xi_N]} \le C \left\| f^{(4)} \right\|_{[\xi_1, \xi_N]} |\xi|^4$$

where

$$|\xi| := \max_{i = 2, \ldots, N} |\xi_i - \xi_{i-1}|$$

For more details, see de Boor (1978, pages 320-322).

Comments

1. Workspace may be explicitly provided, if desired, by use of C2PER/DC2PER. The reference is:

```
CALL C2PER (NDATA, XDATA, FDATA, BREAK, CSCOEF, WK, IWK)
```

   The additional arguments are as follows:

   WK — Work array of length 6 * NDATA.

   IWK — Work array of length NDATA.

2. Informational error

Type	Code	Description
3	1	The data set is not periodic, i.e., the function values at the smallest and largest XDATA points are not equal. The value at the smallest XDATA point is used.

3. The cubic spline can be evaluated using CSVAL and its derivative can be evaluated using CSDER.

Example

In this example, a cubic spline interpolant to a function *f* is computed. The values of this spline are then compared with the exact function values.

```
      USE IMSL_LIBRARIES

      IMPLICIT   NONE
      INTEGER    NDATA
      PARAMETER  (NDATA=11)
!
      INTEGER    I, NINTV, NOUT
      REAL       BREAK(NDATA), CSCOEF(4,NDATA), F,&
                 FDATA(NDATA), FLOAT, H, PI, SIN, X, XDATA(NDATA)
      INTRINSIC  FLOAT, SIN
!
!                                 Define function
      F(X) = SIN(15.0*X)
!                                 Set up a grid
      PI = CONST('PI')
      H = 2.0*PI/15.0/10.0
      DO 10  I=1, NDATA
         XDATA(I) = H*FLOAT(I-1)
         FDATA(I) = F(XDATA(I))
   10 CONTINUE
!                                 Round off will cause FDATA(11) to
!                                 be nonzero; this would produce a
!                                 warning error since FDATA(1) is zero.
!                                 Therefore, the value of FDATA(1) is
!                                 used rather than the value of
!                                 FDATA(11).
      FDATA(NDATA) = FDATA(1)
!
!                                 Compute cubic spline interpolant
      CALL CSPER (XDATA, FDATA, BREAK, CSCOEF)
!                                 Get output unit number
      CALL UMACH (2, NOUT)
!                                 Write heading
      WRITE (NOUT,99999)
99999 FORMAT (13X, 'X', 9X, 'Interpolant', 5X, 'Error')
      NINTV = NDATA - 1
      H     = H/2.0
!                                 Print the interpolant on a finer grid
      DO 20  I=1, 2*NDATA - 1
         X = H*FLOAT(I-1)
         WRITE (NOUT,'(2F15.3,F15.6)') X, CSVAL(X,BREAK,CSCOEF),&
                                     F(X) - CSVAL(X,BREAK,&
                                     CSCOEF)
   20 CONTINUE
      END
```

Output

```
       X         Interpolant     Error
0.000          0.000       0.000000
0.021          0.309       0.000138
0.042          0.588       0.000000
0.063          0.809       0.000362
0.084          0.951       0.000000
0.105          1.000       0.000447
0.126          0.951       0.000000
0.147          0.809       0.000362
```

```
 0.168          0.588       0.000000
 0.188          0.309       0.000138
 0.209          0.000       0.000000
 0.230         -0.309      -0.000138
 0.251         -0.588       0.000000
 0.272         -0.809      -0.000362
 0.293         -0.951       0.000000
 0.314         -1.000      -0.000447
 0.335         -0.951       0.000000
 0.356         -0.809      -0.000362
 0.377         -0.588       0.000000
 0.398         -0.309      -0.000138
 0.419          0.000       0.000000
```

CSVAL

This function evaluates a cubic spline.

Function Return Value

CSVAL — Value of the polynomial at `X`. (Output)

Required Arguments

X — Point at which the spline is to be evaluated. (Input)

BREAK — Array of length `NINTV` + 1 containing the breakpoints for the piecewise cubic representation. (Input)
`BREAK` must be strictly increasing.

CSCOEF — Matrix of size 4 by `NINTV` + 1 containing the local coefficients of the cubic pieces. (Input)

Optional Arguments

NINTV — Number of polynomial pieces. (Input)

FORTRAN 90 Interface

Generic: `CSVAL (X, BREAK, CSCOEF [, …])`

Specific: The specific interface names are `S_CSVAL` and `D_CSVAL`.

FORTRAN 77 Interface

Single: `CSVAL (X, NINTV, BREAK, CSCOEF)`

Double: The double precision function name is `DCSVAL`.

Description

The routine CSVAL evaluates a cubic spline at a given point. It is a special case of the routine PPDER, which evaluates the derivative of a piecewise polynomial. (The value of a piecewise polynomial is its zero-th derivative and a cubic spline is a piecewise polynomial of order 4.) The routine PPDER is based on the routine PPVALU in de Boor (1978, page 89).

Example

For an example of the use of CSVAL, see IMSL routine CSINT.

CSDER

This function evaluates the derivative of a cubic spline.

Function Return Value

CSDER — Value of the IDERIV-th derivative of the polynomial at X. (Output)

Required Arguments

IDERIV — Order of the derivative to be evaluated. (Input)
In particular, IDERIV = 0 returns the value of the polynomial.

X — Point at which the polynomial is to be evaluated. (Input)

BREAK — Array of length NINTV + 1 containing the breakpoints for the piecewise cubic representation. (Input)
BREAK must be strictly increasing.

CSCOEF — Matrix of size 4 by NINTV + 1 containing the local coefficients of the cubic pieces. (Input)

Optional Arguments

NINTV — Number of polynomial pieces. (Input)
Default: NINTV = size (BREAK,1)–1.

FORTRAN 90 Interface

Generic: CSDER (IDERIV, X, BREAK, CSCOEF, CSDER [, …])

Specific: The specific interface names are S_CSDER and D_CSDER.

FORTRAN 77 Interface

Single: CSDER (IDERIV, X, NINTV, BREAK, CSCOEF)

Double: The double precision function name is DCSDER.

Description

The function CSDER evaluates the derivative of a cubic spline at a given point. It is a special case of the routine PPDER, which evaluates the derivative of a piecewise polynomial. (A cubic spline is a piecewise polynomial of order 4.) The routine PPDER is based on the routine PPVALU in de Boor (1978, page 89).

Example

In this example, we compute a cubic spline interpolant to a function *f* using IMSL routine CSINT. The values of the spline and its first and second derivatives are computed using CSDER. These values can then be compared with the corresponding values of the interpolated function.

```
      USE CSDER_INT
      USE CSINT_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    NDATA
      PARAMETER  (NDATA=10)
!
      INTEGER    I, NINTV, NOUT
      REAL       BREAK(NDATA), CDDF, CDF, CF, COS, CSCOEF(4,NDATA),&
                 DDF, DF, F, FDATA(NDATA), FLOAT, SIN, X,&
                 XDATA(NDATA)
      INTRINSIC  COS, FLOAT, SIN
!                                  Define function and derivatives
      F(X)   = SIN(15.0*X)
      DF(X)  = 15.0*COS(15.0*X)
      DDF(X) = -225.0*SIN(15.0*X)
!                                  Set up a grid
      DO 10  I=1, NDATA
         XDATA(I) = FLOAT(I-1)/FLOAT(NDATA-1)
         FDATA(I) = F(XDATA(I))
   10 CONTINUE
!                                  Compute cubic spline interpolant
      CALL CSINT (XDATA, FDATA, BREAK, CSCOEF)
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Write heading
      WRITE (NOUT,99999)
99999 FORMAT (9X, 'X', 8X, 'S(X)', 5X, 'Error', 6X, 'S''(X)', 5X,&
              'Error', 6X, 'S''''(X)', 4X, 'Error', /)
      NINTV = NDATA - 1
!                                  Print the interpolant on a finer grid
      DO 20  I=1, 2*NDATA
         X    = FLOAT(I-1)/FLOAT(2*NDATA-1)
         CF   = CSDER(0,X,BREAK,CSCOEF)
         CDF  = CSDER(1,X,BREAK,CSCOEF)
         CDDF = CSDER(2,X,BREAK,CSCOEF)
         WRITE (NOUT,'(F11.3, 3(F11.3, F11.6))') X, CF, F(X) - CF,&
                                            CDF, DF(X) - CDF,&
                                            CDDF, DDF(X) - CDDF
   20 CONTINUE
      END
```

Output

```
   X         S(X)      Error       S'(X)      Error       S''(X)     Error

 0.000      0.000    0.000000    26.285  -11.284739   -379.458  379.457794
 0.053      0.902   -0.192203     8.841    1.722460   -283.411  123.664734
 0.105      1.019   -0.019333    -3.548    3.425718   -187.364  -37.628586
 0.158      0.617    0.081009   -10.882    0.146207    -91.317  -65.824875
 0.211     -0.037    0.021155   -13.160   -1.837700      4.730   -1.062027
 0.263     -0.674   -0.046945   -10.033   -0.355268    117.916   44.391640
 0.316     -0.985   -0.015060    -0.719    1.086203    235.999  -11.066727
 0.368     -0.682   -0.004651    11.314   -0.409097    154.861   -0.365387
 0.421      0.045   -0.011915    14.708    0.284042    -25.887   18.552732
 0.474      0.708    0.024292     9.508    0.702690   -143.785  -21.041260
 0.526      0.978    0.020854     0.161   -0.771948   -211.402  -13.411087
 0.579      0.673    0.001410   -11.394    0.322443   -163.483   11.674103
 0.632     -0.064    0.015118   -14.937   -0.045511     28.856  -17.856323
 0.684     -0.724   -0.019246    -8.859   -1.170871    163.866    3.435547
 0.737     -0.954   -0.044143     0.301    0.554493    184.217   40.417282
 0.789     -0.675    0.012143    10.307    0.928152    166.021  -16.939514
 0.842      0.027    0.038176    15.015   -0.047344     12.914  -27.575521
 0.895      0.764   -0.010112    11.666   -1.819128   -140.193  -29.538193
 0.947      1.114   -0.116304     0.258   -1.357680   -293.301   68.905701
 1.000      0.650    0.000000   -19.208    7.812407   -446.408  300.092896
```

CS1GD

Evaluates the derivative of a cubic spline on a grid.

Required Arguments

IDERIV — Order of the derivative to be evaluated. (Input)
In particular, `IDERIV` = 0 returns the values of the cubic spline.

XVEC — Array of length `N` containing the points at which the cubic spline is to be evaluated. (Input)
The points in `XVEC` should be strictly increasing.

BREAK — Array of length `NINTV` + 1 containing the breakpoints for the piecewise cubic representation. (Input)
`BREAK` must be strictly increasing.

CSCOEF — Matrix of size 4 by `NINTV` + 1 containing the local coefficients of the cubic pieces. (Input)

VALUE — Array of length `N` containing the values of the `IDERIV`-th derivative of the cubic spline at the points in `XVEC`. (Output)

Optional Arguments

N — Length of vector `XVEC`. (Input)
Default: `N` = size (`XVEC`,1).

NINTV — Number of polynomial pieces. (Input)
Default: `NINTV` = size (`BREAK`,1) –1.

FORTRAN 90 Interface

Generic: `CALL CS1GD (IDERIV, XVEC, BREAK, CSCOEF, VALUE [, …])`

Specific: The specific interface names are `S_CS1GD` and `D_CS1GD`.

FORTRAN 77 Interface

Single: `CALL CS1GD (IDERIV, N, XVEC, NINTV, BREAK, CSCOEF, VALUE)`

Double: The double precision name is `DCS1GD`.

Description

The routine CS1GD evaluates a cubic spline (or its derivative) at a vector of points. That is, given a vector x of length n satisfying $x_i < x_{i+1}$ for $i = 1, \ldots, n - 1$, a derivative value j, and a cubic spline s that is represented by a breakpoint sequence and coefficient matrix this routine returns the values

$$s^{(j)}(x_i) \qquad i = 1, \ldots, n$$

in the array VALUE. The functionality of this routine is the same as that of CSDER called in a loop, however CS1GD should be much more efficient.

Comments

1. Workspace may be explicitly provided, if desired, by use of C21GD/DC21GD. The reference is:

   CALL C21GD (IDERIV, N, XVEC, NINTV, BREAK, CSCOEF, VALUE, IWK, WORK1, WORK2)

   The additional arguments are as follows:

   IWK — Array of length N.

   WORK1 — Array of length N.

   WORK2 — Array of length N.

2. Informational error

Type	Code	Description
4	4	The points in XVEC must be strictly increasing.

Example

To illustrate the use of CS1GD, we modify the example program for CSINT. In this example, a cubic spline interpolant to F is computed. The values of this spline are then compared with the exact function values. The routine CS1GD is based on the routine PPVALU in de Boor (1978, page 89).

```
      USE CS1GD_INT
      USE CSINT_INT
      USE UMACH_INT
      USE CSVAL_INT

      IMPLICIT   NONE
!                                  Specifications
      INTEGER    NDATA, N, IDERIV, J
      PARAMETER  (NDATA=11, N=2*NDATA-1)
!
      INTEGER    I, NINTV, NOUT
      REAL       BREAK(NDATA), CSCOEF(4,NDATA), F,&
                 FDATA(NDATA), FLOAT, SIN, X, XDATA(NDATA),&
```

```
                      FVALUE(N), VALUE(N), XVEC(N)
      INTRINSIC  FLOAT, SIN
!                                  Define function
      F(X) = SIN(15.0*X)
!                                  Set up a grid
      DO 10  I=1, NDATA
         XDATA(I) = FLOAT(I-1)/FLOAT(NDATA-1)
         FDATA(I) = F(XDATA(I))
   10 CONTINUE
!                                  Compute cubic spline interpolant
      CALL CSINT (XDATA, FDATA, BREAK, CSCOEF)
      DO 20  I=1, N
         XVEC(I) = FLOAT(I-1)/FLOAT(2*NDATA-2)
         FVALUE(I) = F(XVEC(I))
   20  CONTINUE
      IDERIV = 0
      NINTV = NDATA - 1
      CALL CS1GD (IDERIV, XVEC, BREAK, CSCOEF, VALUE)
!                                  Get output unit number.
      CALL UMACH (2, NOUT)
!                                  Write heading
      WRITE (NOUT,99999)
99999 FORMAT (13X, 'X', 9X, 'Interpolant', 5X, 'Error')
!                                  Print the interpolant and the error
!                                  on a finer grid
      DO 30 J=1, N
         WRITE (NOUT,'(2F15.3,F15.6)') XVEC(J), VALUE(J),&
                                     FVALUE(J)-VALUE(J)
   30 CONTINUE
      END
```

Output

```
    X         Interpolant     Error
0.000           0.000       0.000000
0.050           0.809      -0.127025
0.100           0.997       0.000000
0.150           0.723       0.055214
0.200           0.141       0.000000
0.250          -0.549      -0.022789
0.300          -0.978       0.000000
0.350          -0.843      -0.016246
0.400          -0.279       0.000000
0.450           0.441       0.009348
0.500           0.938       0.000000
0.550           0.903       0.019947
0.600           0.412       0.000000
0.650          -0.315      -0.004895
0.700          -0.880       0.000000
0.750          -0.938      -0.029541
0.800          -0.537       0.000000
0.850           0.148       0.034693
0.900           0.804       0.000000
0.950           1.086      -0.092559
1.000           0.650       0.000000
```

CSITG

This function evaluates the integral of a cubic spline.

Function Return Value

CSITG — Value of the integral of the spline from A to B. (Output)

Required Arguments

A — Lower limit of integration. (Input)

B — Upper limit of integration. (Input)

BREAK — Array of length NINTV + 1 containing the breakpoints for the piecewise cubic representation. (Input)
BREAK must be strictly increasing.

CSCOEF — Matrix of size 4 by NINTV + 1 containing the local coefficients of the cubic pieces. (Input)

Optional Arguments

NINTV — Number of polynomial pieces. (Input)
Default: NINTV = size (BREAK,1) – 1.

FORTRAN 90 Interface

Generic: CSITG (A, B, BREAK, CSCOEF [, …])

Specific: The specific interface names are S_CSITG and D_CSITG.

FORTRAN 77 Interface

Single: CSITG(A, B, NINTV, BREAK, CSCOEF)

Double: The double precision function name is DCSITG.

Description

The function CSITG evaluates the integral of a cubic spline over an interval. It is a special case of the routine PPITG, which evaluates the integral of a piecewise polynomial. (A cubic spline is a piecewise polynomial of order 4.)

Example

This example computes a cubic spline interpolant to the function x^2 using CSINT and evaluates its integral over the intervals [0., .5] and [0., 2.]. Since CSINT uses the not-a knot condition, the interpolant reproduces x^2, hence the integral values are 1/24 and 8/3, respectively.

```
      USE CSITG_INT
      USE UMACH_INT
      USE CSINT_INT

      IMPLICIT   NONE
      INTEGER    NDATA
      PARAMETER  (NDATA=10)
!
      INTEGER    I, NINTV, NOUT
      REAL       A, B, BREAK(NDATA), CSCOEF(4,NDATA), ERROR,&
                 EXACT, F, FDATA(NDATA), FI, FLOAT, VALUE, X,&
                 XDATA(NDATA)
      INTRINSIC  FLOAT
!                                  Define function and integral
      F(X)  = X*X
      FI(X) = X*X*X/3.0
!                                  Set up a grid
      DO 10  I=1, NDATA
         XDATA(I) = FLOAT(I-1)/FLOAT(NDATA-1)
         FDATA(I) = F(XDATA(I))
   10 CONTINUE
!                                  Compute cubic spline interpolant
      CALL CSINT (XDATA, FDATA, BREAK, CSCOEF)
!                                  Compute the integral of F over
!                                  [0.0,0.5]
      A     = 0.0
      B     = 0.5
      NINTV = NDATA - 1
      VALUE = CSITG(A,B,BREAK,CSCOEF)
      EXACT = FI(B) - FI(A)
      ERROR = EXACT - VALUE
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Print the result
      WRITE (NOUT,99999) A, B, VALUE, EXACT, ERROR
!                                  Compute the integral of F over
!                                  [0.0,2.0]
      A     = 0.0
      B     = 2.0
      VALUE = CSITG(A,B,BREAK,CSCOEF)
      EXACT = FI(B) - FI(A)
      ERROR = EXACT - VALUE
!                                  Print the result
      WRITE (NOUT,99999) A, B, VALUE, EXACT, ERROR
99999 FORMAT (' On the closed interval (', F3.1, ',', F3.1,&
              ') we have :', /, 1X, 'Computed Integral = ', F10.5, /,&
```

```
              1X, 'Exact Integral    = ', F10.5, /, 1X, 'Error          '&
              , '    = ', F10.6, /, /)
       END
```

Output

```
 On the closed interval (0.0,0.5) we have :
 Computed Integral =    0.04167
 Exact Integral    =    0.04167
 Error             =   0.000000

 On the closed interval (0.0,2.0) we have :
 Computed Integral =    2.66666
 Exact Integral    =    2.66667
 Error             =   0.000006
```

SPLEZ

more...

Computes the values of a spline that either interpolates or fits user-supplied data.

Required Arguments

XDATA — Array of length NDATA containing the data point abscissae. (Input)
The data point abscissas must be distinct.

FDATA — Array of length NDATA containing the data point ordinates. (Input)

XVEC — Array of length N containing the points at which the spline function values are desired. (Input)
The entries of XVEC must be distinct.

VALUE — Array of length N containing the spline values. (Output)
VALUE (I) = S(XVEC (I)) if IDER = 0, VALUE(I) = S′(XVEC (I)) if IDER = 1, and so forth, where S is the computed spline.

Optional Arguments

NDATA — Number of data points. (Input)
Default: NDATA = size (XDATA,1).

All choices of ITYPE are valid if NDATA is larger than 6. More specifically,

NDATA > ITYPE	for ITYPE = 1.
NDATA > 3	or ITYPE = 2, 3.
NDATA > (ITYPE − 3)	for ITYPE = 4, 5, 6, 7, 8.
NDATA > 3	for ITYPE = 9, 10, 11, 12.
NDATA > KORDER	for ITYPE = 13, 14, 15.

ITYPE — Type of interpolant desired. (Input)
Default: ITYPE = 1.

ITYPE

1	yields CSINT
2	yields CSAKM
3	yields CSCON
4	yields BSINT-BSNAK K = 2
5	yields BSINT-BSNAK K = 3
6	yields BSINT-BSNAK K = 4
7	yields BSINT-BSNAK K = 5
8	yields BSINT-BSNAK K = 6
9	yields CSSCV
10	yields BSLSQ K = 2
11	yields BSLSQ K = 3
12	yields BSLSQ K = 4
13	yields BSVLS K = 2
14	yields BSVLS K = 3
15	yields BSVLS K = 4

IDER — Order of the derivative desired. (Input)
Default: IDER = 0.

N — Number of function values desired. (Input)
Default: N = size (XVEC,1).

FORTRAN 90 Interface

Generic: CALL SPLEZ (XDATA, FDATA, XVEC, VALUE [, …])

Specific: The specific interface names are S_SPLEZ and D_SPLEZ.

FORTRAN 77 Interface

Single: CALL SPLEZ (NDATA, XDATA, FDATA, ITYPE, IDER, N, XVEC, VALUE)

Double: The double precision name is DSPLEZ.

Description

This routine is designed to let the user experiment with various interpolation and smoothing routines in the library.

The routine SPLEZ computes a spline interpolant to a set of data points (x_i, f_i) for $i = 1, \ldots,$ NDATA if ITYPE = 1, …, 8. If ITYPE ≥ 9, various smoothing or least squares splines are computed. The output for this routine consists of a vector of values of the computed spline or its derivatives. Specifically, let i = IDER, n = N, v = XVEC, and y = VALUE, then if s is the computed spline we set

$$y_j = s^{(i)}(v_j) \quad j = 1, \ldots, n$$

The routines called are listed above under the ITYPE heading. Additional documentation can be found by referring to these routines.

Example

In this example, all the ITYPE parameters are exercised. The values of the spline are then compared with the exact function values and derivatives.

```
      USE IMSL_LIBRARIES

      IMPLICIT   NONE
      INTEGER    NDATA, N
      PARAMETER  (NDATA=21, N=2*NDATA-1)
!                                  Specifications for local variables
      INTEGER    I, IDER, ITYPE, NOUT
      REAL       FDATA(NDATA), FPVAL(N), FVALUE(N),&
                 VALUE(N), XDATA(NDATA), XVEC(N), EMAX1(15),&
                 EMAX2(15), X
!                                  Specifications for intrinsics
      INTRINSIC  FLOAT, SIN, COS
      REAL       FLOAT, SIN, COS
!                                  Specifications for subroutines
!
      REAL       F, FP
!
!                                  Define a function
      F(X)  = SIN(X*X)
      FP(X) = 2*X*COS(X*X)
!
      CALL UMACH (2, NOUT)
!                                  Set up a grid
      DO 10  I=1, NDATA
         XDATA(I) = 3.0*(FLOAT(I-1)/FLOAT(NDATA-1))
         FDATA(I) = F(XDATA(I))
   10 CONTINUE
      DO 20  I=1, N
         XVEC(I)    = 3.0*(FLOAT(I-1)/FLOAT(2*NDATA-2))
         FVALUE(I)  = F(XVEC(I))
         FPVAL(I) = FP(XVEC(I))
   20 CONTINUE
!
      WRITE (NOUT,99999)
!                                  Loop to call SPLEZ for each ITYPE
      DO 40  ITYPE=1, 15
         DO 30  IDER=0, 1
            CALL SPLEZ (XDATA, FDATA, XVEC, VALUE, ITYPE=ITYPE, &
                        IDER=IDER)
!                                 Compute the maximum error
            IF (IDER .EQ. 0) THEN
               CALL SAXPY (N, -1.0, FVALUE, 1, VALUE, 1)
```

```
                 EMAX1(ITYPE) = ABS(VALUE(ISAMAX(N,VALUE,1)))
              ELSE
                 CALL SAXPY (N, -1.0, FPVAL, 1, VALUE, 1)
                 EMAX2(ITYPE) = ABS(VALUE(ISAMAX(N,VALUE,1)))
              END IF
   30  CONTINUE
          WRITE (NOUT,'(I7,2F20.6)') ITYPE, EMAX1(ITYPE), EMAX2(ITYPE)
   40 CONTINUE
!
99999 FORMAT (4X, 'ITYPE', 6X, 'Max error for f', 5X,&
              'Max error for f''', /)
      END
```

Output

```
ITYPE      Max error for f     Max error for f’

 1            0.014082            0.658018
 2            0.024682            0.897757
 3            0.020896            0.813228
 4            0.083615            2.168083
 5            0.010403            0.508043
 6            0.014082            0.658020
 7            0.004756            0.228858
 8            0.001070            0.077159
 9            0.020896            0.813228
10            0.392603            6.047916
11            0.162793            1.983959
12            0.045404            1.582624
13            0.588370            7.680381
14            0.752475            9.673786
15            0.049340            1.713031
```

BSINT

more...

Computes the spline interpolant, returning the B-spline coefficients.

Required Arguments

NDATA — Number of data points. (Input)

XDATA — Array of length NDATA containing the data point abscissas. (Input)

FDATA — Array of length NDATA containing the data point ordinates. (Input)

KORDER — Order of the spline. (Input)
KORDER must be less than or equal to NDATA.

XKNOT — Array of length NDATA + KORDER containing the knot sequence. (Input)
XKNOT must be nondecreasing.

BSCOEF — Array of length NDATA containing the B-spline coefficients. (Output)

FORTRAN 90 Interface

Generic: CALL BSINT (NDATA, XDATA, FDATA, KORDER, XKNOT, BSCOEF)

Specific: The specific interface names are S_BSINT and D_BSINT.

FORTRAN 77 Interface

Single: CALL BSINT (NDATA, XDATA, FDATA, KORDER, XKNOT, BSCOEF)

Double: The double precision name is DBSINT.

Description

Following the notation in de Boor (1978, page 108), let $B_j = B_{j,k,t}$ denote the j-th B-spline of order k with respect to the knot sequence **t**. Then, `BSINT` computes the vector a satisfying

$$\sum_{j=1}^{N} a_j B_j(x_i) = f_i$$

and returns the result in `BSCOEF` = a. This linear system is banded with at most $k - 1$ subdiagonals and $k - 1$ superdiagonals. The matrix

$$A = (B_j(x_i))$$

is totally positive and is invertible if and only if the diagonal entries are nonzero. The routine `BSINT` is based on the routine `SPLINT` by de Boor (1978, page 204).

The routine `BSINT` produces the coefficients of the B-spline interpolant of order `KORDER` with knot sequence `XKNOT` to the data (x_i, f_i) for i = 1 to `NDATA`, where x = `XDATA` and f = `FDATA`. Let **t** = `XKNOT`, k = `KORDER`, and N = `NDATA`. First, `BSINT` sorts the `XDATA` vector and stores the result in x. The elements of the `FDATA` vector are permuted appropriately and stored in f, yielding the equivalent data (x_i, f_i) for i = 1 to N. The following preliminary checks are performed on the data. We verify that

$$x_i < x_{i+1} \quad i = 1,\dots, N - 1$$

$$\mathbf{t}_i < \mathbf{t}_{i+1} \quad i = 1,\dots, N$$

$$\mathbf{t}_i \le \mathbf{t}_{i+k} \quad i = 1,\dots, N + k - 1$$

The first test checks to see that the abscissas are distinct. The second and third inequalities verify that a valid knot sequence has been specified.

In order for the interpolation matrix to be nonsingular, we also check $\mathbf{t}_k \le x \le \mathbf{t}_{N+1}$ for i = 1 to N. This first inequality in the last check is necessary since the method used to generate the entries of the interpolation matrix requires that the k possibly nonzero B-splines at x_i,

$$B_{j-k+1}, \dots, B_j \qquad \text{where } j \text{ satisfies } \mathbf{t}_j \le x_i < \mathbf{t}_{j+1}$$

be well-defined (that is, $j - k + 1 \ge 1$).

General conditions are not known for the exact behavior of the error in spline interpolation, however, if **t** and x are selected properly and the data points arise from the values of a smooth (say C^k) function f, i.e. $f_i = f(x_i)$, then the error will behave in a predictable fashion. The maximum absolute error satisfies

$$\| f - s \|_{\left[\mathbf{t}_k, \mathbf{t}_{N-1}\right]} \leq C \| f^{(k)} \|_{\left[\mathbf{t}_k, \mathbf{t}_{N+1}\right]} | \, \mathbf{t} \, |^k$$

where

$$|\mathbf{t}| := \max_{i = k, \, \ldots \, , N} |\mathbf{t}_{i+1} - \mathbf{t}_i|$$

For more information on this problem, see de Boor (1978, Chapter 13) and the references therein. This routine can be used in place of the IMSL routine CSINT by calling BSNAK to obtain the proper knots, then calling BSINT yielding the B-spline coefficients, and finally calling IMSL routine BSCPP to convert to piecewise polynomial form.

Comments

1. Workspace may be explicitly provided, if desired, by use of B2INT/DB2INT. The reference is:

```
CALL B2INT (NDATA, XDATA, FDATA, KORDER, XKNOT, BSCOEF, WK1,
  WK2, WK3, IWK)
```

The additional arguments are as follows:

WK1 — Work array of length (5 * KORDER – 2) * NDATA.

WK2 — Work array of length NDATA.

WK3 — Work array of length NDATA.

IWK — Work array of length NDATA.

2. Informational errors

Type	Code	Description
3	1	The interpolation matrix is ill-conditioned.
4	3	The XDATA values must be distinct.
4	4	Multiplicity of the knots cannot exceed the order of the spline.
4	5	The knots must be nondecreasing.
4	15	The I-th smallest element of the data point array must be greater than the Ith knot and less than the (I + KORDER)-th knot.
4	16	The largest element of the data point array must be greater than the (NDATA)-th knot and less than or equal to the (NDATA + KORDER)-th knot.
4	17	The smallest element of the data point array must be greater than or equal to the first knot and less than the (KORDER + 1)st knot.

3. The spline can be evaluated using BSVAL, and its derivative can be evaluated using BSDER.

Example

In this example, a spline interpolant *s*, to

$$f(x) = \sqrt{x}$$

is computed. The interpolated values are then compared with the exact function values using the IMSL routine BSVAL.

```
      USE BSINT_INT
      USE BSNAK_INT
      USE UMACH_INT
      USE BSVAL_INT

      IMPLICIT   NONE
      INTEGER    KORDER, NDATA, NKNOT
      PARAMETER  (KORDER=3, NDATA=5, NKNOT=NDATA+KORDER)
!
      INTEGER    I, NCOEF, NOUT
      REAL       BSCOEF(NDATA), BT, F, FDATA(NDATA), FLOAT,&
                 SQRT, X, XDATA(NDATA), XKNOT(NKNOT), XT
      INTRINSIC  FLOAT, SQRT
!                                  Define function
      F(X) = SQRT(X)
!                                  Set up interpolation points
      DO 10  I=1, NDATA
         XDATA(I) = FLOAT(I-1)/FLOAT(NDATA-1)
         FDATA(I) = F(XDATA(I))
   10 CONTINUE
!                                  Generate knot sequence
      CALL BSNAK (NDATA, XDATA, KORDER, XKNOT)
!                                  Interpolate
      CALL BSINT (NDATA, XDATA, FDATA, KORDER, XKNOT, BSCOEF)
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Write heading
      WRITE (NOUT,99999)
!                                  Print on a finer grid
      NCOEF = NDATA
      XT    = XDATA(1)
!                                  Evaluate spline
      BT    = BSVAL(XT,KORDER,XKNOT,NCOEF,BSCOEF)
      WRITE (NOUT,99998) XT, BT, F(XT) - BT
      DO 20  I=2, NDATA
         XT = (XDATA(I-1)+XDATA(I))/2.0
!                                  Evaluate spline
         BT = BSVAL(XT,KORDER,XKNOT,NCOEF,BSCOEF)
         WRITE (NOUT,99998) XT, BT, F(XT) - BT
         XT = XDATA(I)
!                                  Evaluate spline
         BT = BSVAL(XT,KORDER,XKNOT,NCOEF,BSCOEF)
         WRITE (NOUT,99998) XT, BT, F(XT) - BT
   20 CONTINUE
99998 FORMAT (' ', F6.4, 15X, F8.4, 12X, F11.6)
99999 FORMAT (/, 6X, 'X', 19X, 'S(X)', 18X, 'Error', /)
      END
```

Output

```
     X                   S(X)                  Error
0.0000                 0.0000               0.000000
```

```
 0.1250              0.2918             0.061781
 0.2500              0.5000             0.000000
 0.3750              0.6247            -0.012311
 0.5000              0.7071             0.000000
 0.6250              0.7886             0.002013
 0.7500              0.8660             0.000000
 0.8750              0.9365            -0.001092
 1.0000              1.0000             0.000000
```

BSNAK

Computes the "not-a-knot" spline knot sequence.

Required Arguments

NDATA — Number of data points. (Input)

XDATA — Array of length `NDATA` containing the location of the data points. (Input)

KORDER — Order of the spline. (Input)

XKNOT — Array of length `NDATA` + `KORDER` containing the knot sequence. (Output)

FORTRAN 90 Interface

Generic: `CALL BSNAK (NDATA, XDATA, KORDER, XKNOT)`

Specific: The specific interface names are `S_BSNAK` and `D_BSNAK`.

FORTRAN 77 Interface

Single: `CALL BSNAK (NDATA, XDATA, KORDER, XKNOT)`

Double: The double precision name is `DBSNAK`.

Description

Given the data points x = `XDATA` , the order of the spline k = `KORDER`, and the number N = `NDATA` of elements in `XDATA`, the subroutine `BSNAK` returns in $\mathbf{t}$ = `XKNOT` a knot sequence that is appropriate for interpolation of data on x by splines of order k. The vector $\mathbf{t}$ contains the knot sequence in its first $N + k$ positions. If k is even and we assume that the entries in the input vector x are increasing, then $\mathbf{t}$ is returned as

$$\mathbf{t}_i = x_1 \qquad \text{for } i = 1, \ldots, k$$

$$\mathbf{t}_i = x_{i-k/2} \qquad \text{for } i = k + 1, \ldots, N$$

$$\mathbf{t}_i = x_N + \varepsilon \qquad \text{for } i = N + 1, \ldots, N + k$$

where ε is a small positive constant. There is some discussion concerning this selection of knots in de Boor (1978, page 211). If k is odd, then $\mathbf{t}$ is returned as

$$\mathbf{t}_i = x_1 \quad for\ i = 1, \ldots, k$$

$$\mathbf{t}_i = \left(x_{i - \frac{k-1}{2}} + x_{i-1-\frac{k-1}{2}}\right)/2 \quad for\ i = k+1, \ldots, N$$

$$\mathbf{t}_i = x_N + \varepsilon \quad for\ \ i = N+1, \ldots, N+k$$

It is not necessary to sort the values in *x* since this is done in the routine `BSNAK`.

Comments

1. Workspace may be explicitly provided, if desired, by use of `B2NAK/DB2NAK`. The reference is:

   `CALL B2NAK (NDATA, XDATA, KORDER, XKNOT, XSRT, IWK)`

   The additional arguments are as follows:

   XSRT — Work array of length `NDATA` to hold the sorted `XDATA` values. If `XDATA` is not needed, `XSRT` may be the same as `XDATA`.

   IWK — Work array of length `NDATA` to hold the permutation of `XDATA`.

2. Informational error

Type	Code	Description
4	4	The `XDATA` values must be distinct.

3. The first knot is at the left endpoint and the last knot is slightly beyond the last endpoint. Both endpoints have multiplicity `KORDER`.

4. Interior knots have multiplicity one.

Example

In this example, we compute (for $k = 3, \ldots, 8$) six spline interpolants s_k to $F(x) = \sin(10x^3)$ on the interval [0,1]. The routine `BSNAK` is used to generate the knot sequences for s_k and then `BSINT` is called to obtain the interpolant. We evaluate the absolute error

$$|s_k - F|$$

at 100 equally spaced points and print the maximum error for each *k*.

```
      USE IMSL_LIBRARIES

      IMPLICIT   NONE
      INTEGER    KMAX, KMIN, NDATA
      PARAMETER  (KMAX=8, KMIN=3, NDATA=20)
```

```
!
      INTEGER    I, K, KORDER, NOUT
      REAL       ABS, AMAX1, BSCOEF(NDATA), DIF, DIFMAX, F,&
                 FDATA(NDATA), FLOAT, FT, SIN, ST, T, X, XDATA(NDATA),&
                 XKNOT(KMAX+NDATA), XT
      INTRINSIC  ABS, AMAX1, FLOAT, SIN
!                                  Define function and tau function
      F(X) = SIN(10.0*X*X*X)
      T(X) = 1.0 - X*X
!                                  Set up data
      DO 10  I=1, NDATA
         XT       = FLOAT(I-1)/FLOAT(NDATA-1)
         XDATA(I) = T(XT)
         FDATA(I) = F(XDATA(I))
   10 CONTINUE
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Write heading
      WRITE (NOUT,99999)
!                                  Loop over different orders
      DO 30  K=KMIN, KMAX
         KORDER = K
!                                  Generate knots
         CALL BSNAK (NDATA, XDATA, KORDER, XKNOT)
!                                  Interpolate
         CALL BSINT (NDATA, XDATA, FDATA, KORDER, XKNOT, BSCOEF)
         DIFMAX = 0.0
         DO 20  I=1, 100
            XT     = FLOAT(I-1)/99.0
!                                  Evaluate spline
            ST     = BSVAL(XT,KORDER,XKNOT,NDATA,BSCOEF)
            FT     = F(XT)
            DIF    = ABS(FT-ST)
!                                  Compute maximum difference
            DIFMAX = AMAX1(DIF,DIFMAX)
   20  CONTINUE
!                                  Print maximum difference
         WRITE (NOUT,99998) KORDER, DIFMAX
   30 CONTINUE
!
99998 FORMAT (' ', I3, 5X, F9.4)
99999 FORMAT (' KORDER', 5X, 'Maximum difference', /)
      END
```

Output

```
KORDER     Maximum difference
   3         0.0080
   4         0.0026
   5         0.0004
   6         0.0008
   7         0.0010
   8         0.0004
```

BSOPK

more...

Computes the "optimal" spline knot sequence.

Required Arguments

NDATA — Number of data points. (Input)

XDATA — Array of length NDATA containing the location of the data points. (Input)

KORDER — Order of the spline. (Input)

XKNOT — Array of length NDATA + KORDER containing the knot sequence. (Output)

FORTRAN 90 Interface

Generic: CALL BSOPK (NDATA, XDATA, KORDER, XKNOT)

Specific: The specific interface names are S_BSOPK and D_BSOPK.

FORTRAN 77 Interface

Single: CALL BSOPK (NDATA, XDATA, KORDER, XKNOT)

Double: The double precision name is DBSOPK.

Description

Given the abscissas x = XDATA for an interpolation problem and the order of the spline interpolant k = KORDER, BSOPK returns the knot sequence **t** = XKNOT that minimizes the constant in the error estimate

$$\|f - s\| \le c \, \|f^{(k)}\|$$

In the above formula, f is any function in C^k and s is the spline interpolant to f at the abscissas x with knot sequence **t**.

The algorithm is based on a routine described in de Boor (1978, page 204), which in turn is based on a theorem of Micchelli, Rivlin and Winograd (1976).

Comments

1. Workspace may be explicitly provided, if desired, by use of B2OPK/DB2OPK. The reference is:

   CALL B2OPK (NDATA, XDATA, KORDER, XKNOT, MAXIT, WK, IWK)

   The additional arguments are as follows:

   MAXIT — Maximum number of iterations of Newton's Method. (Input) A suggested value is 10.

   WK — Work array of length (NDATA – KORDER) * (3 * KORDER – 2) + 6 * NDATA + 2 * KORDER + 5.

   IWK — Work array of length NDATA.

2. Informational errors

Type	Code	Description
3	6	Newton's method iteration did not converge.
4	3	The XDATA values must be distinct.
4	4	Interpolation matrix is singular. The XDATA values may be too close together.

3. The default value for MAXIT is 10, this can be overridden by calling B2OPK/DB2OPK directly with a larger value.

Example

In this example, we compute (for k = 3, …, 8) six spline interpolants s_k to $F(x) = \sin(10x^3)$ on the interval [0, 1]. The routine BSOPK is used to generate the knot sequences for s_k and then BSINT is called to obtain the interpolant. We evaluate the absolute error

$$|s_k - F|$$

at 100 equally spaced points and print the maximum error for each k.

```
      USE BSOPK_INT
      USE BSINT_INT
      USE UMACH_INT
      USE BSVAL_INT

      IMPLICIT   NONE
      INTEGER    KMAX, KMIN, NDATA
      PARAMETER  (KMAX=8, KMIN=3, NDATA=20)
!
```

```
      INTEGER    I, K, KORDER, NOUT
      REAL       ABS, AMAX1, BSCOEF(NDATA), DIF, DIFMAX, F,&
                 FDATA(NDATA), FLOAT, FT, SIN, ST, T, X, XDATA(NDATA),&
                 XKNOT(KMAX+NDATA), XT
      INTRINSIC  ABS, AMAX1, FLOAT, SIN
!                                  Define function and tau function
      F(X) = SIN(10.0*X*X*X)
      T(X) = 1.0 - X*X
!                                  Set up data
      DO 10  I=1, NDATA
         XT       = FLOAT(I-1)/FLOAT(NDATA-1)
         XDATA(I) = T(XT)
         FDATA(I) = F(XDATA(I))
   10 CONTINUE
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Write heading
      WRITE (NOUT,99999)
!                                  Loop over different orders
      DO 30  K=KMIN, KMAX
         KORDER = K
!                                  Generate knots
         CALL BSOPK (NDATA, XDATA, KORDER, XKNOT)
!                                  Interpolate
         CALL BSINT (NDATA, XDATA, FDATA, KORDER, XKNOT, BSCOEF)
         DIFMAX = 0.0
         DO 20  I=1, 100
            XT     = FLOAT(I-1)/99.0
!                                  Evaluate spline
            ST     = BSVAL(XT,KORDER,XKNOT,NDATA,BSCOEF)
            FT     = F(XT)
            DIF    = ABS(FT-ST)
!                                  Compute maximum difference
            DIFMAX = AMAX1(DIF,DIFMAX)
   20  CONTINUE
!                                  Print maximum difference
         WRITE (NOUT,99998) KORDER, DIFMAX
   30 CONTINUE
!
99998 FORMAT (' ', I3, 5X, F9.4)
99999 FORMAT (' KORDER', 5X, 'Maximum difference', /)
      END
```

Output

```
KORDER   Maximum difference

  3        0.0096
  4        0.0018
  5        0.0005
  6        0.0004
  7        0.0007
  8        0.0035
```

BS2IN

more...

Computes a two-dimensional tensor-product spline interpolant, returning the tensor-product B-spline coefficients.

Required Arguments

XDATA — Array of length NXDATA containing the data points in the X-direction. (Input)
XDATA must be strictly increasing.

YDATA — Array of length NYDATA containing the data points in the Y-direction. (Input)
YDATA must be strictly increasing.

FDATA — Array of size NXDATA by NYDATA containing the values to be interpolated. (Input)
FDATA (I, J) is the value at (XDATA (I), YDATA(J)).

KXORD — Order of the spline in the X-direction. (Input)
KXORD must be less than or equal to NXDATA.

KYORD — Order of the spline in the Y-direction. (Input)
KYORD must be less than or equal to NYDATA.

XKNOT — Array of length NXDATA + KXORD containing the knot sequence in the X-direction. (Input)
XKNOT must be nondecreasing.

YKNOT — Array of length NYDATA + KYORD containing the knot sequence in the Y-direction. (Input)
YKNOT must be nondecreasing.

BSCOEF — Array of length NXDATA * NYDATA containing the tensor-product B-spline coefficients. (Output)
BSCOEF is treated internally as a matrix of size NXDATA by NYDATA.

Optional Arguments

NXDATA — Number of data points in the X-direction. (Input)
Default: NXDATA = size (XDATA,1).

NYDATA — Number of data points in the Y-direction. (Input)
Default: NYDATA = size (YDATA,1).

LDF — The leading dimension of FDATA exactly as specified in the dimension statement of the calling program. (Input)
Default: LDF = size (FDATA,1).

FORTRAN 90 Interface

Generic: CALL BS2IN (XDATA, YDATA, FDATA, KXORD, KYORD, XKNOT, YKNOT, BSCOEF [, …])

Specific: The specific interface names are S_BS2IN and D_BS2IN.

FORTRAN 77 Interface

Single: CALL BS2IN (NXDATA, XDATA, NYDATA, YDATA, FDATA, LDF, KXORD, KYORD, XKNOT, YKNOT, BSCOEF)

Double: The double precision name is DBS2IN.

Description

The routine BS2IN computes a tensor product spline interpolant. The tensor product spline interpolant to data $\{(x_i, y_j, f_{ij})\}$, where $1 \le i \le N_x$ and $1 \le j \le N_y$, has the form

$$\sum_{m=1}^{N_y} B_{n,k_x,\mathbf{t}_x}(x) B_{m,k_y,\mathbf{t}_y}(y)$$

where k_x and k_y are the orders of the splines. (These numbers are passed to the subroutine in KXORD and KYORD, respectively.) Likewise, $\mathbf{t}_x$ and $\mathbf{t}_y$ are the corresponding knot sequences (XKNOT and YKNOT). The algorithm requires that

$$\mathbf{t}_x(k_x) \le x_i \le \mathbf{t}_x(N_x + 1) \qquad 1 \le i \le N_x$$
$$\mathbf{t}_y(k_y) \le y_j \le \mathbf{t}_y(N_y + 1) \qquad 1 \le j \le N_y$$

Tensor product spline interpolants in two dimensions can be computed quite efficiently by solving (repeatedly) two univariate interpolation problems. The computation is motivated by the following observations. It is necessary to solve the system of equations

$$\sum_{m=1}^{N_y}\sum_{n=1}^{N_x} c_{nm} B_{n,k_x,\mathbf{t}_x}(x_i) B_{m,k_y,\mathbf{t}_y}(y_j) = f_{ij}$$

Setting

$$h_{mi} = \sum_{n=1}^{N_x} c_{nm} B_{n,k_x,\mathbf{t}_x}\left(x_i\right)$$

we note that for each fixed *i* from 1 to N_x, we have N_y linear equations in the same number of unknowns as can be seen below:

$$\sum_{m=1}^{N_y} h_{mi} B_{m,k_y,\mathbf{t}_y}\left(y_j\right) = f_{ij}$$

The same matrix appears in all of the equations above:

$$\left[B_{m,k_y,\mathbf{t}_y}\left(y_j\right)\right] 1 \le m, j \le N_y$$

Thus, we need only factor this matrix once and then apply this factorization to the N_x righthand sides. Once this is done and we have computed h_{mi}, then we must solve for the coefficients c_{nm} using the relation

$$\sum_{n=1}^{N_x} c_{nm} B_{n,k_x,\mathbf{t}_x}\left(x_i\right) = h_{mi}$$

for *m* from 1 to N_y, which again involves one factorization and N_y solutions to the different right-hand sides. The routine `BS2IN` is based on the routine `SPLI2D` by de Boor (1978, page 347).

Comments

1. Workspace may be explicitly provided, if desired, by use of `B22IN/DB22IN`. The reference is:

   ```
   CALL B22IN (NXDATA, XDATA, NYDATA, YDATA, FDATA, LDF, KXORD,
      KYORD, XKNOT, YKNOT, BSCOEF, WK, IWK)
   ```

   The additional arguments are as follows:

   WK — Work array of length `NXDATA * NYDATA + MAX((2 * KXORD − 1)` `NXDATA, (2 * KYORD − 1) * NYDATA) + MAX((3 * KXORD − 2) *` `NXDATA, (3 * KYORD − 2) * NYDATA) + 2 * MAX(NXDATA, NYDATA)`.

IWK — Work array of length MAX(NXDATA, NYDATA).

2. Informational errors

Type	Code	Description
3	1	Interpolation matrix is nearly singular. LU factorization failed.
3	2	Interpolation matrix is nearly singular. Iterative refinement failed.
4	6	The XDATA values must be strictly increasing.
4	7	The YDATA values must be strictly increasing.
4	13	Multiplicity of the knots cannot exceed the order of the spline.
4	14	The knots must be nondecreasing.
4	15	The I-th smallest element of the data point array must be greater than the I-th knot and less than the (I + K_ORD)-th knot.
4	16	The largest element of the data point array must be greater than the (N_DATA)-th knot and less than or equal to the (N_DATA + K_ORD)-th knot.
4	17	7 The smallest element of the data point array must be greater than or equal to the first knot and less than the (K_ORD + 1)st knot.

Example

In this example, a tensor product spline interpolant to a function *f* is computed. The values of the interpolant and the error on a 4 × 4 grid are displayed.

```
      USE BS2IN_INT
      USE BSNAK_INT
      USE BS2VL_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                  SPECIFICATIONS FOR PARAMETERS
      INTEGER    KXORD, KYORD, LDF, NXDATA, NXKNOT, NXVEC, NYDATA,&
                 NYKNOT, NYVEC
      PARAMETER  (KXORD=5, KYORD=2, NXDATA=21, NXVEC=4, NYDATA=6,&
                 NYVEC=4, LDF=NXDATA, NXKNOT=NXDATA+KXORD,&
                 NYKNOT=NYDATA+KYORD)
!
      INTEGER    I, J, NOUT, NXCOEF, NYCOEF
      REAL       BSCOEF(NXDATA,NYDATA), F, FDATA(LDF,NYDATA), FLOAT,&
                 X, XDATA(NXDATA), XKNOT(NXKNOT), XVEC(NXVEC), Y,&
                 YDATA(NYDATA), YKNOT(NYKNOT), YVEC(NYVEC),VL
      INTRINSIC  FLOAT
!                                  Define function
      F(X,Y) = X*X*X + X*Y
!                                  Set up interpolation points
      DO 10  I=1, NXDATA
         XDATA(I) = FLOAT(I-11)/10.0
   10 CONTINUE
!                                  Generate knot sequence
      CALL BSNAK (NXDATA, XDATA, KXORD, XKNOT)
!                                  Set up interpolation points
      DO 20  I=1, NYDATA
         YDATA(I) = FLOAT(I-1)/5.0
```

```
   20 CONTINUE
!                                  Generate knot sequence
      CALL BSNAK (NYDATA, YDATA, KYORD, YKNOT)
!                                  Generate FDATA
      DO 40  I=1, NYDATA
         DO 30  J=1, NXDATA
            FDATA(J,I) = F(XDATA(J),YDATA(I))
   30  CONTINUE
   40 CONTINUE
!                                  Interpolate
      CALL BS2IN (XDATA, YDATA, FDATA, KXORD, KYORD, XKNOT, YKNOT,&
                  BSCOEF)
      NXCOEF = NXDATA
      NYCOEF = NYDATA
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Write heading
      WRITE (NOUT,99999)
!                                  Print over a grid of
!                                  [0.0,1.0] x [0.0,1.0] at 16 points.
      DO 50  I=1, NXVEC
         XVEC(I) = FLOAT(I-1)/3.0
   50 CONTINUE
      DO 60  I=1, NYVEC
         YVEC(I) = FLOAT(I-1)/3.0
   60 CONTINUE
!                                  Evaluate spline
      DO 80  I=1, NXVEC
         DO 70  J=1, NYVEC
            VL = BS2VL (XVEC(I), YVEC(J), KXORD, KYORD, XKNOT,&
                 YKNOT, NXCOEF, NYCOEF, BSCOEF)

             WRITE (NOUT,'(3F15.4,F15.6)') XVEC(I), YVEC(J),&
                        VL, (F(XVEC(I),YVEC(J))-VL)
   70  CONTINUE
   80  CONTINUE
99999 FORMAT (13X, 'X', 14X, 'Y', 10X, 'S(X,Y)', 9X, 'Error')
      END
```

Output

```
     X              Y             S(X,Y)         Error
0.0000         0.0000         0.0000        0.000000
0.0000         0.3333         0.0000        0.000000
0.0000         0.6667         0.0000        0.000000
0.0000         1.0000         0.0000        0.000000
0.3333         0.0000         0.0370        0.000000
0.3333         0.3333         0.1481        0.000000
0.3333         0.6667         0.2593        0.000000
0.3333         1.0000         0.3704        0.000000
0.6667         0.0000         0.2963        0.000000
0.6667         0.3333         0.5185        0.000000
0.6667         0.6667         0.7407        0.000000
0.6667         1.0000         0.9630        0.000000
1.0000         0.0000         1.0000        0.000000
1.0000         0.3333         1.3333        0.000000
1.0000         0.6667         1.6667        0.000000
1.0000         1.0000         2.0000        0.000000
```

BS3IN

more...

Computes a three-dimensional tensor-product spline interpolant, returning the tensor-product B-spline coefficients.

Required Arguments

XDATA — Array of length `NXDATA` containing the data points in the x−direction. (Input)
`XDATA` must be increasing.

YDATA — Array of length `NYDATA` containing the data points in the y-direction. (Input)
`YDATA` must be increasing.

ZDATA — Array of length `NZDATA` containing the data points in the z-direction. (Input)
`ZDATA` must be increasing.

FDATA — Array of size `NXDATA` by `NYDATA` by `NZDATA` containing the values to be interpolated. (Input)
`FDATA` (`I`, `J`, `K`) contains the value at (`XDATA` (`I`), `YDATA`(`J`), `ZDATA`(`K`)).

KXORD — Order of the spline in the x-direction. (Input)
`KXORD` must be less than or equal to `NXDATA`.

KYORD — Order of the spline in the y-direction. (Input)
`KYORD` must be less than or equal to `NYDATA`.

KZORD — Order of the spline in the z-direction. (Input)
`KZORD` must be less than or equal to `NZDATA`.

XKNOT — Array of length `NXDATA` + `KXORD` containing the knot sequence in the x-direction. (Input)
`XKNOT` must be nondecreasing.

YKNOT — Array of length `NYDATA` + `KYORD` containing the knot sequence in the y-direction. (Input)
`YKNOT` must be nondecreasing.

ZKNOT — Array of length `NZDATA` + `KZORD` containing the knot sequence in the z-direction. (Input)
`ZKNOT` must be nondecreasing.

BSCOEF — Array of length NXDATA * NYDATA * NZDATA containing the tensor-product B-spline coefficients. (Output)
BSCOEF is treated internally as a matrix of size NXDATA by NYDATA by NZDATA.

Optional Arguments

NXDATA — Number of data points in the *x*-direction. (Input)
Default: NXDATA = size (XDATA,1).

NYDATA — Number of data points in the *y*-direction. (Input)
Default: NYDATA = size (YDATA,1).

NZDATA — Number of data points in the *z*-direction. (Input)
Default: NZDATA = size (ZDATA,1).

LDF — Leading dimension of FDATA exactly as specified in the dimension statement of the calling program. (Input)
Default: LDF = size (FDATA,1).

MDF — Middle dimension of FDATA exactly as specified in the dimension statement of the calling program. (Input)
Default: MDF = size (FDATA,2).

FORTRAN 90 Interface

Generic: CALL BS3IN (XDATA, YDATA, ZDATA, FDATA, KXORD, KYORD, KZORD, XKNOT, YKNOT, ZKNOT, BSCOEF [, …])

Specific: The specific interface names are S_BS3IN and D_BS3IN.

FORTRAN 77 Interface

Single: CALL BS3IN (NXDATA, XDATA, NYDATA, YDATA, NZDATA, ZDATA, FDATA, LDF, MDF, KXORD, KYORD, KZORD, XKNOT, YKNOT, ZKNOT, BSCOEF)

Double: The double precision name is DBS3IN.

Description

The routine BS3IN computes a tensor-product spline interpolant. The tensor-product spline interpolant to data $\{(x_i, y_j, z_k, f_{ijk})\}$, where $1 \le i \le N_x$, $1 \le j \le N_y$, and $1 \le k \le N_z$ has the form

$$\sum_{l=1}^{N_z}\sum_{m=1}^{N_y}\sum_{n=1}^{N_x} c_{nml} B_{n,k_x,\mathbf{t}_x}(x) B_{m,k_y,\mathbf{t}_y}(y) B_{l,k_z,\mathbf{t}_z}(z)$$

where k_x, k_y, and k_z are the orders of the splines (these numbers are passed to the subroutine in `KXORD`, `KYORD`, and `KZORD`, respectively). Likewise, $\mathbf{t}_x$, $\mathbf{t}_y$, and $\mathbf{t}_z$ are the corresponding knot sequences (`XKNOT`, `YKNOT`, and `ZKNOT`). The algorithm requires that

$$\begin{aligned}
\mathbf{t}_x(k_x) &\leq x_i \leq \mathbf{t}_x(N_x+1) \quad 1 \leq i \leq N_x \\
\mathbf{t}_y(k_y) &\leq y_j \leq \mathbf{t}_y(N_y+1) \quad 1 \leq j \leq N_y \\
\mathbf{t}_z(k_z) &\leq z_k \leq \mathbf{t}_z(N_z+1) \quad 1 \leq k \leq N_z
\end{aligned}$$

Tensor-product spline interpolants can be computed quite efficiently by solving (repeatedly) three univariate interpolation problems. The computation is motivated by the following observations. It is necessary to solve the system of equations

$$\sum_{l=1}^{N_z}\sum_{m=1}^{N_y}\sum_{n=1}^{N_x} c_{nml} B_{n,k_x,\mathbf{t}_x}(x_i) B_{m,k_y,\mathbf{t}_y}(y_j) B_{l,k_z,\mathbf{t}_z}(z_k) = f_{ijk}$$

Setting

$$h_{lij} = \sum_{m=1}^{N_y}\sum_{n=1}^{N_x} c_{nml} B_{n,k_x,\mathbf{t}_x}(x_i) B_{m,k_y,\mathbf{t}_y}(y_j)$$

we note that for each fixed pair ij we have N_z linear equations in the same number of unknowns as can be seen below:

$$\sum_{l=1}^{N_z} h_{lij} B_{l,k_z,\mathbf{t}_z}(z_k) = f_{ijk}$$

The same interpolation matrix appears in all of the equations above:

$$\left[B_{l,k_z,\mathbf{t}_z}(z_k) \right] \qquad 1 \leq l,k \leq N_z$$

Thus, we need only factor this matrix once and then apply it to the $N_x N_y$ right-hand sides. Once this is done and we have computed h_{lij}, then we must solve for the coefficients c_{nml} using the relation

$$\sum_{m=1}^{N_y}\sum_{n=1}^{N_x} c_{nml} B_{n,k_x,\mathbf{t}_x}\left(x_i\right) B_{m,k_y,\mathbf{t}_y}\left(y_j\right) = h_{lij}$$

that is the *bivariate* tensor-product problem addressed by the IMSL routine BS2IN. The interested reader should consult the algorithm description in the two-dimensional routine if more detail is desired. The routine BS3IN is based on the routine SPLI2D by de Boor (1978, page 347).

Comments

1. Workspace may be explicitly provided, if desired, by use of B23IN/DB23IN. The reference is:

   ```
   CALL B23IN (NXDATA, XDATA, NYDATA, YDATA, NZDAYA, ZDATA,
     FDATA, LDF, MDF, KXORD, KYORD, KZORD, XKNOT, YKNOT, ZKNOT,
     BSCOEF, WK, IWK)
   ```

   The additional arguments are as follows:

   WK — Work array of length

   ```
   MAX((2 * KXORD – 1) * NXDATA, (2 * KYORD – 1) * NYDATA,
       (2 * KZORD – 1) * NZDATA) +
   MAX((3 * KXORD – 2) * NXDATA, (3 * KYORD – 2) * NYDATA,
       (3 * KZORD – 2) * NZDATA)
   + NXDATA * NYDATA *NZDATA
   + 2 * MAX(NXDATA, NYDATA, NZDATA).
   ```

   IWK — Work array of length MAX(NXDATA, NYDATA, NZDATA).

2. Informational errors

Type	Code	Description
3	1	Interpolation matrix is nearly singular. LU factorization failed.
3	2	Interpolation matrix is nearly singular. Iterative refinement failed.
4	13	Multiplicity of the knots cannot exceed the order of the spline.
4	14	The knots must be nondecreasing.
4	15	The I-th smallest element of the data point array must be greater than the Ith knot and less than the (I + K_ORD)-th knot.
4	16	The largest element of the data point array must be greater than the (N_DATA)-th knot and less than or equal to the (N_DATA + K_ORD)-th knot.
4	17	The smallest element of the data point array must be greater than or equal to the first knot and less than the (K_ORD + 1)st knot.
4	18	The XDATA values must be strictly increasing.
4	19	The YDATA values must be strictly increasing.
4	20	The ZDATA values must be strictly increasing.

Example

In this example, a tensor-product spline interpolant to a function *f* is computed. The values of the interpolant and the error on a 4 × 4 × 2 grid are displayed.

```
      USE BS3IN_INT
      USE BSNAK_INT
      USE UMACH_INT
      USE BS3GD_INT

      IMPLICIT   NONE
!                                  SPECIFICATIONS FOR PARAMETERS
      INTEGER    KXORD, KYORD, KZORD, LDF, MDF, NXDATA, NXKNOT, NXVEC,&
                 NYDATA, NYKNOT, NYVEC, NZDATA, NZKNOT, NZVEC
      PARAMETER  (KXORD=5, KYORD=2, KZORD=3, NXDATA=21, NXVEC=4,&
                 NYDATA=6, NYVEC=4, NZDATA=8, NZVEC=2, LDF=NXDATA,&
                 MDF=NYDATA, NXKNOT=NXDATA+KXORD, NYKNOT=NYDATA+KYORD,&
                 NZKNOT=NZDATA+KZORD)
!
      INTEGER    I, J, K, NOUT, NXCOEF, NYCOEF, NZCOEF
      REAL       BSCOEF(NXDATA,NYDATA,NZDATA), F,&
                 FDATA(LDF,MDF,NZDATA), FLOAT, VALUE(NXVEC,NYVEC,NZVEC)&
                 , X, XDATA(NXDATA), XKNOT(NXKNOT), XVEC(NXVEC), Y,&
                 YDATA(NYDATA), YKNOT(NYKNOT), YVEC(NYVEC), Z,&
                 ZDATA(NZDATA), ZKNOT(NZKNOT), ZVEC(NZVEC)
      INTRINSIC  FLOAT
!                                  Define function.
      F(X,Y,Z) = X*X*X + X*Y*Z
!                                  Set up X-interpolation points
      DO 10  I=1, NXDATA
         XDATA(I) = FLOAT(I-11)/10.0
   10 CONTINUE
!                                  Set up Y-interpolation points
      DO 20  I=1, NYDATA
         YDATA(I) = FLOAT(I-1)/FLOAT(NYDATA-1)
   20 CONTINUE
!                                  Set up Z-interpolation points
      DO 30  I=1, NZDATA
         ZDATA(I) = FLOAT(I-1)/FLOAT(NZDATA-1)
   30 CONTINUE
!                                  Generate knots
      CALL BSNAK (NXDATA, XDATA, KXORD, XKNOT)
      CALL BSNAK (NYDATA, YDATA, KYORD, YKNOT)
      CALL BSNAK (NZDATA, ZDATA, KZORD, ZKNOT)
!                                  Generate FDATA
      DO 50  K=1, NZDATA
         DO 40  I=1, NYDATA
            DO 40  J=1, NXDATA
               FDATA(J,I,K) = F(XDATA(J),YDATA(I),ZDATA(K))
   40  CONTINUE
   50 CONTINUE
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Interpolate
      CALL BS3IN (XDATA, YDATA, ZDATA, FDATA, KXORD, &
                  KYORD, KZORD, XKNOT, YKNOT, ZKNOT, BSCOEF)
!
      NXCOEF = NXDATA
      NYCOEF = NYDATA
      NZCOEF = NZDATA
!                                  Write heading
      WRITE (NOUT,99999)
!                                  Print over a grid of
!                                  [-1.0,1.0] x [0.0,1.0] x [0.0,1.0]
```

```
!                                  at 32 points.
      DO 60  I=1, NXVEC
         XVEC(I) = 2.0*(FLOAT(I-1)/3.0) - 1.0
   60 CONTINUE
      DO 70  I=1, NYVEC
         YVEC(I) = FLOAT(I-1)/3.0
   70 CONTINUE
      DO 80  I=1, NZVEC
         ZVEC(I) = FLOAT(I-1)
   80 CONTINUE
!                                  Call the evaluation routine.
      CALL BS3GD (0, 0, 0, XVEC, YVEC, ZVEC,&
                  KXORD, KYORD, KZORD, XKNOT, YKNOT, ZKNOT, BSCOEF, VALUE)
      DO 110  I=1, NXVEC
         DO 100  J=1, NYVEC
            DO 90  K=1, NZVEC
               WRITE (NOUT,'(4F13.4, F13.6)') XVEC(I), YVEC(K),&
                                             ZVEC(K), VALUE(I,J,K),&
                                             F(XVEC(I),YVEC(J),ZVEC(K))&
                                              - VALUE(I,J,K)
   90       CONTINUE
  100    CONTINUE
  110 CONTINUE
99999 FORMAT (10X, 'X', 11X, 'Y', 10X, 'Z', 10X, 'S(X,Y,Z)', 7X,&
             'Error')
      END
```

Output

```
     X            Y           Z          S(X,Y,Z)       Error
-1.0000       0.0000      0.0000      -1.0000      0.000000
-1.0000       0.3333      1.0000      -1.0000      0.000000
-1.0000       0.0000      0.0000      -1.0000      0.000000
-1.0000       0.3333      1.0000      -1.3333      0.000000
-1.0000       0.0000      0.0000      -1.0000      0.000000
-1.0000       0.3333      1.0000      -1.6667      0.000000
-1.0000       0.0000      0.0000      -1.0000      0.000000
-1.0000       0.3333      1.0000      -2.0000      0.000000
-0.3333       0.0000      0.0000      -0.0370      0.000000
-0.3333       0.3333      1.0000      -0.0370      0.000000
-0.3333       0.0000      0.0000      -0.0370      0.000000
-0.3333       0.3333      1.0000      -0.1481      0.000000
-0.3333       0.0000      0.0000      -0.0370      0.000000
-0.3333       0.3333      1.0000      -0.2593      0.000000
-0.3333       0.0000      0.0000      -0.0370      0.000000
-0.3333       0.3333      1.0000      -0.3704      0.000000
 0.3333       0.0000      0.0000       0.0370      0.000000
 0.3333       0.3333      1.0000       0.0370      0.000000
 0.3333       0.0000      0.0000       0.0370      0.000000
 0.3333       0.3333      1.0000       0.1481      0.000000
 0.3333       0.0000      0.0000       0.0370      0.000000
 0.3333       0.3333      1.0000       0.2593      0.000000
 0.3333       0.0000      0.0000       0.0370      0.000000
 0.3333       0.3333      1.0000       0.3704      0.000000
 1.0000       0.0000      0.0000       1.0000      0.000000
 1.0000       0.3333      1.0000       1.0000      0.000000
 1.0000       0.0000      0.0000       1.0000      0.000000
 1.0000       0.3333      1.0000       1.3333      0.000000
 1.0000       0.0000      0.0000       1.0000      0.000000
 1.0000       0.3333      1.0000       1.6667      0.000000
 1.0000       0.0000      0.0000       1.0000      0.000000
 1.0000       0.3333      1.0000       2.0000      0.000000
```

BSVAL

This function evaluates a spline, given its B-spline representation.

Function Return Value

BSVAL — Value of the spline at X. (Output)

Required Arguments

X — Point at which the spline is to be evaluated. (Input)

KORDER — Order of the spline. (Input)

XKNOT — Array of length KORDER + NCOEF containing the knot sequence. (Input)
XKNOT must be nondecreasing.

NCOEF — Number of B-spline coefficients. (Input)

BSCOEF — Array of length NCOEF containing the B-spline coefficients. (Input)

FORTRAN 90 Interface

Generic: BSVAL (X, KORDER, XKNOT, NCOEF, BSCOEF)

Specific: The specific interface names are S_BSVAL and D_BSVAL.

FORTRAN 77 Interface

Single: BSVAL (X, KORDER, XKNOT, NCOEF, BSCOEF)

Double: The double precision function name is DBSVAL.

Description

The function BSVAL evaluates a spline (given its B-spline representation) at a specific point. It is a special case of the routine BSDER, which evaluates the derivative of a spline given its B-spline representation. The routine BSDER is based on the routine BVALUE by de Boor (1978, page 144).

Specifically, given the knot vector **t**, the number of coefficients *N*, the coefficient vector *a*, and a point *x*, BSVAL returns the number

$$\sum_{j=1}^{N} a_j B_{j,k}(x)$$

where $B_{j,k}$ is the j-th B-spline of order k for the knot sequence **t**. Note that this function routine arbitrarily treats these functions as if they were right continuous near XKNOT(KORDER) and left continuous near XKNOT(NCOEF + 1). Thus, if we have KORDER knots stacked at the left or right end point, and if we try to evaluate at these end points, then we will get the value of the limit from the interior of the interval.

Comments

1. Workspace may be explicitly provided, if desired, by use of B2VAL/DB2VAL. The reference is:

   CALL B2VAL (X, KORDER, XKNOT, NCOEF, BSCOEF, WK1, WK2, WK3)

   The additional arguments are as follows:

   WK1 — Work array of length KORDER.

   WK2 — Work array of length KORDER.

   WK3 — Work array of length KORDER.

2. Informational errors

Type	Code	Description
4	4	Multiplicity of the knots cannot exceed the order of the spline.
4	5	The knots must be nondecreasing.

Example

For an example of the use of BSVAL, see IMSL routine BSINT.

BSDER

This function evaluates the derivative of a spline, given its B-spline representation.

Function Return Value

BSDER — Value of the IDERIV-th derivative of the spline at X. (Output)

Required Arguments

IDERIV — Order of the derivative to be evaluated. (Input)
In particular, IDERIV = 0 returns the value of the spline.

X — Point at which the spline is to be evaluated. (Input)

KORDER — Order of the spline. (Input)

XKNOT — Array of length NCOEF + KORDER containing the knot sequence. (Input)
XKNOT must be nondecreasing.

NCOEF — Number of B-spline coefficients. (Input)

BSCOEF — Array of length NCOEF containing the B-spline coefficients. (Input)

FORTRAN 90 Interface

Generic: BSDER (IDERIV, X, KORDER, XKNOT, NCOEF, BSCOEF)

Specific: The specific interface names are S_BSDER and D_BSDER.

FORTRAN 77 Interface

Single: BSDER (IDERIV, X, KORDER, XKNOT, NCOEF, BSCOEF)

Double: The double precision function name is DBSDER.

Description

The function BSDER produces the value of a spline or one of its derivatives (given its B-spline representation) at a specific point. The function BSDER is based on the routine BVALUE by de Boor (1978, page 144).

Specifically, given the knot vector **t**, the number of coefficients *N*, the coefficient vector *a*, the order of the derivative *i* and a point *x*, BSDER returns the number

$$\sum_{j=1}^{N} a_j B_{j,k}^{(i)}(x)$$

where $B_{j,k}$ is the *j*-th B-spline of order *k* for the knot sequence **t**. Note that this function routine arbitrarily treats these functions as if they were right continuous near XKNOT(KORDER) and left continuous near XKNOT(NCOEF + 1). Thus, if we have KORDER knots stacked at the left or right end point, and if we try to evaluate at these end points, then we will get the value of the limit from the interior of the interval.

Comments

1. Workspace may be explicitly provided, if desired, by use of B2DER/DB2DER. The reference is:

   CALL B2DER (IDERIV, X, KORDER, XKNOT, NCOEF, BSCOEF, WK1, WK2, WK3)

   The additional arguments are as follows:

   WK1 — Array of length KORDER.

   WK2 — Array of length KORDER.

   WK3 — Array of length KORDER.

2. Informational errors

Type	Code	Description
4	4	Multiplicity of the knots cannot exceed the order of the spline.
4	5	The knots must be nondecreasing.

Example

A spline interpolant to the function

$$f(x) = \sqrt{x}$$

is constructed using BSINT. The B-spline representation, which is returned by the IMSL routine BSINT, is then used by BSDER to compute the value and derivative of the interpolant. The output consists of the interpolation values and the error at the data points and the midpoints. In addition, we display the value of the derivative and the error at these same points.

```
      USE BSDER_INT
      USE BSINT_INT
      USE BSNAK_INT
      USE UMACH_INT
```

```
      IMPLICIT   NONE
      INTEGER    KORDER, NDATA, NKNOT
      PARAMETER  (KORDER=3, NDATA=5, NKNOT=NDATA+KORDER)
!
      INTEGER    I, NCOEF, NOUT
      REAL       BSCOEF(NDATA), BT0, BT1, DF, F, FDATA(NDATA),&
                 FLOAT, SQRT, X, XDATA(NDATA), XKNOT(NKNOT), XT
      INTRINSIC  FLOAT, SQRT
!                                  Define function and derivative
      F(X)   = SQRT(X)
      DF(X) = 0.5/SQRT(X)
!                                  Set up interpolation points
      DO 10  I=1, NDATA
         XDATA(I) = FLOAT(I)/FLOAT(NDATA)
         FDATA(I) = F(XDATA(I))
   10 CONTINUE
!                                  Generate knot sequence
      CALL BSNAK (NDATA, XDATA, KORDER, XKNOT)
!                                  Interpolate
      CALL BSINT (NDATA, XDATA, FDATA, KORDER, XKNOT, BSCOEF)
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Write heading
      WRITE (NOUT,99999)
!                                  Print on a finer grid
      NCOEF = NDATA
      XT    = XDATA(1)
!                                  Evaluate spline
      BT0   = BSDER(0,XT,KORDER,XKNOT,NCOEF,BSCOEF)
      BT1   = BSDER(1,XT,KORDER,XKNOT,NCOEF,BSCOEF)
      WRITE (NOUT,99998) XT, BT0, F(XT) - BT0, BT1, DF(XT) - BT1
      DO 20  I=2, NDATA
         XT  = (XDATA(I-1)+XDATA(I))/2.0
!                                  Evaluate spline
         BT0 = BSDER(0,XT,KORDER,XKNOT,NCOEF,BSCOEF)
         BT1 = BSDER(1,XT,KORDER,XKNOT,NCOEF,BSCOEF)
         WRITE (NOUT,99998) XT, BT0, F(XT) - BT0, BT1, DF(XT) - BT1
         XT  = XDATA(I)
!                                  Evaluate spline
         BT0 = BSDER(0,XT,KORDER,XKNOT,NCOEF,BSCOEF)
         BT1 = BSDER(1,XT,KORDER,XKNOT,NCOEF,BSCOEF)
         WRITE (NOUT,99998) XT, BT0, F(XT) - BT0, BT1, DF(XT) - BT1
   20 CONTINUE
99998 FORMAT (' ', F6.4, 5X, F7.4, 3X, F10.6, 5X, F8.4, 3X, F10.6)


99999 FORMAT (6X, 'X', 8X, 'S(X)', 7X, 'Error', 8X, 'S''(X)', 8X,&
              'Error', /)
      END
```

Output

```
     X         S(X)        Error         S’(X)         Error

0.2000      0.4472     0.000000      1.0423     0.075738
0.3000      0.5456     0.002084      0.9262    -0.013339
0.4000      0.6325     0.000000      0.8101    -0.019553
0.5000      0.7077    -0.000557      0.6940     0.013071
0.6000      0.7746     0.000000      0.6446     0.000869
0.7000      0.8366     0.000071      0.5952     0.002394
0.8000      0.8944     0.000000      0.5615    -0.002525
0.9000      0.9489    -0.000214      0.5279    -0.000818
1.0000      1.0000     0.000000      0.4942     0.005814
```

BS1GD

Evaluates the derivative of a spline on a grid, given its B-spline representation.

Required Arguments

IDERIV — Order of the derivative to be evaluated. (Input)
In particular, IDERIV = 0 returns the value of the spline.

XVEC — Array of length N containing the points at which the spline is to be evaluated. (Input)
XVEC should be strictly increasing.

KORDER — Order of the spline. (Input)

XKNOT — Array of length NCOEF + KORDER containing the knot sequence. (Input)
XKNOT must be nondecreasing.

BSCOEF — Array of length NCOEF containing the B-spline coefficients. (Input)

VALUE — Array of length N containing the values of the IDERIV-th derivative of the spline at the points in XVEC. (Output)

Optional Arguments

N — Length of vector XVEC. (Input)
Default: N = size (XVEC,1).

NCOEF — Number of B-spline coefficients. (Input)
Default: NCOEF = size (BSCOEF,1).

FORTRAN 90 Interface

Generic: CALL BS1GD (IDERIV, XVEC, KORDER, XKNOT, BSCOEF, VALUE [, …])

Specific: The specific interface names are S_BS1GD and D_BS1GD.

FORTRAN 77 Interface

Single: CALL BS1GD (IDERIV, N, XVEC, KORDER, XKNOT, NCOEF, BSCOEF, VALUE)

Double: The double precision name is DBS1GD.

Description

The routine BS1GD evaluates a B-spline (or its derivative) at a vector of points. That is, given a vector x of length n satisfying $x_i < x_{i+1}$ for $i = 1, \ldots, n - 1$, a derivative value j, and a B-spline s that is represented by a knot sequence and coefficient sequence, this routine returns the values

$$s^{(j)}(x_i) \quad i = 1, \ldots, n$$

in the array VALUE. The functionality of this routine is the same as that of BSDER called in a loop, however BS1GD should be much more efficient. This routine converts the B-spline representation to piecewise polynomial form using the IMSL routine BSCPP, and then uses the IMSL routine PPVAL for evaluation.

Comments

1. Workspace may be explicitly provided, if desired, by use of B21GD/DB21GD. The reference is:

   ```
   CALL B21GD (IDERIV, N, XVEC, KORDER, XKNOT, NCOEF, BSCOEF,
     VALUE, RWK1, RWK2, IWK3, RWK4, RWK5, RWK6)
   ```

   The additional arguments are as follows:

   RWK1 — Real array of length KORDER * (NCOEF – KORDER + 1).

   RWK2 — Real array of length NCOEF – KORDER + 2.

   IWK3 — Integer array of length N.

   RWK4 — Real array of length N.

   RWK5 — Real array of length N.

   RWK6 — Real array of length (KORDER + 3) * KORDER

2. Informational error

Type	Code	Description
4	5	The points in XVEC must be strictly increasing.

Example

To illustrate the use of BS1GD, we modify the example program for BSDER. In this example, a quadratic (order 3) spline interpolant to F is computed. The values and derivatives of this spline are then compared with the exact function and derivative values. The routine BS1GD is based on the routines BSPLPP and PPVALU in de Boor (1978, page 89).

```
      USE BS1GD_INT
      USE BSINT_INT
      USE BSNAK_INT
```

```
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    KORDER, NDATA, NKNOT, NFGRID
      PARAMETER  (KORDER=3, NDATA=5, NKNOT=NDATA+KORDER, NFGRID = 9)
!                                  SPECIFICATIONS FOR LOCAL VARIABLES
      INTEGER    I, NCOEF, NOUT
      REAL       ANS0(NFGRID), ANS1(NFGRID), BSCOEF(NDATA),&
                 FDATA(NDATA),&
                 X, XDATA(NDATA), XKNOT(NKNOT), XVEC(NFGRID)
!                                  SPECIFICATIONS FOR INTRINSICS
      INTRINSIC  FLOAT, SQRT
      REAL       FLOAT, SQRT
!                                  SPECIFICATIONS FOR SUBROUTINES
      REAL       DF, F
!
      F(X)  = SQRT(X)
      DF(X) = 0.5/SQRT(X)
!
      CALL UMACH (2, NOUT)
!                                  Set up interpolation points
      DO 10  I=1, NDATA
         XDATA(I) = FLOAT(I)/FLOAT(NDATA)
         FDATA(I) = F(XDATA(I))
   10 CONTINUE
      CALL BSNAK (NDATA, XDATA, KORDER, XKNOT)
!                                  Interpolate
      CALL BSINT (NDATA, XDATA, FDATA, KORDER, XKNOT, BSCOEF)
      WRITE (NOUT,99999)
!                                  Print on a finer grid
      NCOEF   = NDATA
      XVEC(1) = XDATA(1)
      DO 20  I=2, 2*NDATA - 2, 2
         XVEC(I)   = (XDATA(I/2+1)+XDATA(I/2))/2.0
         XVEC(I+1) = XDATA(I/2+1)
   20 CONTINUE
      CALL BS1GD (0, XVEC, KORDER, XKNOT, BSCOEF, ANS0)
      CALL BS1GD (1, XVEC, KORDER, XKNOT, BSCOEF, ANS1)
      DO 30  I=1, 2*NDATA - 1
         WRITE (NOUT,99998) XVEC(I), ANS0(I), F(XVEC(I)) - ANS0(I),&
                           ANS1(I), DF(XVEC(I)) - ANS1(I)
   30 CONTINUE
99998 FORMAT (' ', F6.4, 5X, F7.4, 5X, F8.4, 5X, F8.4, 5X, F8.4)
99999 FORMAT (6X, 'X', 8X, 'S(X)', 7X, 'Error', 8X, 'S''(X)', 8X,&
             'Error', /)
      END
```

Output

```
     X         S(X)        Error         S’(X)        Error

0.2000      0.4472      0.0000       1.0423       0.0757
0.3000      0.5456      0.0021       0.9262      -0.0133
0.4000      0.6325      0.0000       0.8101      -0.0196
0.5000      0.7077     -0.0006       0.6940       0.0131
0.6000      0.7746      0.0000       0.6446       0.0009
0.7000      0.8366      0.0001       0.5952       0.0024
0.8000      0.8944      0.0000       0.5615      -0.0025
0.9000      0.9489     -0.0002       0.5279      -0.0008
1.0000      1.0000      0.0000       0.4942       0.0058
```

BSITG

This function evaluates the integral of a spline, given its B-spline representation.

Function Return Value

BSITG — Value of the integral of the spline from A to B. (Output)

Required Arguments

A — Lower limit of integration. (Input)

B — Upper limit of integration. (Input)

KORDER — Order of the spline. (Input)

XKNOT — Array of length KORDER + NCOEF containing the knot sequence. (Input)
XKNOT must be nondecreasing.

NCOEF — Number of B-spline coefficients. (Input)

BSCOEF — Array of length NCOEF containing the B-spline coefficients. (Input)

FORTRAN 90 Interface

Generic: BSITG (A, B, KORDER, XKNOT, NCOEF, BSCOEF)

Specific: The specific interface names are S_BSITG and D_BSITG.

FORTRAN 77 Interface

Single: BSITG (A, B, KORDER, XKNOT, NCOEF, BSCOEF)

Double: The double precision function name is DBSITG.

Description

The function BSITG computes the integral of a spline given its B-spline representation. Specifically, given the knot sequence $\mathbf{t}$ = XKNOT, the order k = KORDER, the coefficients a = BSCOEF , n = NCOEF and an interval [a, b], BSITG returns the value

$$\int_a^b \sum_{i=1}^{n} a_i B_{i,k,\mathbf{t}}(x)\,dx$$

This routine uses the identity (22) on page 151 of de Boor (1978), and it assumes that $\mathbf{t}_1 = \ldots = \mathbf{t}_k$ and $\mathbf{t}_{n+1} = \ldots = \mathbf{t}_{n+k}$.

Comments

1. Workspace may be explicitly provided, if desired, by use of `B2ITG/DB2ITG`. The reference is:

```
CALL B2ITG(A, B, KORDER, XKNOT, NCOEF, BSCOEF, TCOEF, AJ,
   DL, DR)
```

The additional arguments are as follows:

TCOEF — Work array of length `KORDER + 1`.

AJ — Work array of length `KORDER + 1`.

DL — Work array of length `KORDER + 1`.

DR — Work array of length `KORDER + 1`.

2. Informational errors

Type	Code	Description
3	7	The upper and lower endpoints of integration are equal.
3	8	The lower limit of integration is less than `XKNOT(KORDER)`.
3	9	The upper limit of integration is greater than `XKNOT(NCOEF` + 1).
4	4	Multiplicity of the knots cannot exceed the order of the spline.
4	5	The knots must be nondecreasing.

Example

We integrate the quartic (k = 5) spline that interpolates x^3 at the points $\{i/10 : i = -10, \ldots, 10\}$ over the interval [0, 1]. The exact answer is 1/4 since the interpolant reproduces cubic polynomials.

```
      USE BSITG_INT
      USE BSNAK_INT
      USE BSINT_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    KORDER, NDATA, NKNOT
      PARAMETER  (KORDER=5, NDATA=21, NKNOT=NDATA+KORDER)
!
      INTEGER    I, NCOEF, NOUT
      REAL       A, B, BSCOEF(NDATA), ERROR, EXACT, F,&
```

```
                  FDATA(NDATA), FI, FLOAT, VAL, X, XDATA(NDATA),&
                  XKNOT(NKNOT)
      INTRINSIC  FLOAT
!                                  Define function and integral
      F(X)  = X*X*X
      FI(X) = X**4/4.0
!                                  Set up interpolation points
      DO 10  I=1, NDATA
         XDATA(I) = FLOAT(I-11)/10.0
         FDATA(I) = F(XDATA(I))
   10 CONTINUE
!                                  Generate knot sequence
      CALL BSNAK (NDATA, XDATA, KORDER, XKNOT)
!                                  Interpolate
      CALL BSINT (NDATA, XDATA, FDATA, KORDER, XKNOT, BSCOEF)
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!
      NCOEF = NDATA
      A     = 0.0
      B     = 1.0
!                                  Integrate from A to B
      VAL   = BSITG(A,B,KORDER,XKNOT,NCOEF,BSCOEF)
      EXACT = FI(B) - FI(A)
      ERROR = EXACT - VAL
!                                  Print results
      WRITE (NOUT,99999) A, B, VAL, EXACT, ERROR
99999 FORMAT (' On the closed interval (', F3.1, ',', F3.1,&
             ') we have :', /, 1X, 'Computed Integral = ', F10.5, /,&
             1X, 'Exact Integral    = ', F10.5, /, 1X, 'Error           '&
             , '    = ', F10.6, /, /)
      END
```

Output

```
On the closed interval (0.0,1.0) we have :
Computed Integral =    0.25000
Exact Integral    =    0.25000
Error             =   0.000000
```

BS2VL

This function evaluates a two-dimensional tensor-product spline, given its tensor-product B-spline representation.

Function Return Value

BS2VL — Value of the spline at (X, Y). (Output)

Required Arguments

X — X-coordinate of the point at which the spline is to be evaluated. (Input)

Y — Y-coordinate of the point at which the spline is to be evaluated. (Input)

KXORD — Order of the spline in the X-direction. (Input)

KYORD — Order of the spline in the Y-direction. (Input)

XKNOT — Array of length NXCOEF + KXORD containing the knot sequence in the X-direction. (Input)
XKNOT must be nondecreasing.

YKNOT — Array of length NYCOEF + KYORD containing the knot sequence in the Y-direction. (Input)
YKNOT must be nondecreasing.

NXCOEF — Number of B-spline coefficients in the X-direction. (Input)

NYCOEF — Number of B-spline coefficients in the Y-direction. (Input)

BSCOEF — Array of length NXCOEF * NYCOEF containing the tensor-product B-spline coefficients. (Input)
BSCOEF is treated internally as a matrix of size NXCOEF by NYCOEF.

FORTRAN 90 Interface

Generic: BS2VL (X, Y, KXORD, KYORD, XKNOT, YKNOT, NXCOEF, NYCOEF, BSCOEF)

Specific: The specific interface names are S_BS2VL and D_BS2VL.

FORTRAN 77 Interface

Single: BS2VL (X, Y, KXORD, KYORD, XKNOT, YKNOT, NXCOEF, NYCOEF, BSCOEF)

Double: The double precision function name is DBS2VL.

Description

The function BS2VL evaluates a bivariate tensor product spline (represented as a linear combination of tensor product B-splines) at a given point. This routine is a special case of the routine BS2DR, which evaluates partial derivatives of such a spline. (The value of a spline is its zero-th derivative.) For more information see de Boor (1978, pages 351– 353).

This routine returns the value of the function *s* at a point (*x*, *y*) given the coefficients *c* by computing

$$s(x,y) = \sum_{m=1}^{N_y} \sum_{n=1}^{N_x} c_{nm} B_{n,k_x,\mathbf{t}_x}(x) B_{m,k_y,\mathbf{t}_y}(y)$$

where k_x and k_y are the orders of the splines. (These numbers are passed to the subroutine in KXORD and KYORD, respectively.) Likewise, $\mathbf{t}_x$ and $\mathbf{t}_y$ are the corresponding knot sequences (XKNOT and YKNOT).

Comments

Workspace may be explicitly provided, if desired, by use of B22VL/DB22VL. The reference is:

```
CALL B22VL (X, Y, KXORD, KYORD, XKNOT, YKNOT, NXCOEF, NYCOEF, BSCOEF,
   WK)
```

The additional argument is

WK — Work array of length 3 * MAX (KXORD, KYORD) + KYORD.

Example

For an example of the use of BS2VL, see IMSL routine BS2IN.

BS2DR

This function evaluates the derivative of a two-dimensional tensor-product spline, given its tensor-product B-spline representation.

Function Return Value

BS2DR — Value of the (IXDER, IYDER) derivative of the spline at (X, Y). (Output)

Required Arguments

IXDER — Order of the derivative in the X−direction. (Input)

IYDER — Order of the derivative in the Y−direction. (Input)

X — X−coordinate of the point at which the spline is to be evaluated. (Input)

Y — Y−coordinate of the point at which the spline is to be evaluated. (Input)

KXORD — Order of the spline in the X−direction. (Input)

KYORD — Order of the spline in the Y−direction. (Input)

XKNOT — Array of length NXCOEF + KXORD containing the knot sequence in the X−direction. (Input)
XKNOT must be nondecreasing.

YKNOT — Array of length NYCOEF + KYORD containing the knot sequence in the Y−direction. (Input)
YKNOT must be nondecreasing.

NXCOEF — Number of B-spline coefficients in the X−direction. (Input)

NYCOEF — Number of B-spline coefficients in the Y−direction. (Input)

BSCOEF — Array of length NXCOEF * NYCOEF containing the tensor-product B-spline coefficients. (Input)
BSCOEF is treated internally as a matrix of size NXCOEF by NYCOEF.

FORTRAN 90 Interface

Generic:	BS2DR (IXDER, IYDER, X, Y, KXORD, KYORD, XKNOT, YKNOT, NXCOEF, NYCOEF, BSCOEF)
Specific:	The specific interface names are S_BS2DR and D_BS2DR.

FORTRAN 77 Interface

Single: `BS2DR (IXDER, IYDER, X, Y, KXORD, KYORD, XKNOT, YKNOT, NXCOEF, NYCOEF, BSCOEF)`

Double: The double precision function name is `DBS2DR`.

Description

The routine `BS2DR` evaluates a partial derivative of a bivariate tensor-product spline (represented as a linear combination of tensor product B-splines) at a given point; see de Boor (1978, pages 351 – 353).

This routine returns the value of $s^{(p,q)}$ at a point (x, y) given the coefficients c by computing

$$s^{(p,q)}(x,y) = \sum_{m=1}^{N_y}\sum_{n=1}^{N_x} c_{nm} B^{(p)}{}_{n,k_x,\mathbf{t}_x}(x) B^{(q)}{}_{m,k_y,\mathbf{t}_y}(y)$$

where k_x and k_y are the orders of the splines. (These numbers are passed to the subroutine in `KXORD` and `KYORD`, respectively.) Likewise, $\mathbf{t}_x$ and $\mathbf{t}_y$ are the corresponding knot sequences (`XKNOT` and `YKNOT`.)

Comments

1. Workspace may be explicitly provided, if desired, by use of `B22DR/DB22DR`. The reference is:

```
CALL B22DR(IXDER, IYDER, X, Y, KXORD, KYORD, XKNOT, YKNOT,
   NXCOEF, NYCOEF, BSCOEF, WK)
```

   The additional argument is:

   WK — Work array of length `3 * MAX(KXORD, KYORD) + KYORD`.

2. Informational errors

Type	Code	Description
3	1	The point `X` does not satisfy `XKNOT(KXORD) .LE. X .LE. XKNOT(NXCOEF + 1)`.
3	2	The point `Y` does not satisfy `YKNOT(KYORD) .LE. Y .LE. YKNOT(NYCOEF + 1)`.

Example

In this example, a spline interpolant *s* to a function *f* is constructed. We use the IMSL routine BS2IN to compute the interpolant and then BS2DR is employed to compute $s^{(2,1)}(x, y)$. The values of this partial derivative and the error are computed on a 4 × 4 grid and then displayed.

```
      USE BS2DR_INT
      USE BSNAK_INT
      USE UMACH_INT
      USE BS2IN_INT

      IMPLICIT   NONE
!                                  SPECIFICATIONS FOR PARAMETERS
      INTEGER    KXORD, KYORD, LDF, NXDATA, NXKNOT, NYDATA, NYKNOT
      PARAMETER  (KXORD=5, KYORD=3, NXDATA=21, NYDATA=6, LDF=NXDATA,&
                 NXKNOT=NXDATA+KXORD, NYKNOT=NYDATA+KYORD)
!
      INTEGER    I, J, NOUT, NXCOEF, NYCOEF
      REAL       BSCOEF(NXDATA,NYDATA), F, F21,&
                 FDATA(LDF,NYDATA), FLOAT, S21, X, XDATA(NXDATA),&
                 XKNOT(NXKNOT), Y, YDATA(NYDATA), YKNOT(NYKNOT)
      INTRINSIC  FLOAT

!                                  Define function and (2,1) derivative
      F(X,Y)   = X*X*X*X + X*X*X*Y*Y
      F21(X,Y) = 12.0*X*Y
!                                  Set up interpolation points
      DO 10  I=1, NXDATA
         XDATA(I) = FLOAT(I-11)/10.0
   10 CONTINUE
!                                  Generate knot sequence
      CALL BSNAK (NXDATA, XDATA, KXORD, XKNOT)
!                                  Set up interpolation points
      DO 20  I=1, NYDATA
         YDATA(I) = FLOAT(I-1)/5.0
   20 CONTINUE
!                                  Generate knot sequence
      CALL BSNAK (NYDATA, YDATA, KYORD, YKNOT)
!                                  Generate FDATA
      DO 40  I=1, NYDATA
         DO 30  J=1, NXDATA
            FDATA(J,I) = F(XDATA(J),YDATA(I))
   30  CONTINUE
   40 CONTINUE
!                                  Interpolate
      CALL BS2IN (XDATA, YDATA, FDATA, KXORD, KYORD, XKNOT, &
                  YKNOT, BSCOEF)
      NXCOEF = NXDATA
      NYCOEF = NYDATA
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Write heading
      WRITE (NOUT,99999)
!                                  Print (2,1) derivative over a
!                                  grid of [0.0,1.0] x [0.0,1.0]
!                                  at 16 points.
      DO 60  I=1, 4
         DO 50  J=1, 4
            X    = FLOAT(I-1)/3.0
            Y    = FLOAT(J-1)/3.0
!                                  Evaluate spline
            S21 = BS2DR(2,1,X,Y,KXORD,KYORD,XKNOT,YKNOT,NXCOEF,NYCOEF,&
                  BSCOEF)
```

```
              WRITE (NOUT,'(3F15.4, F15.6)') X, Y, S21, F21(X,Y) - S21
   50  CONTINUE
   60 CONTINUE
99999 FORMAT (39X, '(2,1)', /, 13X, 'X', 14X, 'Y', 10X, 'S     (X,Y)',&
                5X, 'Error')
      END
```

Output

```
                               (2,1)
    X              Y              S     (X,Y)     Error
 0.0000         0.0000         0.0000        0.000000
 0.0000         0.3333         0.0000        0.000000
 0.0000         0.6667         0.0000        0.000000
 0.0000         1.0000         0.0000        0.000001
 0.3333         0.0000         0.0000        0.000000
 0.3333         0.3333         1.3333        0.000002
 0.3333         0.6667         2.6667       -0.000002
 0.3333         1.0000         4.0000        0.000008
 0.6667         0.0000         0.0000        0.000006
 0.6667         0.3333         2.6667       -0.000011
 0.6667         0.6667         5.3333        0.000028
 0.6667         1.0000         8.0001       -0.000134
 1.0000         0.0000        -0.0004        0.000439
 1.0000         0.3333         4.0003       -0.000319
 1.0000         0.6667         7.9996        0.000363
 1.0000         1.0000        12.0005       -0.000458
```

BS2GD

Evaluates the derivative of a two-dimensional tensor-product spline, given its tensor-product B-spline representation on a grid.

Required Arguments

IXDER — Order of the derivative in the X-direction. (Input)

IYDER — Order of the derivative in the Y-direction. (Input)

XVEC — Array of length NX containing the X-coordinates at which the spline is to be evaluated. (Input)
The points in XVEC should be strictly increasing.

YVEC — Array of length NY containing the Y-coordinates at which the spline is to be evaluated. (Input)
The points in YVEC should be strictly increasing.

KXORD — Order of the spline in the X-direction. (Input)

KYORD — Order of the spline in the Y-direction. (Input)

XKNOT — Array of length NXCOEF + KXORD containing the knot sequence in the X-direction. (Input)
XKNOT must be nondecreasing.

YKNOT — Array of length NYCOEF + KYORD containing the knot sequence in the Y-direction. (Input)
YKNOT must be nondecreasing.

BSCOEF — Array of length NXCOEF * NYCOEF containing the tensor-product B-spline coefficients. (Input)
BSCOEF is treated internally as a matrix of size NXCOEF by NYCOEF.

VALUE — Value of the (IXDER, IYDER) derivative of the spline on the NX by NY grid. (Output)
VALUE (I, J) contains the derivative of the spline at the point (XVEC(I), YVEC(J)).

Optional Arguments

NX — Number of grid points in the X-direction. (Input)
Default: NX = size (XVEC,1).

NY — Number of grid points in the Y-direction. (Input)
Default: NY = size (YVEC,1).

NXCOEF — Number of B-spline coefficients in the X-direction. (Input)
Default: NXCOEF = size (XKNOT,1) – KXORD.

NYCOEF — Number of B-spline coefficients in the Y-direction. (Input)
Default: NYCOEF = size (YKNOT,1) – KYORD.

LDVALU — Leading dimension of VALUE exactly as specified in the dimension statement of the calling program. (Input)
Default: LDVALU = SIZE (VALUE,1).

FORTRAN 90 Interface

Generic:	CALL BS2GD (IXDER, IDER, XVEC, YVEC, KXORD, KYORD, XKNOT, YKNOT, BSCOEF, VALUE [, …])
Specific:	The specific interface names are S_BS2GD and D_BS2GD.

FORTRAN 77 Interface

Single:	CALL BS2GD (IXDER, IYDER, NX, XVEC, NY, YVEC, KXORD, KYORD, XKNOT, YKNOT, NXCOEF, NYCOEF, BSCOEF, VALUE, LDVALU)
Double:	The double precision name is DBS2GD.

Description

The routine BS2GD evaluates a partial derivative of a bivariate tensor-product spline (represented as a linear combination of tensor-product B-splines) on a grid of points; see de Boor (1978, pages 351-353).

This routine returns the values of $s^{(p,q)}$ on the grid (x_i, y_j) for $i = 1, \ldots, nx$ and $j = 1, \ldots, ny$ given the coefficients c by computing (for all (x, y) in the grid)

$$s^{(p,q)}(x,y) = \sum_{m=1}^{N_y} \sum_{n=1}^{N_x} c_{nm} B_{n,k_x,\mathbf{t}_x}^{(p)}(x) B_{m,k_y,\mathbf{t}_y}^{(q)}(y)$$

where k_x and k_y are the orders of the splines. (These numbers are passed to the subroutine in KXORD and KYORD, respectively.) Likewise, $\mathbf{t}_x$ and $\mathbf{t}_y$ are the corresponding knot sequences (XKNOT and YKNOT). The grid must be ordered in the sense that $x_i < x_{i+1}$ and $y_j < y_{j+1}$.

Comments

1. Workspace may be explicitly provided, if desired, by use of B22GD/DB22GD. The reference is:

   CALL B22GD (IXDER, IYDER, NX, XVEC, NY, YVEC, KXORD, KYORD, XKNOT, YKNOT, NXCOEF, NYCOEF, BSCOEF, VALUE, LDVALU, LEFTX, LEFTY, A, B, DBIATX, DBIATY, BX, BY)

   The additional arguments are as follows:

   LEFTX — Integer work array of length NX.

   LEFTY — Integer work array of length NY.

   A — Work array of length KXORD * KXORD.

   B — Work array of length KYORD * KYORD.

   DBIATX — Work array of length KXORD * (IXDER + 1).

   DBIATY — Work array of length KYORD * (IYDER + 1).

   BX — Work array of length KXORD * NX.

   BY — Work array of length KYORD * NY.

2 Informational errors

Type	Code	Description
3	1	XVEC(I) does not satisfy XKNOT (KXORD) .LE. XVEC(I) .LE. XKNOT(NXCOEF + 1)
3	2	YVEC(I) does not satisfyYKNOT (KYORD) .LE. YVEC(I) .LE. YKNOT(NYCOEF + 1)
4	3	XVEC is not strictly increasing.
4	4	YVEC is not strictly increasing.

Example

In this example, a spline interpolant *s* to a function *f* is constructed. We use the IMSL routine BS2IN to compute the interpolant and then BS2GD is employed to compute $s^{(2,1)}(x, y)$ on a grid. The values of this partial derivative and the error are computed on a 4 × 4 grid and then displayed.

```
      USE BS2GD_INT
      USE BS2IN_INT
      USE BSNAK_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                  SPECIFICATIONS FOR LOCAL VARIABLES
      INTEGER    I, J, KXORD, KYORD, LDF, NOUT, NXCOEF, NXDATA,&
                 NYCOEF, NYDATA
      REAL       DCCFD(21,6), DOCBSC(21,6), DOCXD(21), DOCXK(26),&
                 DOCYD(6), DOCYK(9), F, F21, FLOAT, VALUE(4,4),&
                 X, XVEC(4), Y, YVEC(4)
```

```
      INTRINSIC  FLOAT
!                                  Define function and derivative
      F(X,Y)   = X*X*X*X + X*X*X*Y*Y
      F21(X,Y) = 12.0*X*Y
!                                  Initialize/Setup
      CALL UMACH (2, NOUT)
      KXORD  = 5
      KYORD  = 3
      NXDATA = 21
      NYDATA = 6
      LDF    = NXDATA
!                                  Set up interpolation points
      DO 10  I=1, NXDATA
         DOCXD(I) = FLOAT(I-11)/10.0
   10 CONTINUE
!                                  Set up interpolation points
      DO 20  I=1, NYDATA
         DOCYD(I) = FLOAT(I-1)/5.0
   20 CONTINUE
!                                  Generate knot sequence
      CALL BSNAK (NXDATA, DOCXD, KXORD, DOCXK)
!                                  Generate knot sequence
      CALL BSNAK (NYDATA, DOCYD, KYORD, DOCYK)
!                                  Generate FDATA
      DO 40  I=1, NYDATA
         DO 30  J=1, NXDATA
            DCCFD(J,I) = F(DOCXD(J),DOCYD(I))
   30  CONTINUE
   40 CONTINUE
!                                  Interpolate
      CALL BS2IN (DOCXD, DOCYD, DCCFD, KXORD, KYORD, &
                  DOCXK, DOCYK, DOCBSC)
!                                  Print (2,1) derivative over a
!                                  grid of [0.0,1.0] x [0.0,1.0]
!                                  at 16 points.
      NXCOEF = NXDATA
      NYCOEF = NYDATA
      WRITE (NOUT,99999)
      DO 50  I=1, 4
         XVEC(I) = FLOAT(I-1)/3.0
         YVEC(I) = XVEC(I)
   50 CONTINUE
      CALL BS2GD (2, 1, XVEC, YVEC, KXORD, KYORD, DOCXK, DOCYK,&
                  DOCBSC, VALUE)
      DO 70  I=1, 4
         DO 60  J=1, 4
            WRITE (NOUT,'(3F15.4,F15.6)') XVEC(I), YVEC(J),&
                                         VALUE(I,J),&
                                         F21(XVEC(I),YVEC(J)) -&
                                         VALUE(I,J)
   60  CONTINUE
   70 CONTINUE
99999 FORMAT (39X, '(2,1)', /, 13X, 'X', 14X, 'Y', 10X, 'S    (X,Y)',&
             5X, 'Error')
      END
```

Output

```
                          (2,1)
    X              Y          S    (X,Y)      Error
0.0000         0.0000         0.0000       0.000000
0.0000         0.3333         0.0000       0.000000
0.0000         0.6667         0.0000       0.000000
0.0000         1.0000         0.0000       0.000001
0.3333         0.0000         0.0000      -0.000001
```

```
 0.3333          0.3333          1.3333        0.000001
 0.3333          0.6667          2.6667       -0.000004
 0.3333          1.0000          4.0000        0.000008
 0.6667          0.0000          0.0000       -0.000001
 0.6667          0.3333          2.6667       -0.000008
 0.6667          0.6667          5.3333        0.000038
 0.6667          1.0000          8.0001       -0.000113
 1.0000          0.0000         -0.0005        0.000488
 1.0000          0.3333          4.0004       -0.000412
 1.0000          0.6667          7.9995        0.000488
 1.0000          1.0000         12.0002       -0.000244
```

BS2IG

This function evaluates the integral of a tensor-product spline on a rectangular domain, given its tensor-product B-spline representation.

Function Return Value

BS2IG — Integral of the spline over the rectangle (A, B) by (C, D). (Output)

Required Arguments

A — Lower limit of the X-variable. (Input)

B — Upper limit of the X-variable. (Input)

C — Lower limit of the Y-variable. (Input)

D — Upper limit of the Y-variable. (Input)

KXORD — Order of the spline in the X-direction. (Input)

KYORD — Order of the spline in the Y-direction. (Input)

XKNOT — Array of length NXCOEF + KXORD containing the knot sequence in the X-direction. (Input)
XKNOT must be nondecreasing.

YKNOT — Array of length NYCOEF + KYORD containing the knot sequence in the Y-direction. (Input)
YKNOT must be nondecreasing.

BSCOEF — Array of length NXCOEF * NYCOEF containing the tensor-product B-spline coefficients. (Input)
BSCOEF is treated internally as a matrix of size NXCOEF by NYCOEF.

Optional Arguments

NXCOEF — Number of B-spline coefficients in the X-direction. (Input)
Default: NXCOEF = size (XKNOT,1) – KXORD.

NYCOEF — Number of B-spline coefficients in the Y-direction. (Input)
Default: NYCOEF = size (YKNOT,1) – KYORD.

FORTRAN 90 Interface

Generic: `BS2IG (A, B, C, D, KXORD, KYORD, XKNOT, YKNOT, BSCOEF [, …])`

Specific: The specific interface names are `S_BS2IG` and `D_BS2IG`.

FORTRAN 77 Interface

Single: `BS2IG (A, B, C, D, KXORD, KYORD, XKNOT, YKNOT, NXCOEF, NYCOEF, BSCOEF)`

Double: The double precision function name is `DBS2IG`.

Description

The function `BS2IG` computes the integral of a tensor-product two-dimensional spline given its B-spline representation. Specifically, given the knot sequence $\mathbf{t}_x$ = `XKNOT`, $\mathbf{t}_y$ = `YKNOT`, the order k_x = `KXORD`, k_y = `KYORD`, the coefficients $\boldsymbol{\beta}$ = `BSCOEF`, the number of coefficients n_x = `NXCOEF`, n_y = `NYCOEF` and a rectangle $[a, b]$ by $[c, d]$, `BS2IG` returns the value

$$\int_a^b \int_c^d \sum_{i=1}^{n_x} \sum_{j=1}^{n_y} \beta_{ij} B_{ij} dy dx$$

where

$$B_{i,j}(x,y) = B_{i,k_x,\mathbf{t}_x}(x) B_{j,k_y,\mathbf{t}_y}(y)$$

This routine uses the identity (22) on page 151 of de Boor (1978). It assumes (for all knot sequences) that the first and last k knots are stacked, that is, $t_1 = \ldots = t_k$ and $t_{n+1} = \ldots = t_{n+k}$, where k is the order of the spline in the x or y direction.

Comments

1. Workspace may be explicitly provided, if desired, by use of `B22IG/DB22IG`. The reference is:

```
CALL B22IG(A, B, C, D, KXORD, KYORD, XKNOT, YKNOT, NXCOEF,
   NYCOEF, BSCOEF, WK)
```

The additional argument is:

WK — Work array of length `4 * (MAX(KXORD, KYORD) + 1) + NYCOEF`.

2. Informational errors

Type	Code	Description
3	1	The lower limit of the X-integration is less than XKNOT(KXORD).
3	2	The upper limit of the X-integration is greater than XKNOT(NXCOEF + 1).
3	3	The lower limit of the Y-integration is less than YKNOT(KYORD).
3	4	The upper limit of the Y-integration is greater than YKNOT(NYCOEF + 1).
4	13	Multiplicity of the knots cannot exceed the order of the spline.
4	14	The knots must be nondecreasing.

Example

We integrate the two-dimensional tensor-product quartic (k_x = 5) by linear (k_y = 2) spline that interpolates $x^3 + xy$ at the points $\{(i/10, j/5) : i = -10, \ldots, 10$ and $j = 0, \ldots, 5\}$ over the rectangle $[0, 1] \times [.5, 1]$. The exact answer is 5/16.

```
      USE BS2IG_INT
      USE BSNAK_INT
      USE BS2IN_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                  SPECIFICATIONS FOR PARAMETERS
      INTEGER    KXORD, KYORD, LDF, NXDATA, NXKNOT, NYDATA, NYKNOT
      PARAMETER  (KXORD=5, KYORD=2, NXDATA=21, NYDATA=6, LDF=NXDATA,&
                 NXKNOT=NXDATA+KXORD, NYKNOT=NYDATA+KYORD)
!
      INTEGER    I, J, NOUT, NXCOEF, NYCOEF
      REAL       A, B, BSCOEF(NXDATA,NYDATA), C , D, F,&
                 FDATA(LDF,NYDATA), FI, FLOAT, VAL, X, XDATA(NXDATA),&
                 XKNOT(NXKNOT), Y, YDATA(NYDATA), YKNOT(NYKNOT)
      INTRINSIC  FLOAT
!                                  Define function and integral
      F(X,Y)      = X*X*X + X*Y
      FI(A,B,C ,D) = .25*((B**4-A**4)*(D-C )+(B*B-A*A)*(D*D-C *C ))
!                                  Set up interpolation points
      DO 10  I=1, NXDATA
         XDATA(I) = FLOAT(I-11)/10.0
   10 CONTINUE
!                                  Generate knot sequence
      CALL BSNAK (NXDATA, XDATA, KXORD, XKNOT)
!                                  Set up interpolation points
      DO 20  I=1, NYDATA
         YDATA(I) = FLOAT(I-1)/5.0
   20 CONTINUE
!                                  Generate knot sequence
      CALL BSNAK (NYDATA, YDATA, KYORD, YKNOT)
!                                  Generate FDATA
      DO 40  I=1, NYDATA
         DO 30  J=1, NXDATA
            FDATA(J,I) = F(XDATA(J),YDATA(I))
   30  CONTINUE
   40 CONTINUE
!                                  Interpolate
      CALL BS2IN (XDATA, YDATA, FDATA, KXORD,&
                  KYORD, XKNOT, YKNOT, BSCOEF)
```

```
!                                   Integrate over rectangle
!                                   [0.0,1.0] x [0.0,0.5]
      NXCOEF = NXDATA
      NYCOEF = NYDATA
      A      = 0.0
      B      = 1.0
      C       = 0.5
      D      = 1.0
      VAL    = BS2IG(A,B,C ,D,KXORD,KYORD,XKNOT,YKNOT,BSCOEF)
!                                   Get output unit number
      CALL UMACH (2, NOUT)
!                                   Print results
      WRITE (NOUT,99999) VAL, FI(A,B,C ,D), FI(A,B,C ,D) - VAL
99999 FORMAT (' Computed Integral = ', F10.5, /, ' Exact Integral    '&
             , '= ', F10.5, /, ' Error             '&
             , '= ', F10.6, /)
      END
```

Output

```
Computed Integral =    0.31250
Exact Integral    =    0.31250
Error             =   0.000000
```

BS3VL

This function Evaluates a three-dimensional tensor-product spline, given its tensor-product B-spline representation.

Function Return Value

BS3VL — Value of the spline at (X, Y, Z). (Output)

Required Arguments

X — X-coordinate of the point at which the spline is to be evaluated. (Input)

Y — Y-coordinate of the point at which the spline is to be evaluated. (Input)

Z — Z-coordinate of the point at which the spline is to be evaluated. (Input)

KXORD — Order of the spline in the X-direction. (Input)

KYORD — Order of the spline in the Y-direction. (Input)

KZORD — Order of the spline in the Z-direction. (Input)

XKNOT — Array of length NXCOEF + KXORD containing the knot sequence in the X-direction. (Input)
XKNOT must be nondecreasing.

YKNOT — Array of length NYCOEF + KYORD containing the knot sequence in the Y-direction. (Input)
YKNOT must be nondecreasing.

ZKNOT — Array of length NZCOEF + KZORD containing the knot sequence in the Z-direction. (Input)
ZKNOT must be nondecreasing.

NXCOEF — Number of B-spline coefficients in the X-direction. (Input)

NYCOEF — Number of B-spline coefficients in the Y-direction. (Input)

NZCOEF — Number of B-spline coefficients in the Z-direction. (Input)

BSCOEF — Array of length NXCOEF * NYCOEF * NZCOEF containing the tensor-product B-spline coefficients. (Input)
BSCOEF is treated internally as a matrix of size NXCOEF by NYCOEF by NZCOEF.

FORTRAN 90 Interface

Generic: BS3VL (X, Y, Z, KXORD, KYORD, KZORD, XKNOT, YKNOT, ZKNOT, NXCOEF, NYCOEF, NZCOEF, BSCOEF)

Specific: The specific interface names are S_BS3VL and D_BS3VL.

FORTRAN 77 Interface

Single: BS3VL (X, Y, Z, KXORD, KYORD, KZORD, XKNOT, YKNOT, ZKNOT, NXCOEF, NYCOEF, NZCOEF, BSCOEF)

Double: The double precision function name is DBS3VL.

Description

The function BS3VL evaluates a trivariate tensor-product spline (represented as a linear combination of tensor-product B-splines) at a given point. This routine is a special case of the IMSL routine BS3DR, which evaluates a partial derivative of such a spline. (The value of a spline is its zero-th derivative.) For more information, see de Boor (1978, pages 351 – 353).

This routine returns the value of the function *s* at a point (*x*, *y*, *z*) given the coefficients *c* by computing

$$s(x,y,z) = \sum_{l=1}^{N_z} \sum_{m=1}^{N_y} \sum_{n=1}^{N_x} c_{nml} B_{n,k_x,\mathbf{t}_x}(x) B_{m,k_y,\mathbf{t}_y}(y) B_{l,k_z,\mathbf{t}_z}(z)$$

where k_x, k_y, and k_z are the orders of the splines. (These numbers are passed to the subroutine in KXORD, KYORD, and KZORD, respectively.) Likewise, $\mathbf{t}_x$, $\mathbf{t}_y$, and $\mathbf{t}_z$ are the corresponding knot sequences (XKNOT, YKNOT, and ZKNOT).

Comments

Workspace may be explicitly provided, if desired, by use of B23VL/DB23VL. The reference is:

```
CALL B23VL (X, Y, Z, KXORD, KYORD, KZORD, XKNOT, YKNOT,
   ZKNOT, NXCOEF, NYCOEF, NZCOEF, BSCOEF, WK)
```

The additional argument is:

WK — Work array of length 3 * MAX(KXORD, KYORD, KZORD) + KYORD * KZORD + KZORD.

Example

For an example of the use of BS3VL, see IMSL routine BS3IN.

BS3DR

This function evaluates the derivative of a three-dimensional tensor-product spline, given its tensor-product B-spline representation.

Function Return Value

BS3DR — Value of the (IXDER, IYDER, IZDER) derivative of the spline at (X, Y, Z). (Output)

Required Arguments

IXDER — Order of the X-derivative. (Input)

IYDER — Order of the Y-derivative. (Input)

IZDER — Order of the Z-derivative. (Input)

X — X-coordinate of the point at which the spline is to be evaluated. (Input)

Y — Y-coordinate of the point at which the spline is to be evaluated. (Input)

Z — Z-coordinate of the point at which the spline is to be evaluated. (Input)

KXORD — Order of the spline in the X-direction. (Input)

KYORD — Order of the spline in the Y-direction. (Input)

KZORD — Order of the spline in the Z-direction. (Input)

XKNOT — Array of length NXCOEF + KXORD containing the knot sequence in the X-direction. (Input)
KNOT must be nondecreasing.

YKNOT — Array of length NYCOEF + KYORD containing the knot sequence in the Y-direction. (Input)
YKNOT must be nondecreasing.

ZKNOT — Array of length NZCOEF + KZORD containing the knot sequence in the Z-direction. (Input)
ZKNOT must be nondecreasing.

NXCOEF — Number of B-spline coefficients in the X-direction. (Input)

NYCOEF — Number of B-spline coefficients in the Y-direction. (Input)

NZCOEF — Number of B-spline coefficients in the Z-direction. (Input)

BSCOEF — Array of length NXCOEF * NYCOEF * NZCOEF containing the tensor-product B-spline coefficients. (Input)
BSCOEF is treated internally as a matrix of size NXCOEF by NYCOEF by NZCOEF.

FORTRAN 90 Interface

Generic: BS3DR (IXDER, IYDER, IZDER, X, Y, Z, KXORD, KYORD, KZORD, XKNOT, YKNOT, ZKNOT, NXCOEF, NYCOEF, NZCOEF, BSCOEF)

Specific: The specific interface names are S_BS3DR and D_BS3DR.

FORTRAN 77 Interface

Single: BS3DR (IXDER, IYDER, IZDER, X, Y, Z, KXORD, KYORD, KZORD, XKNOT, YKNOT, ZKNOT, NXCOEF, NYCOEF, NZCOEF, BSCOEF)

Double: The double precision function name is DBS3DR.

Description

The function BS3DR evaluates a partial derivative of a trivariate tensor-product spline (represented as a linear combination of tensor-product B-splines) at a given point. For more information, see de Boor (1978, pages 351–353).

This routine returns the value of the function $s^{(p,q,r)}$ at a point (x, y, z) given the coefficients c by computing

$$s^{(p,q,r)}(x,y,z) = \sum_{l=1}^{N_z}\sum_{m=1}^{N_y}\sum_{n=1}^{N_x} c_{nml} B_{n,k_x,\mathbf{t}_x}^{(p)}(x) B_{m,k_y,\mathbf{t}_y}^{(q)}(y) B_{l,k_z,\mathbf{t}_z}^{(r)}(z)$$

where k_x, k_y, and k_z are the orders of the splines. (These numbers are passed to the subroutine in KXORD, KYORD, and KZORD, respectively.) Likewise, $\mathbf{t}_x$, $\mathbf{t}_y$, and $\mathbf{t}_z$ are the corresponding knot sequences (XKNOT, YKNOT, and ZKNOT).

Comments

1. Workspace may be explicitly provided, if desired, by use of B23DR/DB23DR. The reference is:

```
CALL B23DR(IXDER, IYDER, IZDER, X, Y, Z, KXORD, KYORD,
   KZORD, XKNOT, YKNOT, ZKNOT, NXCOEF, NYCOEF, NZCOEF,
   BSCOEF, WK)
```

The additional argument is:

WK — Work array of length 3 * `MAX0 (KXORD, KYORD, KZORD) + KYORD * KZORD + KZORD`.

2. Informational errors

Type	Code	Description
3	1	The point `X` does not satisfy `XKNOT(KXORD) .LE. X .LE. XKNOT(NXCOEF + 1)`.
3	2	The point `Y` does not satisfy `YKNOT(KYORD) .LE. Y .LE. YKNOT(NYCOEF + 1)`.
3	3	The point `Z` does not satisfy `ZKNOT(KZORD) .LE. Z .LE. ZKNOT(NZCOEF + 1)`.

Example

In this example, a spline interpolant *s* to a function $f(x, y, z) = x^4 + y(xz)^3$ is constructed using `BS3IN`. Next, `BS3DR` is used to compute $s^{(2,0,1)}(x, y, z)$. The values of this partial derivative and the error are computed on a 4 × 4 × 2 grid and then displayed.

```
      USE BS3DR_INT
      USE BS3IN_INT
      USE BSNAK_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                  SPECIFICATIONS FOR PARAMETERS
      INTEGER    KXORD, KYORD, KZORD, LDF, MDF, NXDATA, NXKNOT,&
                 NYDATA, NYKNOT, NZDATA, NZKNOT
      PARAMETER  (KXORD=5, KYORD=2, KZORD=3, NXDATA=21, NYDATA=6,&
                 NZDATA=8, LDF=NXDATA, MDF=NYDATA,&
                 NXKNOT=NXDATA+KXORD, NYKNOT=NYDATA+KYORD,&
                 NZKNOT=NZDATA+KZORD)
!
      INTEGER    I, J, K, L, NOUT, NXCOEF, NYCOEF, NZCOEF
      REAL       BSCOEF(NXDATA,NYDATA,NZDATA), F, F201,&
                 FDATA(LDF,MDF,NZDATA), FLOAT, S201, X, XDATA(NXDATA),&
                 XKNOT(NXKNOT), Y, YDATA(NYDATA), YKNOT(NYKNOT), Z,&
                 ZDATA(NZDATA), ZKNOT(NZKNOT)
      INTRINSIC  FLOAT
!                                  Define function and (2,0,1)
!                                  derivative
      F(X,Y,Z)     = X*X*X*X + X*X*X*Y*Z*Z*Z
      F201(X,Y,Z)  = 18.0*X*Y*Z
!                                  Set up X-interpolation points
      DO 10  I=1, NXDATA
         XDATA(I)  = FLOAT(I-11)/10.0
   10 CONTINUE
!                                  Set up Y-interpolation points
      DO 20  I=1, NYDATA
         YDATA(I)  = FLOAT(I-1)/FLOAT(NYDATA-1)
   20 CONTINUE
!                                  Set up Z-interpolation points
      DO 30  I=1, NZDATA
         ZDATA(I)  = FLOAT(I-1)/FLOAT(NZDATA-1)
   30 CONTINUE
```

```
!                                  Generate knots
      CALL BSNAK (NXDATA, XDATA, KXORD, XKNOT)
      CALL BSNAK (NYDATA, YDATA, KYORD, YKNOT)
      CALL BSNAK (NZDATA, ZDATA, KZORD, ZKNOT)
!                                  Generate FDATA
      DO 50  K=1, NZDATA
         DO 40  I=1, NYDATA
            DO 40  J=1, NXDATA
               FDATA(J,I,K) = F(XDATA(J),YDATA(I),ZDATA(K))
   40  CONTINUE
   50 CONTINUE
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Interpolate&
      CALL BS3IN (XDATA, YDATA, ZDATA, FDATA, KXORD, KYORD, KZORD, XKNOT, &
                  YKNOT, ZKNOT, BSCOEF)
!
      NXCOEF = NXDATA
      NYCOEF = NYDATA
      NZCOEF = NZDATA
!                                  Write heading
      WRITE (NOUT,99999)
!                                  Print over a grid of
!                                  [-1.0,1.0] x [0.0,1.0] x [0.0,1.0]
!                                  at 32 points.
      DO 80  I=1, 4
         DO 70  J=1, 4
            DO 60  L=1, 2
               X    = 2.0*(FLOAT(I-1)/3.0) - 1.0
               Y    = FLOAT(J-1)/3.0
               Z    = FLOAT(L-1)
!                                  Evaluate spline
               S201 = BS3DR(2,0,1,X,Y,Z,KXORD,KYORD,KZORD,XKNOT,YKNOT,&
                      ZKNOT,NXCOEF,NYCOEF,NZCOEF,BSCOEF)
               WRITE (NOUT,'(3F12.4,2F12.6)') X, Y, Z, S201,&
                      F201(X,Y,Z) - S201
   60     CONTINUE
   70  CONTINUE
   80 CONTINUE
99999 FORMAT (38X, '(2,0,1)', /, 9X, 'X', 11X,&
             'Y', 11X, 'Z', 4X, 'S     (X,Y,Z)    Error')
      END
```

Output

```
                                   (2,0,1)
     X           Y           Z     S      (X,Y,Z)    Error
-1.0000      0.0000      0.0000   -0.000107    0.000107
-1.0000      0.0000      1.0000    0.000053   -0.000053
-1.0000      0.3333      0.0000    0.064051   -0.064051
-1.0000      0.3333      1.0000   -5.935941   -0.064059
-1.0000      0.6667      0.0000    0.127542   -0.127542
-1.0000      0.6667      1.0000  -11.873034   -0.126966
-1.0000      1.0000      0.0000    0.191166   -0.191166
-1.0000      1.0000      1.0000  -17.808527   -0.191473
-0.3333      0.0000      0.0000   -0.000002    0.000002
-0.3333      0.0000      1.0000    0.000000    0.000000
-0.3333      0.3333      0.0000    0.021228   -0.021228
-0.3333      0.3333      1.0000   -1.978768   -0.021232
-0.3333      0.6667      0.0000    0.042464   -0.042464
-0.3333      0.6667      1.0000   -3.957536   -0.042464
-0.3333      1.0000      0.0000    0.063700   -0.063700
-0.3333      1.0000      1.0000   -5.936305   -0.063694
 0.3333      0.0000      0.0000   -0.000003    0.000003
 0.3333      0.0000      1.0000    0.000000    0.000000
```

```
   0.3333      0.3333      0.0000   -0.021229    0.021229
   0.3333      0.3333      1.0000    1.978763    0.021238
   0.3333      0.6667      0.0000   -0.042465    0.042465
   0.3333      0.6667      1.0000    3.957539    0.042462
   0.3333      1.0000      0.0000   -0.063700    0.063700
   0.3333      1.0000      1.0000    5.936304    0.063697
   1.0000      0.0000      0.0000   -0.000098    0.000098
   1.0000      0.0000      1.0000    0.000053   -0.000053
   1.0000      0.3333      0.0000   -0.063855    0.063855
   1.0000      0.3333      1.0000    5.936146    0.063854
   1.0000      0.6667      0.0000   -0.127631    0.127631
   1.0000      0.6667      1.0000   11.873067    0.126933
   1.0000      1.0000      0.0000   -0.191442    0.191442
   1.0000      1.0000      1.0000   17.807940    0.192060
```

BS3GD

Evaluates the derivative of a three-dimensional tensor-product spline, given its tensor-product B-spline representation on a grid.

Required Arguments

IXDER — Order of the X-derivative. (Input)

IYDER — Order of the Y-derivative. (Input)

IZDER — Order of the Z-derivative. (Input)

XVEC — Array of length NX containing the *x*-coordinates at which the spline is to be evaluated. (Input)
The points in XVEC should be strictly increasing.

YVEC — Array of length NY containing the *y*-coordinates at which the spline is to be evaluated. (Input)
The points in YVEC should be strictly increasing.

ZVEC — Array of length NZ containing the *z*-coordinates at which the spline is to be evaluated. (Input)
The points in ZVEC should be strictly increasing.

KXORD — Order of the spline in the *x*-direction. (Input)

KYORD — Order of the spline in the *y*-direction. (Input)

KZORD — Order of the spline in the *z*-direction. (Input)

XKNOT — Array of length NXCOEF + KXORD containing the knot sequence in the *x*-direction. (Input)
XKNOT must be nondecreasing.

YKNOT — Array of length NYCOEF + KYORD containing the knot sequence in the *y*-direction. (Input)
YKNOT must be nondecreasing.

ZKNOT — Array of length NZCOEF + KZORD containing the knot sequence in the *z*-direction. (Input)
ZKNOT must be nondecreasing.

BSCOEF — Array of length NXCOEF * NYCOEF * NZCOEF containing the tensor-product B-spline coefficients. (Input)
BSCOEF is treated internally as a matrix of size NXCOEF by NYCOEF by NZCOEF.

VALUE — Array of size NX by NY by NZ containing the values of the (IXDER, IYDER, IZDER) derivative of the spline on the NX by NY by NZ grid. (Output)
VALUE(I, J, K) contains the derivative of the spline at the point (XVEC(I), YVEC(J), ZVEC(K)).

Optional Arguments

NX — Number of grid points in the *x*-direction. (Input)
Default: NX = size (XVEC,1).

NY — Number of grid points in the *y*-direction. (Input)
Default: NY = size (YVEC,1).

NZ — Number of grid points in the *z*-direction. (Input)
Default: NZ = size (ZVEC,1).

NXCOEF — Number of B-spline coefficients in the *x*-direction. (Input)
Default: NXCOEF = size (XKNOT,1) – KXORD.

NYCOEF — Number of B-spline coefficients in the *y*-direction. (Input)
Default: NYCOEF = size (YKNOT,1) – KYORD.

NZCOEF — Number of B-spline coefficients in the *z*-direction. (Input)
Default: NZCOEF = size (ZKNOT,1) – KZORD.

LDVALU — Leading dimension of VALUE exactly as specified in the dimension statement of the calling program. (Input)
Default: LDVALU = SIZE (VALUE,1).

MDVALU — Middle dimension of VALUE exactly as specified in the dimension statement of the calling program. (Input)
Default: MDVALU = SIZE (VALUE,2).

FORTRAN 90 Interface

Generic: CALL BS3GD (IXDER, IYDER, IZDER, XVEC, YVEC, ZVEC, KXORD, KYORD, KZORD, XKNOT, YKNOT, ZKNOT, BSCOEF, VALUE [, …])

Specific: The specific interface names are S_BS3GD and D_BS3GD.

FORTRAN 77 Interface

Single: CALL BS3GD (IXDER, IYDER, IZDER, NX, XVEC, NY, YVEC, NZ, ZVEC, KXORD, KYORD, KZORD, XKNOT, YKNOT, ZKNOT, NXCOEF, NYCOEF, NZCOEF, BSCOEF, VALUE, LDVALU, MDVALU)

Double: The double precision name is DBS3GD.

Description

The routine BS3GD evaluates a partial derivative of a trivariate tensor-product spline (represented as a linear combination of tensor-product B-splines) on a grid. For more information, see de Boor (1978, pages 351 – 353).

This routine returns the value of the function $s^{(p,q,r)}$ on the grid (x_i, y_j, z_k) for $i = 1, \ldots, nx$, $j = 1, \ldots, ny$, and $k = 1, \ldots, nz$ given the coefficients c by computing (for all (x, y, z) on the grid)

$$s^{(p,q,r)}(x,y,z) = \sum_{l=1}^{N_z}\sum_{m=1}^{N_y}\sum_{n=1}^{N_x} c_{nml} B_{n,k_x,\mathbf{t}_x}^{(p)}(x) B_{m,k_y,\mathbf{t}_y}^{(q)}(y) B_{l,k_z,\mathbf{t}_z}^{(r)}(z)$$

where k_x, k_y, and k_z are the orders of the splines. (These numbers are passed to the subroutine in KXORD, KYORD, and KZORD, respectively.) Likewise, $\mathbf{t}_x$, $\mathbf{t}_y$, and $\mathbf{t}_z$ are the corresponding knot sequences (XKNOT, YKNOT, and ZKNOT). The grid must be ordered in the sense that $x_i < x_{i+1}$, $y_j < y_{j+1}$, and $z_k < z_{k+1}$.

Comments

1. Workspace may be explicitly provided, if desired, by use of B23GD/DB23GD. The reference is:

```
CALL B23GD ((IXDER, IYDER, IZDER, NX, XVEC, NY, YVEC, NZ,
   ZVEC, KXORD, KYORD, KZORD, XKNOT, YKNOT, ZKNOT, NXCOEF,
   NYCOEF, NZCOEF, BSCOEF, VALUE, LDVALU, MDVALU, LEFTX,
   LEFTY, LEFTZ, A, B, C, DBIATX, DBIATY, DBIATZ, BX, BY, BZ)
```

The additional arguments are as follows:

LEFTX — Work array of length NX.

LEFTY — Work array of length NY.

LEFTZ — Work array of length NZ.

A — Work array of length KXORD * KXORD.

B — Work array of length KYORD * KYORD.

C — Work array of length KZORD * KZORD.

DBIATX — Work array of length KXORD * (IXDER + 1).

DBIATY — Work array of length KYORD * (IYDER + 1).

DBIATZ — Work array of length KZORD * (IZDER + 1).

BX — Work array of length KXORD * NX.

BY — Work array of length KYORD * NY.

BZ — Work array of length KZORD * NZ.

2. Informational errors

Type	Code	Description
3	1	XVEC(I) does not satisfy XKNOT(KXORD) ≤ XVEC(I) ≤ XKNOT(NXCOEF + 1).
3	2	YVEC(I) does not satisfy YKNOT(KYORD) ≤ YVEC(I) ≤ YKNOT(NYCOEF + 1).
3	3	ZVEC(I) does not satisfy ZKNOT(KZORD) ≤ ZVEC(I) ≤ ZKNOT(NZCOEF + 1).
4	4	XVEC is not strictly increasing.
4	5	YVEC is not strictly increasing.
4	6	ZVEC is not strictly increasing.

Example

In this example, a spline interpolant *s* to a function $f(x, y, z) = x^4 + y(xz)^3$ is constructed using BS3IN. Next, BS3GD is used to compute $s^{(2,0,1)}(x, y, z)$ on the grid. The values of this partial derivative and the error are computed on a $4 \times 4 \times 2$ grid and then displayed.

```
      USE BS3GD_INT
      USE BS3IN_INT
      USE BSNAK_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    KXORD, KYORD, KZORD, LDF, LDVAL, MDF, MDVAL, NXDATA,&
                 NXKNOT, NYDATA, NYKNOT, NZ, NZDATA, NZKNOT
      PARAMETER  (KXORD=5, KYORD=2, KZORD=3, LDVAL=4, MDVAL=4,&
                 NXDATA=21, NYDATA=6, NZ=2, NZDATA=8, LDF=NXDATA,&
                 MDF=NYDATA, NXKNOT=NXDATA+KXORD, NYKNOT=NYDATA+KYORD,&
                 NZKNOT=NZDATA+KZORD)
!
      INTEGER    I, J, K, L, NOUT, NXCOEF, NYCOEF, NZCOEF
      REAL       BSCOEF(NXDATA,NYDATA,NZDATA), F, F201,&
                 FDATA(LDF,MDF,NZDATA), FLOAT, VALUE(LDVAL,MDVAL,NZ),&
                 X, XDATA(NXDATA), XKNOT(NXKNOT), XVEC(LDVAL), Y,&
                 YDATA(NYDATA), YKNOT(NYKNOT), YVEC(MDVAL), Z,&
                 ZDATA(NZDATA), ZKNOT(NZKNOT), ZVEC(NZ)
      INTRINSIC  FLOAT
!
!
!
      F(X,Y,Z)    = X*X*X*X + X*X*X*Y*Z*Z*Z
      F201(X,Y,Z) = 18.0*X*Y*Z
!
      CALL UMACH (2, NOUT)
!                                 Set up X interpolation points
      DO 10  I=1, NXDATA
         XDATA(I) = 2.0*(FLOAT(I-1)/FLOAT(NXDATA-1)) - 1.0
   10 CONTINUE
!                                 Set up Y interpolation points
      DO 20  I=1, NYDATA
         YDATA(I) = FLOAT(I-1)/FLOAT(NYDATA-1)
   20 CONTINUE
!                                 Set up Z interpolation points
      DO 30  I=1, NZDATA
         ZDATA(I) = FLOAT(I-1)/FLOAT(NZDATA-1)
   30 CONTINUE
```

```
!                                  Generate knots
      CALL BSNAK (NXDATA, XDATA, KXORD, XKNOT)
      CALL BSNAK (NYDATA, YDATA, KYORD, YKNOT)
      CALL BSNAK (NZDATA, ZDATA, KZORD, ZKNOT)
!                                  Generate FDATA
      DO 50  K=1, NZDATA
         DO 40  I=1, NYDATA
            DO 40  J=1, NXDATA
               FDATA(J,I,K) = F(XDATA(J),YDATA(I),ZDATA(K))
   40  CONTINUE
   50 CONTINUE
!                                  Interpolate
      CALL BS3IN (XDATA, YDATA, ZDATA, FDATA, KXORD, KYORD,&
                  KZORD, XKNOT, YKNOT, ZKNOT, BSCOEF)
!
      NXCOEF = NXDATA
      NYCOEF = NYDATA
      NZCOEF = NZDATA
!                                  Print over a grid of
!                                  [-1.0,1.0] x [0.0,1.0] x [0.0,1.0]
!                                  at 32 points.
      DO 60  I=1, 4
         XVEC(I) = 2.0*(FLOAT(I-1)/3.0) - 1.0
   60 CONTINUE
      DO 70  J=1, 4
         YVEC(J) = FLOAT(J-1)/3.0
   70 CONTINUE
      DO 80  L=1, 2
         ZVEC(L) = FLOAT(L-1)
   80 CONTINUE
      CALL BS3GD (2, 0, 1, XVEC, YVEC, ZVEC, KXORD, KYORD,&
                  KZORD, XKNOT, YKNOT, ZKNOT, BSCOEF, VALUE)
!
!
      WRITE (NOUT,99999)
      DO 110  I=1, 4
         DO 100  J=1, 4
            DO 90  L=1, 2
               WRITE (NOUT,'(5F13.4)') XVEC(I), YVEC(J), ZVEC(L),&
                                      VALUE(I,J,L),&
                                      F201(XVEC(I),YVEC(J),ZVEC(L)) -&
                                      VALUE(I,J,L)
   90   CONTINUE
  100 CONTINUE
  110 CONTINUE
99999 FORMAT (44X, '(2,0,1)', /, 10X, 'X', 11X, 'Y', 10X, 'Z', 10X,&
             'S      (X,Y,Z)   Error')
      STOP
      END
```

Output

```
                                            (2,0,1)
          X           Y          Z          S      (X,Y,Z)   Error
      -1.0000      0.0000      0.0000     -0.0005      0.0005
      -1.0000      0.0000      1.0000      0.0002     -0.0002
      -1.0000      0.3333      0.0000      0.0641     -0.0641
      -1.0000      0.3333      1.0000     -5.9360     -0.0640
      -1.0000      0.6667      0.0000      0.1274     -0.1274
      -1.0000      0.6667      1.0000    -11.8730     -0.1270
      -1.0000      1.0000      0.0000      0.1911     -0.1911
      -1.0000      1.0000      1.0000    -17.8086     -0.1914
      -0.3333      0.0000      0.0000      0.0000      0.0000
      -0.3333      0.0000      1.0000      0.0000      0.0000
      -0.3333      0.3333      0.0000      0.0212     -0.0212
```

```
      -0.3333         0.3333         1.0000        -1.9788        -0.0212
      -0.3333         0.6667         0.0000         0.0425        -0.0425
      -0.3333         0.6667         1.0000        -3.9575        -0.0425
      -0.3333         1.0000         0.0000         0.0637        -0.0637
      -0.3333         1.0000         1.0000        -5.9363        -0.0637
       0.3333         0.0000         0.0000         0.0000         0.0000
       0.3333         0.0000         1.0000         0.0000         0.0000
       0.3333         0.3333         0.0000        -0.0212         0.0212
       0.3333         0.3333         1.0000         1.9788         0.0212
       0.3333         0.6667         0.0000        -0.0425         0.0425
       0.3333         0.6667         1.0000         3.9575         0.0425
       0.3333         1.0000         0.0000        -0.0637         0.0637
       0.3333         1.0000         1.0000         5.9363         0.0637
       1.0000         0.0000         0.0000        -0.0005         0.0005
       1.0000         0.0000         1.0000         0.0000         0.0000
       1.0000         0.3333         0.0000        -0.0637         0.0637
       1.0000         0.3333         1.0000         5.9359         0.0641
       1.0000         0.6667         0.0000        -0.1273         0.1273
       1.0000         0.6667         1.0000        11.8733         0.1267
       1.0000         1.0000         0.0000        -0.1912         0.1912
       1.0000         1.0000         1.0000        17.8096         0.1904
```

BS3IG

This function evaluates the integral of a tensor-product spline in three dimensions over a three-dimensional rectangle, given its tensor-product B-spline representation.

Function Return Value

BS3IG — Integral of the spline over the three-dimensional rectangle (A, B) by (C, D) by (E, F). (Output)

Required Arguments

A — Lower limit of the X-variable. (Input)

B — Upper limit of the X-variable. (Input)

C — Lower limit of the Y-variable. (Input)

D — Upper limit of the Y-variable. (Input)

E — Lower limit of the Z-variable. (Input)

F — Upper limit of the Z-variable. (Input)

KXORD — Order of the spline in the X-direction. (Input)

KYORD — Order of the spline in the Y-direction. (Input)

KZORD — Order of the spline in the Z-direction. (Input)

XKNOT — Array of length NXCOEF + KXORD containing the knot sequence in the X-direction. (Input) XKNOT must be nondecreasing.

YKNOT — Array of length NYCOEF + KYORD containing the knot sequence in the Y-direction. (Input) YKNOT must be nondecreasing.

ZKNOT — Array of length NZCOEF + KZORD containing the knot sequence in the Z-direction. (Input) ZKNOT must be nondecreasing.

NXCOEF — Number of B-spline coefficients in the X-direction. (Input)

NYCOEF — Number of B-spline coefficients in the Y-direction. (Input)

NZCOEF — Number of B-spline coefficients in the Z-direction. (Input)

BSCOEF — Array of length NXCOEF * NYCOEF * NZCOEF containing the tensor-product B-spline coefficients. (Input)
BSCOEF is treated internally as a matrix of size NXCOEF by NYCOEF by NZCOEF.

FORTRAN 90 Interface

Generic: BS3IG (A, B, C, D, E, F, KXORD, KYORD, KZORD, XKNOT, YKNOT, ZKNOT, NXCOEF, NYCOEF, NZCOEF, BSCOEF)

Specific: The specific interface names are S_BS3IG and D_BS3IG.

FORTRAN 77 Interface

Single: BS3IG (A, B, C, D, E, F, KXORD, KYORD, KZORD, XKNOT, YKNOT, ZKNOT, NXCOEF, NYCOEF, NZCOEF, BSCOEF)

Double: The double precision function name is DBS3IG.

Description

The routine BS3IG computes the integral of a tensor-product three-dimensional spline, given its B-spline representation. Specifically, given the knot sequence $\mathbf{t}_x$ = XKNOT, $\mathbf{t}_y$ = YKNOT, $\mathbf{t}_z$ = ZKNOT, the order k_x = KXORD, k_y = KYORD, k_z = KZORD, the coefficients β = BSCOEF, the number of coefficients n_x = NXCOEF, n_y = NYCOEF, n_z = NZCOEF, and a three-dimensional rectangle $[a, b]$ by $[c, d]$ by $[e, f]$, BS3IG returns the value

$$\int_a^b\int_c^d\int_e^f\sum_{i=1}^{n_x}\sum_{j=1}^{n_y}\sum_{m=1}^{n_z}\beta_{ijm}\, B_{ijm}\; dz\; dy\; dx$$

where

$$B_{ijm}\left(x,y,z\right) = B_{i,k_x,\mathbf{t}_x}\left(x\right)B_{j,k_y,\mathbf{t}_y}\left(y\right)B_{m,k_z\mathbf{t}_z}\left(z\right)$$

This routine uses the identity (22) on page 151 of de Boor (1978). It assumes (for all knot sequences) that the first and last k knots are stacked, that is, $\mathbf{t}_1 = \ldots = \mathbf{t}_k$ and $\mathbf{t}_{n+1} = \ldots = \mathbf{t}_{n+k}$, where k is the order of the spline in the x, y, or z direction.

Comments

1. Workspace may be explicitly provided, if desired, by use of B23IG/DB23IG. The reference is:

```
CALL B23IG(A, B, C, D, E, F, KXORD, KYORD, KZORD, XKNOT,
   YKNOT, ZKNOT, NXCOEF, NYCOEF, NZCOEF, BSCOEF, WK)
```

The additional argument is:

WK — Work array of length
`4 * (MAX(KXORD, KYORD, KZORD) + 1) + NYCOEF + NZCOEF`.

2. Informational errors

Type	**Code**	**Description**
3	1	The lower limit of the `X`-integration is less than `XKNOT`(`KXORD`).
3	2	The upper limit of the `X`-integration is greater than `XKNOT`(`NXCOEF` + 1).
3	3	The lower limit of the `Y`-integration is less than `YKNOT`(`KYORD`).
3	4	The upper limit of the `Y`-integration is greater than `YKNOT`(`NYCOEF` + 1).
3	5	The lower limit of the `Z`- integration is less than `ZKNOT`(`KZORD`).
3	6	The upper limit of the `Z`-integration is greater than `ZKNOT`(`NZCOEF` + 1).
4	13	Multiplicity of the knots cannot exceed the order of the spline.
4	14	The knots must be nondecreasing.

Example

We integrate the three-dimensional tensor-product quartic (k_x = 5) by linear (k_y = 2) by quadratic (k_z = 3) spline which interpolates $x^3 + xyz$ at the points

$$\{(i/10, j/5, m/7) : = -10, \ldots, 10, j = 0, \ldots, 5, \text{ and } m = 0, \ldots, 7\}$$

over the rectangle [0, 1] × [.5, 1] × [0, .5]. The exact answer is 11/128.

```
      USE BS3IG_INT
      USE BS3IN_INT
      USE BSNAK_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                  SPECIFICATIONS FOR PARAMETERS
      INTEGER    KXORD, KYORD, KZORD, LDF, MDF, NXDATA, NXKNOT,&
                 NYDATA, NYKNOT, NZDATA, NZKNOT
      PARAMETER  (KXORD=5, KYORD=2, KZORD=3, NXDATA=21, NYDATA=6,&
                 NZDATA=8, LDF=NXDATA, MDF=NYDATA,&
                 NXKNOT=NXDATA+KXORD, NYKNOT=NYDATA+KYORD,&
                 NZKNOT=NZDATA+KZORD)
!
      INTEGER    I, J, K, NOUT, NXCOEF, NYCOEF, NZCOEF
      REAL       A, B, BSCOEF(NXDATA,NYDATA,NZDATA), C , D, E,&
                 F, FDATA(LDF,MDF,NZDATA), FF, FIG, FLOAT, G, H, RI,&
                 RJ, VAL, X, XDATA(NXDATA), XKNOT(NXKNOT), Y,&
                 YDATA(NYDATA), YKNOT(NYKNOT), Z, ZDATA(NZDATA),&
                 ZKNOT(NZKNOT)
      INTRINSIC  FLOAT
```

```
!                                  Define function
      F(X,Y,Z) = X*X*X + X*Y*Z
!                                  Set up interpolation points
      DO 10  I=1, NXDATA
         XDATA(I) = FLOAT(I-11)/10.0
   10 CONTINUE
!                                  Generate knot sequence
      CALL BSNAK (NXDATA, XDATA, KXORD, XKNOT)
!                                  Set up interpolation points
      DO 20  I=1, NYDATA
         YDATA(I) = FLOAT(I-1)/FLOAT(NYDATA-1)
   20 CONTINUE
!                                  Generate knot sequence
      CALL BSNAK (NYDATA, YDATA, KYORD, YKNOT)
!                                  Set up interpolation points
      DO 30  I=1, NZDATA
         ZDATA(I) = FLOAT(I-1)/FLOAT(NZDATA-1)
   30 CONTINUE
!                                  Generate knot sequence
      CALL BSNAK (NZDATA, ZDATA, KZORD, ZKNOT)
!                                  Generate FDATA
      DO 50  K=1, NZDATA
         DO 40  I=1, NYDATA
            DO 40  J=1, NXDATA
               FDATA(J,I,K) = F(XDATA(J),YDATA(I),ZDATA(K))
   40  CONTINUE
   50 CONTINUE
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Interpolate
      CALL BS3IN (XDATA, YDATA, ZDATA, FDATA, KXORD, KYORD, KZORD, XKNOT, &
                  YKNOT, ZKNOT, BSCOEF)
!
      NXCOEF = NXDATA
      NYCOEF = NYDATA
      NZCOEF = NZDATA
      A      = 0.0
      B      = 1.0
      C      = 0.5
      D      = 1.0
      E      = 0.0
      FF     = 0.5
!                                  Integrate
      VAL    = BS3IG(A,B,C ,D,E,FF,KXORD,KYORD,KZORD,XKNOT,YKNOT,ZKNOT,&
               NXCOEF,NYCOEF,NZCOEF,BSCOEF)
!                                  Calculate integral directly
      G   = .5*(B**4-A**4)
      H   = (B-A)*(B+A)
      RI  = G*(D-C )
      RJ  = .5*H*(D-C )*(D+C )
      FIG = .5*(RI*(FF-E)+.5*RJ*(FF-E)*(FF+E))
!                                  Print results
      WRITE (NOUT,99999) VAL, FIG, FIG - VAL
99999 FORMAT (' Computed Integral = ', F10.5, /, ' Exact Integral    '&
             , '= ', F10.5,/, ' Error             '&
             , '= ', F10.6, /)
      END
```

Output

```
Computed Integral =    0.08594
Exact Integral    =    0.08594
Error             =   0.000000
```

BSCPP

Converts a spline in B-spline representation to piecewise polynomial representation.

Required Arguments

KORDER — Order of the spline. (Input)

XKNOT — Array of length KORDER + NCOEF containing the knot sequence. (Input)
XKNOT must be nondecreasing.

NCOEF — Number of B-spline coefficients. (Input)

BSCOEF — Array of length NCOEF containing the B-spline coefficients. (Input)

NPPCF — Number of piecewise polynomial pieces. (Output)
NPPCF is always less than or equal to NCOEF − KORDER + 1.

BREAK — Array of length (NPPCF + 1) containing the breakpoints of the piecewise polynomial representation. (Output)
BREAK must be dimensioned at least NCOEF − KORDER + 2.

PPCOEF — Array of length KORDER * NPPCF containing the local coefficients of the polynomial pieces. (Output)
PPCOEF is treated internally as a matrix of size KORDER by NPPCF.

FORTRAN 90 Interface

Generic: CALL BSCPP (KORDER, XKNOT, NCOEF, BSCOEF, NPPCF, BREAK, PPCOEF)

Specific: The specific interface names are S_BSCPP and D_BSCPP.

FORTRAN 77 Interface

Single: CALL BSCPP (KORDER, XKNOT, NCOEF, BSCOEF, NPPCF, BREAK, PPCOEF)

Double: The double precision name is DBSCPP.

Description

The routine BSCPP is based on the routine BSPLPP by de Boor (1978, page 140). This routine is used to convert a spline in B-spline representation to a piecewise polynomial (pp) representation which can then be evaluated more efficiently. There is some overhead in converting from the
B-spline representation to the pp representation, but the conversion to pp form is recommended when 3 or more function values are needed per polynomial piece.

Comments

1. Workspace may be explicitly provided, if desired, by use of B2CPP/DB2CPP. The reference is:

```
CALL B2CPP (KORDER, XKNOT, NCOEF, BSCOEFF, NPPCF, BREAK,
   PPCOEF, WK)
```

The additional argument is

WK — Work array of length (KORDER + 3) * KORDER.

2. Informational errors

Type	Code	Description
4	4	Multiplicity of the knots cannot exceed the order of the spline.
4	5	The knots must be nondecreasing.

Example

For an example of the use of BSCPP, see PPDER.

PPVAL

This function evaluates a piecewise polynomial.

Function Return Value

PPVAL — Value of the piecewise polynomial at X. (Output)

Required Arguments

X — Point at which the polynomial is to be evaluated. (Input)

BREAK — Array of length NINTV + 1 containing the breakpoints of the piecewise polynomial representation. (Input)
BREAK must be strictly increasing.

PPCOEF — Array of size KORDER * NINTV containing the local coefficients of the piecewise polynomial pieces. (Input)
PPCOEF is treated internally as a matrix of size KORDER by NINTV.

Optional Arguments

KORDER — Order of the polynomial. (Input)
Default: KORDER = size (PPCOEF,1).

NINTV — Number of polynomial pieces. (Input)
Default: NINTV = size (PPCOEF,2).

FORTRAN 90 Interface

Generic: PPVAL (X, BREAK, PPCOEF [, …])

Specific: The specific interface names are S_PPVAL and D_PPVAL.

FORTRAN 77 Interface

Single: PPVAL (X, KORDER, NINTV, BREAK, PPCOEF)

Double: The double precision function name is DPPVAL.

Description

The routine PPVAL evaluates a piecewise polynomial at a given point. This routine is a special case of the routine PPDER, which evaluates the derivative of a piecewise polynomial. (The value of a piecewise polynomial is its zero-th derivative.)

The routine PPDER is based on the routine PPVALU in de Boor (1978, page 89).

Example

In this example, a spline interpolant to a function *f* is computed using the IMSL routine BSINT. This routine represents the interpolant as a linear combination of B-splines. This representation is then converted to piecewise polynomial representation by calling the IMSL routine BSCPP. The piecewise polynomial is evaluated using PPVAL. These values are compared to the corresponding values of *f*.

```
      USE PPVAL_INT
      USE BSNAK_INT
      USE BSCPP_INT
      USE BSINT_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    KORDER, NCOEF, NDATA, NKNOT
      PARAMETER  (KORDER=4, NCOEF=20, NDATA=20, NKNOT=NDATA+KORDER)
!
      INTEGER    I, NOUT, NPPCF
      REAL       BREAK(NCOEF), BSCOEF(NCOEF), EXP, F, FDATA(NDATA),&
                 FLOAT, PPCOEF(KORDER,NCOEF), S, X, XDATA(NDATA),&
                 XKNOT(NKNOT)
      INTRINSIC  EXP, FLOAT
!                                  Define function
      F(X) = X*EXP(X)
!                                  Set up interpolation points
      DO 30  I=1, NDATA
         XDATA(I) = FLOAT(I-1)/FLOAT(NDATA-1)
         FDATA(I) = F(XDATA(I))
   30 CONTINUE
!                                  Generate knot sequence
      CALL BSNAK (NDATA, XDATA, KORDER, XKNOT)
!                                  Compute the B-spline interpolant
      CALL BSINT (NCOEF, XDATA, FDATA, KORDER, XKNOT, BSCOEF)
!                                  Convert to piecewise polynomial
      CALL BSCPP (KORDER, XKNOT, NCOEF, BSCOEF, NPPCF, BREAK, PPCOEF)
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Write heading
      WRITE (NOUT,99999)
!                                  Print the interpolant on a uniform
!                                  grid
      DO 40  I=1, NDATA
         X = FLOAT(I-1)/FLOAT(NDATA-1)
!                                  Compute value of the piecewise
!                                  polynomial
         S = PPVAL(X,BREAK,PPCOEF)
         WRITE (NOUT,'(2F12.3, E14.3)') X, S, F(X) - S
```

```
   40 CONTINUE
99999 FORMAT (11X, 'X', 8X, 'S(X)', 7X, 'Error')
      END
```

Output

```
    X        S(X)       Error
0.000       0.000     0.000E+00
0.053       0.055    -0.745E-08
0.105       0.117     0.000E+00
0.158       0.185     0.000E+00
0.211       0.260    -0.298E-07
0.263       0.342     0.298E-07
0.316       0.433     0.000E+00
0.368       0.533     0.000E+00
0.421       0.642     0.000E+00
0.474       0.761     0.596E-07
0.526       0.891     0.000E+00
0.579       1.033     0.000E+00
0.632       1.188     0.000E+00
0.684       1.356     0.000E+00
0.737       1.540    -0.119E-06
0.789       1.739     0.000E+00
0.842       1.955     0.000E+00
0.895       2.189     0.238E-06
0.947       2.443     0.238E-06
1.000       2.718     0.238E-06
```

PPDER

This function evaluates the derivative of a piecewise polynomial.

Function Return Value

PPDER — Value of the IDERIV-th derivative of the piecewise polynomial at X. (Output)

Required Arguments

X — Point at which the polynomial is to be evaluated. (Input)

BREAK — Array of length NINTV + 1 containing the breakpoints of the piecewise polynomial representation. (Input)
BREAK must be strictly increasing.

PPCOEF — Array of size KORDER * NINTV containing the local coefficients of the piecewise polynomial pieces. (Input)
PPCOEF is treated internally as a matrix of size KORDER by NINTV.

Optional Arguments

IDERIV — Order of the derivative to be evaluated. (Input)
In particular, IDERIV = 0 returns the value of the polynomial.
Default: IDERIV = 1.

KORDER — Order of the polynomial. (Input)
Default: KORDER = size (PPCOEF,1).

NINTV — Number of polynomial pieces. (Input)
Default: NINTV = size (PPCOEF,2).

FORTRAN 90 Interface

Generic: PPDER (X, BREAK, PPCOEF [, …])

Specific: The specific interface names are S_PPDER and D_PPDER.

FORTRAN 77 Interface

Single: PPDER (IDERIV, X, KORDER, NINTV, BREAK, PPCOEF)

Double: The double precision function name is DPPDER.

Description

The routine PPDER evaluates the derivative of a piecewise polynomial function *f* at a given point. This routine is based on the subroutine PPVALU by de Boor (1978, page 89). In particular, if the breakpoint sequence is stored in ξ (a vector of length N = NINTV + 1), and if the coefficients of the piecewise polynomial representation are stored in **c**, then the value of the *j*-th derivative of *f* at *x* in$[\xi_i, \xi_{i+1})$ is

$$f^{(j)}(x) = \sum_{m=j}^{k-1} c_{m+1,i} \frac{(x-\xi_i)^{m-j}}{(m-j)!}$$

when $j = 0$ to $k - 1$ and zero otherwise. Notice that this representation forces the function to be right continuous. If *x* is less than ξ_1, then *i* is set to 1 in the above formula; if *x* is greater than or equal to ξ_N, then *i* is set to $N - 1$. This has the effect of extending the piecewise polynomial representation to the real axis by extrapolation of the first and last pieces.

Example

In this example, a spline interpolant to a function *f* is computed using the IMSL routine BSINT. This routine represents the interpolant as a linear combination of B-splines. This representation is then converted to piecewise polynomial representation by calling the IMSL routine BSCPP. The piecewise polynomial's zero-th and first derivative are evaluated using PPDER. These values are compared to the corresponding values of *f*.

```
      USE IMSL_LIBRARIES

      IMPLICIT   NONE
      INTEGER    KORDER, NCOEF, NDATA, NKNOT
      PARAMETER  (KORDER=4, NCOEF=20, NDATA=20, NKNOT=NDATA+KORDER)
!
      INTEGER    I, NOUT, NPPCF
      REAL       BREAK(NCOEF), BSCOEF(NCOEF), DF, DS, EXP, F,&
                 FDATA(NDATA), FLOAT, PPCOEF(KORDER,NCOEF), S,&
                 X, XDATA(NDATA), XKNOT(NKNOT)
      INTRINSIC  EXP, FLOAT
!
      F(X)   = X*EXP(X)
      DF(X)  = (X+1.)*EXP(X)
!                                  Set up interpolation points
      DO 10  I=1, NDATA
         XDATA(I) = FLOAT(I-1)/FLOAT(NDATA-1)
         FDATA(I) = F(XDATA(I))
   10 CONTINUE
!                                  Generate knot sequence
```

```
      CALL BSNAK (NDATA, XDATA, KORDER, XKNOT)
!                                 Compute the B-spline interpolant
      CALL BSINT (NCOEF, XDATA, FDATA, KORDER, XKNOT, BSCOEF)
!                                 Convert to piecewise polynomial
      CALL BSCPP (KORDER, XKNOT, NCOEF, BSCOEF, NPPCF, BREAK, PPCOEF)
!                                 Get output unit number
      CALL UMACH (2, NOUT)
!                                 Write heading
      WRITE (NOUT,99999)
!                                 Print the interpolant on a uniform
!                                 grid
      DO 20  I=1, NDATA
         X = FLOAT(I-1)/FLOAT(NDATA-1)
!                                 Compute value of the piecewise
!                                 polynomial
         S = PPDER(X,BREAK,PPCOEF, IDERIV=0, NINTV=NPPCF)
!                                 Compute derivative of the piecewise
!                                 polynomial
         DS = PPDER(X,BREAK,PPCOEF, IDERIV=1, NINTV=NPPCF)
         WRITE (NOUT,'(2F12.3,F12.6,F12.3,F12.6)') X, S, F(X) - S, DS,&
                DF(X), DS
   20 CONTINUE
99999 FORMAT (11X, 'X', 8X, 'S(X)', 7X, 'Error', 7X, 'S''(X)', 7X,&
              'Error')
      END
```

Output

```
    X        S(X)       Error        S’(X)       Error
0.000       0.000    0.000000       1.000   -0.000112
0.053       0.055    0.000000       1.109    0.000030
0.105       0.117    0.000000       1.228   -0.000008
0.158       0.185    0.000000       1.356    0.000002
0.211       0.260    0.000000       1.494    0.000000
0.263       0.342    0.000000       1.643    0.000000
0.316       0.433    0.000000       1.804   -0.000001
0.368       0.533    0.000000       1.978    0.000002
0.421       0.642    0.000000       2.165    0.000001
0.474       0.761    0.000000       2.367    0.000000
0.526       0.891    0.000000       2.584   -0.000001
0.579       1.033    0.000000       2.817    0.000001
0.632       1.188    0.000000       3.068    0.000001
0.684       1.356    0.000000       3.338    0.000001
0.737       1.540    0.000000       3.629    0.000001
0.789       1.739    0.000000       3.941    0.000000
0.842       1.955    0.000000       4.276   -0.000006
0.895       2.189    0.000000       4.636    0.000024
0.947       2.443    0.000000       5.022   -0.000090
1.000       2.718    0.000000       5.436    0.000341
```

PP1GD

Evaluates the derivative of a piecewise polynomial on a grid.

Required Arguments

XVEC — Array of length `N` containing the points at which the piecewise polynomial is to be evaluated. (Input)
The points in `XVEC` should be strictly increasing.

BREAK — Array of length `NINTV` + 1 containing the breakpoints for the piecewise polynomial representation. (Input)
`BREAK` must be strictly increasing.

PPCOEF — Matrix of size `KORDER` by `NINTV` containing the local coefficients of the polynomial pieces. (Input)

VALUE — Array of length `N` containing the values of the `IDERIV`-th derivative of the piecewise polynomial at the points in `XVEC`. (Output)

Optional Arguments

IDERIV — Order of the derivative to be evaluated. (Input)
In particular, `IDERIV` = 0 returns the values of the piecewise polynomial.
Default: `IDERIV` = 1.

N — Length of vector `XVEC`. (Input)
Default: `N` = size (`XVEC`,1).

KORDER — Order of the polynomial. (Input)
Default: `KORDER` = size (`PPCOEF`,1).

NINTV — Number of polynomial pieces. (Input)
Default: `NINTV` = size (`PPCOEF`,2).

FORTRAN 90 Interface

Generic: `CALL PP1GD (XVEC, BREAK, PPCOEF, VALUE [, …])`

Specific: The specific interface names are `S_PP1GD` and `D_PP1GD`.

FORTRAN 77 Interface

Single: CALL PP1GD (IDERIV, N, XVEC, KORDER, NINTV, BREAK, PPCOEF, VALUE)

Double: The double precision name is DPP1GD.

Description

The routine PP1GD evaluates a piecewise polynomial function *f* (or its derivative) at a vector of points. That is, given a vector *x* of length *n* satisfying $x_i < x_{i+1}$ for $i = 1, \ldots, n - 1$, a derivative value *j*, and a piecewise polynomial function *f* that is represented by a breakpoint sequence and coefficient matrix this routine returns the values

$$f^{(j)}(x_i) \qquad i = 1, \ldots, n$$

in the array VALUE. The functionality of this routine is the same as that of PPDER called in a loop, however PP1GD is much more efficient.

Comments

1. Workspace may be explicitly provided, if desired, by use of P21GD/DP21GD. The reference is:

```
CALL P21GD (IDERIV, N, XVEC, KORDER, NINTV, BREAK, PPCOEF,
   VALUE, IWK, WORK1, WORK2)
```

   The additional arguments are as follows:

   IWK — Array of length N.

   WORK1 — Array of length N.

   WORK2 — Array of length N.

2. Informational error

Type	Code	Description
4	4	The points in XVEC must be strictly increasing.

Example

To illustrate the use of PP1GD, we modify the example program for PPDER. In this example, a piecewise polynomial interpolant to *F* is computed. The values of this polynomial are then compared with the exact function values. The routine PP1GD is based on the routine PPVALU in de Boor (1978, page 89).

```
      USE IMSL_LIBRARIES

      IMPLICIT   NONE
      INTEGER    KORDER, N, NCOEF, NDATA, NKNOT
```

```
      PARAMETER  (KORDER=4, N=20, NCOEF=20, NDATA=20,&
                 NKNOT=NDATA+KORDER)
!
      INTEGER    I, NINTV, NOUT, NPPCF
      REAL       BREAK(NCOEF), BSCOEF(NCOEF), DF, EXP, F,&
                 FDATA(NDATA), FLOAT, PPCOEF(KORDER,NCOEF), VALUE1(N),&
                 VALUE2(N), X, XDATA(NDATA), XKNOT(NKNOT), XVEC(N)
      INTRINSIC  EXP, FLOAT
!
      F(X)   = X*EXP(X)
      DF(X) = (X+1.)*EXP(X)
!                                  Set up interpolation points
      DO 10  I=1, NDATA
         XDATA(I) = FLOAT(I-1)/FLOAT(NDATA-1)
         FDATA(I) = F(XDATA(I))
   10 CONTINUE
!                                  Generate knot sequence
      CALL BSNAK (NDATA, XDATA, KORDER, XKNOT)
!                                  Compute the B-spline interpolant
      CALL BSINT (NCOEF, XDATA, FDATA, KORDER, XKNOT, BSCOEF)
!                                  Convert to piecewise polynomial
      CALL BSCPP (KORDER, XKNOT, NCOEF, BSCOEF, NPPCF, BREAK, PPCOEF)
!                                  Compute evaluation points
      DO 20  I=1, N
         XVEC(I) = FLOAT(I-1)/FLOAT(N-1)
   20 CONTINUE
!                                  Compute values of the piecewise
!                                  polynomial
      NINTV = NPPCF
      CALL PP1GD (XVEC, BREAK, PPCOEF, VALUE1, IDERIV=0, NINTV=NINTV)
!                                  Compute the values of the first
!                                  derivative of the piecewise
!                                  polynomial
      CALL PP1GD (XVEC, BREAK, PPCOEF, VALUE2, IDERIV=1, NINTV=NINTV)
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Write heading
      WRITE (NOUT,99998)
!                                  Print the results on a uniform
!                                  grid
      DO 30  I=1, N
         WRITE (NOUT,99999) XVEC(I), VALUE1(I), F(XVEC(I)) - VALUE1(I)&
                          , VALUE2(I), DF(XVEC(I)) - VALUE2(I)
   30 CONTINUE
99998 FORMAT (11X, 'X', 8X, 'S(X)', 7X, 'Error', 7X, 'S''(X)', 7X,&
             'Error')
99999 FORMAT (' ', 2F12.3, F12.6, F12.3, F12.6)
      END
```

Output

```
   X        S(X)      Error       S'(X)      Error
0.000       0.000    0.000000      1.000   -0.000112
0.053       0.055    0.000000      1.109    0.000030
0.105       0.117    0.000000      1.228   -0.000008
0.158       0.185    0.000000      1.356    0.000002
0.211       0.260    0.000000      1.494    0.000000
0.263       0.342    0.000000      1.643    0.000000
0.316       0.433    0.000000      1.804   -0.000001
0.368       0.533    0.000000      1.978    0.000002
0.421       0.642    0.000000      2.165    0.000001
0.474       0.761    0.000000      2.367    0.000000
0.526       0.891    0.000000      2.584   -0.000001
0.579       1.033    0.000000      2.817    0.000001
0.632       1.188    0.000000      3.068    0.000001
```

```
  0.684        1.356    0.000000        3.338    0.000001
  0.737        1.540    0.000000        3.629    0.000001
  0.789        1.739    0.000000        3.941    0.000000
  0.842        1.955    0.000000        4.276   -0.000006
  0.895        2.189    0.000000        4.636    0.000024
  0.947        2.443    0.000000        5.022   -0.000090
  1.000        2.718    0.000000        5.436    0.000341
```

PPITG

This function evaluates the integral of a piecewise polynomial.

Function Return Value

PPITG — Value of the integral from A to B of the piecewise polynomial. (Output)

Required Arguments

A — Lower limit of integration. (Input)

B — Upper limit of integration. (Input)

BREAK — Array of length NINTV + 1 containing the breakpoints for the piecewise polynomial. (Input)
BREAK must be strictly increasing.

PPCOEF — Array of size KORDER * NINTV containing the local coefficients of the piecewise polynomial pieces. (Input)
PPCOEF is treated internally as a matrix of size KORDER by NINTV.

Optional Arguments

KORDER — Order of the polynomial. (Input)
Default: KORDER = size (PPCOEF,1).

NINTV — Number of piecewise polynomial pieces. (Input)
Default: NINTV = size (PPCOEF,2).

FORTRAN 90 Interface

Generic: PP1TG (A, B, BREAK, PPCOEF [, …])

Specific: The specific interface names are S_PP1TG and D_PP1TG.

FORTRAN 77 Interface

Single: PP1TG (A, B, KORDER, NINTV, BREAK, PPCOEF)

Double: The double precision function name is DPP1TG.

Description

The routine PPITG evaluates the integral of a piecewise polynomial over an interval.

Example

In this example, we compute a quadratic spline interpolant to the function x^2 using the IMSL routine BSINT. We then evaluate the integral of the spline interpolant over the intervals [0, 1/2] and [0, 2]. The interpolant reproduces x^2, and hence, the values of the integrals are 1/24 and 8/3, respectively.

```
      USE IMSL_LIBRARIES

      IMPLICIT   NONE
      INTEGER    KORDER, NDATA, NKNOT
      PARAMETER  (KORDER=3, NDATA=10, NKNOT=NDATA+KORDER)
!
      INTEGER    I, NOUT, NPPCF
      REAL       A, B, BREAK(NDATA), BSCOEF(NDATA), EXACT, F,&
                 FDATA(NDATA), FI, FLOAT, PPCOEF(KORDER,NDATA),&
                 VALUE, X, XDATA(NDATA), XKNOT(NKNOT)
      INTRINSIC  FLOAT
!
      F(X)  = X*X
      FI(X) = X*X*X/3.0
!                                  Set up interpolation points
      DO 10  I=1, NDATA
         XDATA(I) = FLOAT(I-1)/FLOAT(NDATA-1)
         FDATA(I) = F(XDATA(I))
   10 CONTINUE
!                                  Generate knot sequence
      CALL BSNAK (NDATA, XDATA, KORDER, XKNOT)
!                                  Interpolate
      CALL BSINT (NDATA, XDATA, FDATA, KORDER, XKNOT, BSCOEF)
!                                  Convert to piecewise polynomial
      CALL BSCPP (KORDER, XKNOT, NDATA, BSCOEF, NPPCF, BREAK, PPCOEF)
!                                  Compute the integral of F over
!                                  [0.0,0.5]
      A     = 0.0
      B     = 0.5
      VALUE = PPITG(A,B,BREAK,PPCOEF,NINTV=NPPCF)
      EXACT = FI(B) - FI(A)
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Print the result
      WRITE (NOUT,99999) A, B, VALUE, EXACT, EXACT - VALUE
!                                  Compute the integral of F over
!                                  [0.0,2.0]
      A     = 0.0
      B     = 2.0
      VALUE = PPITG(A,B,BREAK,PPCOEF,NINTV=NPPCF)
      EXACT = FI(B) - FI(A)
!                                  Print the result
      WRITE (NOUT,99999) A, B, VALUE, EXACT, EXACT - VALUE
99999 FORMAT (' On the closed interval (', F3.1, ',', F3.1,&
              ') we have :', /, 1X, 'Computed Integral = ', F10.5, /,&
             1X, 'Exact Integral    = ', F10.5, /, 1X, 'Error          '&
             , '    = ', F10.6, /, /)
!
      END
```

Output

```
On the closed interval (0.0,0.5) we have :
Computed Integral =    0.04167
Exact Integral    =    0.04167
Error             =   0.000000

On the closed interval (0.0,2.0) we have :
Computed Integral =    2.66667
Exact Integral    =    2.66667
Error             =   0.000001
```

QDVAL

This function evaluates a function defined on a set of points using quadratic interpolation.

Function Return Value

QDVAL — Value of the quadratic interpolant at X. (Output)

Required Arguments

X — Coordinate of the point at which the function is to be evaluated. (Input)

XDATA — Array of length NDATA containing the location of the data points. (Input)
XDATA must be strictly increasing.

FDATA — Array of length NDATA containing the function values. (Input)
FDATA(I) is the value of the function at XDATA(I).

Optional Arguments

NDATA — Number of data points. (Input)
NDATA must be at least 3.
Default: NDATA = size (XDATA,1).

CHECK — Logical variable that is .TRUE. if checking of XDATA is required or .FALSE. if checking is not required. (Input)
Default: CHECK = .TRUE.

FORTRAN 90 Interface

Generic:	QDVAL (X, XDATA, FDATA [, …])
Specific:	The specific interface names are S_QDVAL and D_QDVAL.

FORTRAN 77 Interface

Single:	QDVAL (X, NDATA, XDATA, FDATA, CHECK)
Double:	The double precision name is DQDVAL.

Description

The function QDVAL interpolates a table of values, using quadratic polynomials, returning an approximation to the tabulated function. Let (x_i, f_i) for $i = 1, \ldots, n$ be the tabular data. Given a number x at which an interpolated value is desired, we first find the nearest interior grid point x_i. A quadratic interpolant q is then formed using the three points (x_{i-1}, f_{i-1}), (x_i, f_i), and (x_{i+1}, f_{i+1}). The number returned by QDVAL is $q(x)$.

Comments

Informational error

Type	Code	Description
4	3	The XDATA values must be strictly increasing.

Example

In this example, the value of sin x is approximated at π/4 by using QDVAL on a table of 33 equally spaced values.

```
      USE IMSL_LIBRARIES

      IMPLICIT   NONE
      INTEGER    NDATA
      PARAMETER  (NDATA=33)
!
      INTEGER    I, NOUT
      REAL       F, FDATA(NDATA), H, PI, QT, SIN, X,&
                 XDATA(NDATA)
      INTRINSIC  SIN
!                                  Define function
      F(X) = SIN(X)
!                                  Generate data points
      XDATA(1) = 0.0
      FDATA(1) = F(XDATA(1))
      H        = 1.0/32.0
      DO 10  I=2, NDATA
         XDATA(I) = XDATA(I-1) + H
         FDATA(I) = F(XDATA(I))
   10 CONTINUE
!                                  Get value of PI and set X
      PI = CONST('PI')
      X  = PI/4.0
!                                  Evaluate at PI/4
      QT = QDVAL(X,XDATA,FDATA)
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Print results
      WRITE (NOUT,99999) X, F(X), QT, (F(X)-QT)
!
99999 FORMAT (15X, 'X', 6X, 'F(X)', 6X, 'QDVAL', 5X, 'ERROR', //, 6X,&
             4F10.3, /)
      END
```

Output

```
     X       F(X)       QDVAL      ERROR
  0.785      0.707      0.707      0.000
```

QDDER

This function evaluates the derivative of a function defined on a set of points using quadratic interpolation.

Function Return Value

QDDER — Value of the IDERIV-th derivative of the quadratic interpolant at X. (Output)

Required Arguments

IDERIV — Order of the derivative. (Input)

X — Coordinate of the point at which the function is to be evaluated. (Input)

XDATA — Array of length NDATA containing the location of the data points. (Input) XDATA must be strictly increasing.

FDATA — Array of length NDATA containing the function values. (Input)
FDATA(I) is the value of the function at XDATA(I).

Optional Arguments

NDATA — Number of data points. (Input)
NDATA must be at least three.
Default: NDATA = size (XDATA,1).

CHECK — Logical variable that is .TRUE. if checking of XDATA is required or .FALSE. if checking is not required. (Input)
Default: CHECK = .TRUE.

FORTRAN 90 Interface

Generic: QDDER(IDERIV, X, XDATA, FDATA [, …])

Specific: The specific interface names are S_QDDER and D_QDDER.

FORTRAN 77 Interface

Single: QDDER(IDERIV, X, NDATA, XDATA, FDATA, CHECK)

Double: The double precision function name is DQDDER.

Description

The function QDDER interpolates a table of values, using quadratic polynomials, returning an approximation to the derivative of the tabulated function. Let (x_i, f_i) for $i = 1, \ldots, n$ be the tabular data. Given a number x at which an interpolated value is desired, we first find the nearest interior grid point x_i. A quadratic interpolant q is then formed using the three points $(x_{i-1}, f_{i-1})(x_i, f_i)$, and (x_{i+1}, f_{i+1}). The number returned by QDDER is $q^{(j)}(x)$, where j = IDERIV.

Comments

1. Informational error

Type	Code	Description
4	3	The XDATA values must be strictly increasing.

2. Because quadratic interpolation is used, if the order of the derivative is greater than two, then the returned value is zero.

Example

In this example, the value of sin x and its derivatives are approximated at $\pi/4$ by using QDDER on a table of 33 equally spaced values.

```
      USE IMSL_LIBRARIES

      IMPLICIT   NONE
      INTEGER    NDATA
      PARAMETER  (NDATA=33)
!
      INTEGER    I, IDERIV, NOUT
      REAL       COS, F, F1, F2, FDATA(NDATA), H, PI,&
                 QT, SIN, X, XDATA(NDATA)
      LOGICAL CHECK
      INTRINSIC  COS, SIN
!                                 Define function and derivatives
      F(X)   = SIN(X)
      F1(X)  = COS(X)
      F2(X)  = -SIN(X)
!                                 Generate data points
      XDATA(1)  = 0.0
      FDATA(1)  = F(XDATA(1))
      H         = 1.0/32.0
      DO 10  I=2, NDATA
         XDATA(I) = XDATA(I-1) + H
         FDATA(I) = F(XDATA(I))
```

```
   10 CONTINUE
!                                   Get value of PI and set X
      PI = CONST('PI')
      X  = PI/4.0
!                                   Check XDATA
      CHECK = .TRUE.
!                                   Get output unit number
      CALL UMACH (2, NOUT)
!                                   Write heading
      WRITE (NOUT,99998)
!                                   Evaluate quadratic at PI/4
      IDERIV = 0
      QT     = QDDER(IDERIV,X,XDATA,FDATA, CHECK=CHECK)
      WRITE (NOUT,99999) X, IDERIV, F(X), QT, (F(X)-QT)
      CHECK = .FALSE.
!                                   Evaluate first derivative at PI/4
      IDERIV = 1
      QT     = QDDER(IDERIV,X,XDATA,FDATA)
      WRITE (NOUT,99999) X, IDERIV, F1(X), QT, (F1(X)-QT)
!                                   Evaluate second derivative at PI/4
      IDERIV = 2
      QT     = QDDER(IDERIV,X,XDATA,FDATA, CHECK=CHECK)
      WRITE (NOUT,99999) X, IDERIV, F2(X), QT, (F2(X)-QT)
!
99998 FORMAT (33X, 'IDER', /, 15X, 'X', 6X, 'IDER', 6X, 'F    (X)',&
             5X, 'QDDER', 6X, 'ERROR', //)
99999 FORMAT (7X, F10.3, I8, 3F12.3/)
      END
```

Output

```
                        IDER
   X       IDER       F     (X)      QDDER        ERROR

0.785        0        0.707        0.707        0.000

0.785        1        0.707        0.707        0.000

0.785        2       -0.707       -0.704       -0.003
```

QD2VL

This function evaluates a function defined on a rectangular grid using quadratic interpolation.

Function Return Value

QD2VL — Value of the function at (X, Y). (Output)

Required Arguments

X — *x*-coordinate of the point at which the function is to be evaluated. (Input)

Y — *y*-coordinate of the point at which the function is to be evaluated. (Input)

XDATA — Array of length NXDATA containing the location of the data points in the *x*-direction. (Input)
XDATA must be increasing.

YDATA — Array of length NYDATA containing the location of the data points in the *y*-direction. (Input)
YDATA must be increasing.

FDATA — Array of size NXDATA by NYDATA containing function values. (Input)
FDATA (I, J) is the value of the function at (XDATA (I), YDATA(J)).

Optional Arguments

NXDATA — Number of data points in the *x*-direction. (Input)
NXDATA must be at least three.
Default: NXDATA = size (XDATA,1).

NYDATA — Number of data points in the *y*-direction. (Input)
NYDATA must be at least three.
Default: NYDATA = size (YDATA,1).

LDF — Leading dimension of FDATA exactly as specified in the dimension statement of the calling program. (Input)
LDF must be at least as large as NXDATA.
Default: LDF = size (FDATA,1).

CHECK — Logical variable that is `.TRUE.` if checking of `XDATA` and `YDATA` is required or `.FALSE.` if checking is not required. (Input)
Default: `CHECK` = `.TRUE.`

FORTRAN 90 Interface

Generic: `QD2VL(X, Y, XDATA, YDATA, FDATA [, …])`

Specific: The specific interface names are `S_QD2VL` and `D_QD2VL`.

FORTRAN 77 Interface

Single: `QD2VL(X, Y, NXDATA, XDATA, NYDATA, YDATA, FDATA, LDF, CHECK)`

Double: The double precision function name is `DQD2VL`.

Description

The function `QD2VL` interpolates a table of values, using quadratic polynomials, returning an approximation to the tabulated function. Let (x_i, y_j, f_{ij}) for $i = 1, \ldots, n_x$ and $j = 1, \ldots, n_y$ be the tabular data. Given a point (x, y) at which an interpolated value is desired, we first find the nearest interior grid point (x_i, y_j). A bivariate quadratic interpolant q is then formed using six points near (x, y). Five of the six points are (x_i, y_j), $(x_{i\pm1}, y_j)$, and $(x_i, y_{j\pm1})$. The sixth point is the nearest point to (x, y) of the grid points $(x_{i\pm1}, y_{j\pm1})$. The value $q(x, y)$ is returned by `QD2VL`.

Comments

Informational errors

Type	Code	Description
4	6	The `XDATA` values must be strictly increasing.
4	7	The `YDATA` values must be strictly increasing.

Example

In this example, the value of $\sin(x + y)$ at $x = y = \pi/4$ is approximated by using `QDVAL` on a table of size 21×42 equally spaced values on the unit square.

```
      USE IMSL_LIBRARIES

      IMPLICIT   NONE
      INTEGER    LDF, NXDATA, NYDATA
      PARAMETER  (NXDATA=21, NYDATA=42, LDF=NXDATA)
```

```
!
      INTEGER    I, J, NOUT
      REAL       F, FDATA(LDF,NYDATA), FLOAT, PI, Q, &
                 SIN, X, XDATA(NXDATA), Y, YDATA(NYDATA)
      INTRINSIC  FLOAT, SIN
!                                  Define function
      F(X,Y) = SIN(X+Y)
!                                  Set up X-grid
      DO 10  I=1, NXDATA
         XDATA(I) = FLOAT(I-1)/FLOAT(NXDATA-1)
   10 CONTINUE
!                                  Set up Y-grid
      DO 20  I=1, NYDATA
         YDATA(I) = FLOAT(I-1)/FLOAT(NYDATA-1)
   20 CONTINUE
!                                  Evaluate function on grid
      DO 30  I=1, NXDATA
         DO 30  J=1, NYDATA
            FDATA(I,J) = F(XDATA(I),YDATA(J))
   30 CONTINUE
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Write heading
      WRITE (NOUT,99999)
!                                  Get value for PI and set X and Y
      PI = CONST('PI')
      X  = PI/4.0
      Y  = PI/4.0
!                                  Evaluate quadratic at (X,Y)
      Q = QD2VL(X,Y,XDATA,YDATA,FDATA)
!                                  Print results
      WRITE (NOUT,'(5F12.4)') X, Y, F(X,Y), Q, (Q-F(X,Y))
99999 FORMAT (10X, 'X', 11X, 'Y', 7X, 'F(X,Y)', 7X, 'QD2VL', 9X,&
             'DIF')
      END
```

Output

```
     X           Y        F(X,Y)       QD2VL         DIF
0.7854      0.7854      1.0000      1.0000      0.0000
```

QD2DR

This function evaluates the derivative of a function defined on a rectangular grid using quadratic interpolation.

Function Return Value

QD2DR — Value of the (IXDER, IYDER) derivative of the function at (X, Y). (Output)

Required Arguments

IXDER — Order of the *x*-derivative. (Input)

IYDER — Order of the *y*-derivative. (Input)

X — X-coordinate of the point at which the function is to be evaluated. (Input)

Y — Y-coordinate of the point at which the function is to be evaluated. (Input)

XDATA — Array of length NXDATA containing the location of the data points in the *x*-direction. (Input)
XDATA must be increasing.

YDATA — Array of length NYDATA containing the location of the data points in the *y*-direction. (Input)
YDATA must be increasing.

FDATA — Array of size NXDATA by NYDATA containing function values. (Input)
FDATA(I, J) is the value of the function at (XDATA(I), YDATA(J)).

Optional Arguments

NXDATA — Number of data points in the *x*-direction. (Input)
NXDATA must be at least three.
Default: NXDATA = size (XDATA,1).

NYDATA – Number of data points in the *y*-direction. (Input)
NYDATA must be at least three.
Default: NYDATA = size (YDATA,1).

LDF — Leading dimension of FDATA exactly as specified in the dimension statement of the calling program. (Input)
LDF must be at least as large as NXDATA.
Default: LDF = size (FDATA,1).

CHECK — Logical variable that is .TRUE. if checking of XDATA and YDATA is required or .FALSE. if checking is not required. (Input)
Default: CHECK = .TRUE.

FORTRAN 90 Interface

Generic: QD2DR (IXDER, IYDER, X, Y, XDATA, YDATA, FDATA [, …])

Specific: The specific interface names are S_QD2DR and D_QD2DR.

FORTRAN 77 Interface

Single: QD2DR (IXDER, IYDER, X, Y, NXDATA, XDATA, NYDATA, YDATA, FDATA, LDF, CHECK)

Double: The double precision function name is DQD2DR.

Description

The function QD2DR interpolates a table of values, using quadratic polynomials, returning an approximation to the tabulated function. Let (x_i, y_j, f_{ij}) for $i = 1, \ldots, n_x$ and $j = 1, \ldots, n_y$ be the tabular data. Given a point (x, y) at which an interpolated value is desired, we first find the nearest interior grid point (x_i, y_j). A bivariate quadratic interpolant q is then formed using six points near (x, y). Five of the six points are (x_i, y_j), $(x_{i\pm1}, y_j)$, and $(x_i, y_{j\pm1})$. The sixth point is the nearest point to (x, y) of the grid points $(x_{i\pm1}, y_{j\pm1})$. The value $q^{(p,\, r)}(x, y)$ is returned by QD2DR, where p = IXDER and r = IYDER.

Comments

1. Informational errors

Type	Code	Description
4	6	The XDATA values must be strictly increasing.
4	7	The YDATA values must be strictly increasing.

2. Because quadratic interpolation is used, if the order of any derivative is greater than two, then the returned value is zero.

Example

In this example, the partial derivatives of $\sin(x + y)$ at $x = y = \pi/3$ are approximated by using QD2DR on a table of size 21×42 equally spaced values on the rectangle $[0, 2] \times [0, 2]$.

```
      USE IMSL_LIBRARIES

      IMPLICIT   NONE
      INTEGER    LDF, NXDATA, NYDATA
      PARAMETER  (NXDATA=21, NYDATA=42, LDF=NXDATA)
!
      INTEGER    I, IXDER, IYDER, J, NOUT
      REAL       F, FDATA(LDF,NYDATA), FLOAT, FU, FUNC, PI, Q,&
                 SIN, X, XDATA(NXDATA), Y, YDATA(NYDATA)
      INTRINSIC  FLOAT, SIN
      EXTERNAL   FUNC
!                                  Define function
      F(X,Y) = SIN(X+Y)
!                                  Set up X-grid
      DO 10  I=1, NXDATA
         XDATA(I) = 2.0*(FLOAT(I-1)/FLOAT(NXDATA-1))
   10 CONTINUE
!                                  Set up Y-grid
      DO 20  I=1, NYDATA
         YDATA(I) = 2.0*(FLOAT(I-1)/FLOAT(NYDATA-1))
   20 CONTINUE
!                                  Evaluate function on grid
      DO 30  I=1, NXDATA
         DO 30  J=1, NYDATA
            FDATA(I,J) = F(XDATA(I),YDATA(J))
   30 CONTINUE
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Write heading
      WRITE (NOUT,99998)
!                                  Check XDATA and YDATA
!                                  Get value for PI and set X and Y
      PI = CONST('PI')
      X  = PI/3.0
      Y  = PI/3.0
!                                  Evaluate and print the function
!                                  and its derivatives at X=PI/3 and
!                                  Y=PI/3.
      DO 40  IXDER=0, 1
         DO 40  IYDER=0, 1
            Q  = QD2DR(IXDER,IYDER,X,Y,XDATA,YDATA,FDATA)
            FU = FUNC(IXDER,IYDER,X,Y)
            WRITE (NOUT,99999) X, Y, IXDER, IYDER, FU, Q, (FU-Q)
   40 CONTINUE
!
99998 FORMAT (32X, '(IDX,IDY)', /, 8X, 'X', 8X, 'Y', 3X, 'IDX', 2X,&
             'IDY', 3X, 'F       (X,Y)', 3X, 'QD2DR', 6X, 'ERROR')
99999 FORMAT (2F9.4, 2I5, 3X, F9.4, 2X, 2F11.4)
      END
      REAL FUNCTION FUNC (IX, IY, X, Y)
      INTEGER    IX, IY
      REAL       X, Y
!
      REAL       COS, SIN
      INTRINSIC  COS, SIN
!
      IF (IX.EQ.0 .AND. IY.EQ.0) THEN
!                                  Define (0,0) derivative
         FUNC = SIN(X+Y)
      ELSE IF (IX.EQ.0 .AND. IY.EQ.1) THEN
!                                  Define (0,1) derivative
         FUNC = COS(X+Y)
      ELSE IF (IX.EQ.1 .AND. IY.EQ.0) THEN
!                                  Define (1,0) derivative
         FUNC = COS(X+Y)
```

```
      ELSE IF (IX.EQ.1 .AND. IY.EQ.1) THEN
!                                 Define (1,1) derivative
         FUNC = -SIN(X+Y)
      ELSE
         FUNC = 0.0
      END IF
      RETURN
      END
```

Output

```
                             (IDX,IDY)
     X         Y    IDX   IDY   F        (X,Y)   QD2DR      ERROR
1.0472   1.0472     0     0      0.8660       0.8661    -0.0001
1.0472   1.0472     0     1     -0.5000      -0.4993    -0.0007
1.0472   1.0472     1     0     -0.5000      -0.4995    -0.0005
1.0472   1.0472     1     1     -0.8660      -0.8634    -0.0026
```

QD3VL

This function evaluates a function defined on a rectangular three-dimensional grid using quadratic interpolation.

Function Return Value

QD3VL — Value of the function at (X, Y, Z). (Output)

Required Arguments

X — *x*-coordinate of the point at which the function is to be evaluated. (Input)

Y — *y*-coordinate of the point at which the function is to be evaluated. (Input)

Z — *z*-coordinate of the point at which the function is to be evaluated. (Input)

XDATA — Array of length NXDATA containing the location of the data points in the *x*-direction. (Input)
XDATA must be increasing.

YDATA — Array of length NYDATA containing the location of the data points in the *y*-direction. (Input)
YDATA must be increasing.

ZDATA — Array of length NZDATA containing the location of the data points in the *z*-direction. (Input)
ZDATA must be increasing.

FDATA — Array of size NXDATA by NYDATA by NZDATA containing function values. (Input)
FDATA(I, J, K) is the value of the function at (XDATA(I), YDATA(J), ZDATA(K)).

Optional Arguments

NXDATA — Number of data points in the *x*-direction. (Input)
NXDATA must be at least three.
Default: NXDATA = size (XDATA,1).

NYDATA — Number of data points in the *y*-direction. (Input)
NYDATA must be at least three.
Default: NYDATA = size (YDATA,1).

NZDATA — Number of data points in the *z*-direction. (Input)
NZDATA must be at least three.
Default: NZDATA = size (ZDATA,1).

LDF — Leading dimension of FDATA exactly as specified in the dimension statement of the calling program. (Input)
LDF must be at least as large as NXDATA.
Default: LDF = size (FDATA,1).

MDF — Middle (second) dimension of FDATA exactly as specified in the dimension statement of the calling program. (Input)
MDF must be at least as large as NYDATA.
Default: MDF = size (FDATA,2).

CHECK — Logical variable that is .TRUE. if checking of XDATA, YDATA, and ZDATA is required or .FALSE. if checking is not required. (Input)
Default: CHECK = .TRUE.

FORTRAN 90 Interface

Generic: QD3VL (X, Y, Z, XDATA, YDATA, ZDATA, FDATA [, …])

Specific: The specific interface names are S_QD3VL and D_QD3VL.

FORTRAN 77 Interface

Single: QD3VL(X, Y, Z, NXDATA, XDATA, NYDATA, YDATA, NZDATA, ZDATA, FDATA, LDF, MDF, CHECK)

Double: The double precision function name is DQD3VL.

Description

The function QD3VL interpolates a table of values, using quadratic polynomials, returning an approximation to the tabulated function. Let (x_i, y_j, z_k, f_{ijk}) for $i = 1, \ldots, n_x$, $j = 1, \ldots, n_y$, and $k = 1, \ldots, n_z$ be the tabular data. Given a point (x, y, z) at which an interpolated value is desired, we first find the nearest interior grid point (x_i, y_j, z_k). A trivariate quadratic interpolant q is then formed. Ten points are needed for this purpose. Seven points have the form

$$\left(x_i, y_j, z_k\right), \left(x_{i\pm1}, y_j, z_k\right), \left(x_i, y_{j\pm1}, z_k\right) \text{and} \left(x_i, y_j, z_{k\pm1}\right)$$

The last three points are drawn from the vertices of the octant containing (x, y, z). There are four of these vertices remaining, and we choose to exclude the vertex farthest from the center. This has the slightly deleterious effect of not reproducing the tabular data at the eight exterior corners of the table. The value $q(x, y, z)$ is returned by QD3VL.

Comments

Informational errors

Type	Code	Description
4	9	The XDATA values must be strictly increasing.
4	10	The YDATA values must be strictly increasing.
4	11	The ZDATA values must be strictly increasing.

Example

In this example, the value of sin($x + y + z$) at $x = y = z = \pi/3$ is approximated by using QD3VL on a grid of size 21 × 42 × 18 equally spaced values on the cube $[0, 2]^3$.

```
      USE IMSL_LIBRARIES

      IMPLICIT   NONE
      INTEGER    LDF, MDF, NXDATA, NYDATA, NZDATA
      PARAMETER  (NXDATA=21, NYDATA=42, NZDATA=18, LDF=NXDATA,&
                 MDF=NYDATA)
!
      INTEGER    I, J, K, NOUT
      REAL       F, FDATA(LDF,MDF,NZDATA), FLOAT, PI, Q, &
                 SIN, X, XDATA(NXDATA), Y, YDATA(NYDATA), Z,&
                 ZDATA(NZDATA)
      INTRINSIC  FLOAT, SIN
!                                  Define function
      F(X,Y,Z) = SIN(X+Y+Z)
!                                  Set up X-grid
      DO 10  I=1, NXDATA
         XDATA(I) = 2.0*(FLOAT(I-1)/FLOAT(NXDATA-1))
   10 CONTINUE
!                                  Set up Y-grid
      DO 20  J=1, NYDATA
         YDATA(J) = 2.0*(FLOAT(J-1)/FLOAT(NYDATA-1))
   20 CONTINUE
!                                  Set up Z-grid
      DO 30  K=1, NZDATA
         ZDATA(K) = 2.0*(FLOAT(K-1)/FLOAT(NZDATA-1))
   30 CONTINUE
!                                  Evaluate function on grid
      DO 40  I=1, NXDATA
         DO 40  J=1, NYDATA
            DO 40  K=1, NZDATA
               FDATA(I,J,K) = F(XDATA(I),YDATA(J),ZDATA(K))
   40 CONTINUE
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Write heading
      WRITE (NOUT,99999)
!                                  Get value for PI and set values
!                                  for X, Y, and Z
      PI = CONST('PI')
      X  = PI/3.0
      Y  = PI/3.0
      Z  = PI/3.0
!                                  Evaluate quadratic at (X,Y,Z)
```

```
      Q = QD3VL(X,Y,Z,XDATA,YDATA,ZDATA,FDATA)
!                                  Print results
      WRITE (NOUT,'(6F11.4)') X, Y, Z, F(X,Y,Z), Q, (Q-F(X,Y,Z))
99999 FORMAT (10X, 'X', 10X, 'Y', 10X, 'Z', 5X, 'F(X,Y,Z)', 4X,&
             'QD3VL', 6X, 'ERROR')
      END
```

Output

```
      X          Y          Z     F(X,Y,Z)    QD3VL      ERROR
 1.0472     1.0472     1.0472     0.0000     0.0001     0.0001
```

QD3DR

This function evaluates the derivative of a function defined on a rectangular three-dimensional grid using quadratic interpolation.

Function Return Value

QD3DR — Value of the appropriate derivative of the function at (X, Y, Z). (Output)

Required Arguments

IXDER — Order of the *x*-derivative. (Input)

IYDER — Order of the *y*-derivative. (Input)

IZDER — Order of the *z*-derivative. (Input)

X — *x*-coordinate of the point at which the function is to be evaluated. (Input)

Y — *y*-coordinate of the point at which the function is to be evaluated. (Input)

Z — *z*-coordinate of the point at which the function is to be evaluated. (Input)

XDATA — Array of length NXDATA containing the location of the data points in the *x*-direction. (Input)
XDATA must be increasing.

YDATA — Array of length NYDATA containing the location of the data points in the *y*-direction. (Input)
YDATA must be increasing.

ZDATA — Array of length NZDATA containing the location of the data points in the *z*-direction. (Input)
ZDATA must be increasing.

FDATA — Array of size NXDATA by NYDATA by NZDATA containing function values. (Input)
FDATA(I, J, K) is the value of the function at (XDATA(I), YDATA(J), ZDATA(K)).

Optional Arguments

NXDATA — Number of data points in the *x*-direction. (Input)
NXDATA must be at least three.
Default: NXDATA = size (XDATA,1).

NYDATA — Number of data points in the *y*-direction. (Input)
NYDATA must be at least three.
Default: NYDATA = size (YDATA,1).

NZDATA — Number of data points in the *z*-direction. (Input)
NZDATA must be at least three.
Default: NZDATA = size (ZDATA,1).

LDF — Leading dimension of FDATA exactly as specified in the dimension statement of the calling program. (Input)
LDF must be at least as large as NXDATA.
Default: LDF = size (FDATA,1).

MDF — Middle (second) dimension of FDATA exactly as specified in the dimension statement of the calling program. (Input)
MDF must be at least as large as NYDATA.
Default: MDF = size (FDATA,2).

CHECK — Logical variable that is .TRUE. if checking of XDATA, YDATA, and ZDATA is required or .FALSE. if checking is not required. (Input)
Default: CHECK = .TRUE.

FORTRAN 90 Interface

Generic:	QD3DR (IXDER, IYDER, IZDER, X, Y, Z, XDATA, YDATA, ZDATA, FDATA [, …])
Specific:	The specific interface names are S_QD3DR and D_QD3DR.

FORTRAN 77 Interface

Single:	QD3DR (IXDER, IYDER, IZDER, X, Y, Z, NXDATA, XDATA, NYDATA, YDATA, NZDATA, ZDATA, FDATA, LDF, MDF, CHECK)
Double:	The double precision function name is DQD3DR.

Description

The function QD3DR interpolates a table of values, using quadratic polynomials, returning an approximation to the partial derivatives of the tabulated function. Let

$$(x_i, y_j, z_k, f_{ijk})$$

for $i = 1, \ldots, n_x$, $j = 1, \ldots, n_y$, and $k = 1, \ldots, n_z$ be the tabular data. Given a point (x, y, z) at which an interpolated value is desired, we first find the nearest interior grid point (x_i, y_j, z_k). A trivariate quadratic interpolant q is then formed. Ten points are needed for this purpose. Seven points have the form

$$\left(x_i, y_j, z_k\right), \left(x_{i\pm1}, y_j, z_k\right), \left(x_i, y_{j\pm1}, z_k\right) \text{and} \left(x_i, y_j, z_{k\pm1}\right)$$

The last three points are drawn from the vertices of the octant containing (x, y, z). There are four of these vertices remaining, and we choose to exclude the vertex farthest from the center. This has the slightly deleterious effect of not reproducing the tabular data at the eight exterior corners of the table. The value $q^{(p,r,t)}(x, y, z)$ is returned by `QD3DR`, where p = `IXDER`, r = `IYDER`, and t = `IZDER`.

Comments

1. Informational errors

Type	Code	Description
4	9	The `XDATA` values must be strictly increasing.
4	10	The `YDATA` values must be strictly increasing.
4	11	The `ZDATA` values must be strictly increasing.

2. Because quadratic interpolation is used, if the order of any derivative is greater than two, then the returned value is zero.

Example

In this example, the derivatives of $\sin(x + y + z)$ at $x = y = z = \pi/5$ are approximated by using `QD3DR` on a grid of size $21 \times 42 \times 18$ equally spaced values on the cube $[0, 2]^3$.

```
      USE IMSL_LIBRARIES

      IMPLICIT   NONE
      INTEGER    LDF, MDF, NXDATA, NYDATA, NZDATA
      PARAMETER  (NXDATA=21, NYDATA=42, NZDATA=18, LDF=NXDATA,&
                 MDF=NYDATA)
!
      INTEGER    I, IXDER, IYDER, IZDER, J, K, NOUT
      REAL       F, FDATA(NXDATA,NYDATA,NZDATA), FLOAT, FU,&
                 FUNC, PI, Q, SIN, X, XDATA(NXDATA), Y,&
                 YDATA(NYDATA), Z, ZDATA(NZDATA)
      INTRINSIC  FLOAT, SIN
      EXTERNAL   FUNC
!                                  Define function
      F(X,Y,Z) = SIN(X+Y+Z)
!                                   Set up X-grid
      DO 10  I=1, NXDATA
         XDATA(I) = 2.0*(FLOAT(I-1)/FLOAT(NXDATA-1))
```

```
   10 CONTINUE
!                                  Set up Y-grid
      DO 20  J=1, NYDATA
         YDATA(J) = 2.0*(FLOAT(J-1)/FLOAT(NYDATA-1))
   20 CONTINUE
!                                  Set up Z-grid
      DO 30  K=1, NZDATA
         ZDATA(K) = 2.0*(FLOAT(K-1)/FLOAT(NZDATA-1))
   30 CONTINUE
!                                  Evaluate function on grid
      DO 40  I=1, NXDATA
         DO 40  J=1, NYDATA
            DO 40  K=1, NZDATA
               FDATA(I,J,K) = F(XDATA(I),YDATA(J),ZDATA(K))
   40 CONTINUE
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Write heading
      WRITE (NOUT,99999)
!                                  Get value for PI and set X, Y, and Z
      PI = CONST('PI')
      X  = PI/5.0
      Y  = PI/5.0
      Z  = PI/5.0
!                                  Compute derivatives at (X,Y,Z)
!                                  and print results
      DO 50  IXDER=0, 1
         DO 50  IYDER=0, 1
            DO 50  IZDER=0, 1
               Q  = QD3DR(IXDER,IYDER,IZDER,X,Y,Z,XDATA,YDATA,ZDATA,FDATA)
               FU = FUNC(IXDER,IYDER,IZDER,X,Y,Z)
               WRITE (NOUT,99998) X, Y, Z, IXDER, IYDER, IZDER, FU, Q,&
                                  (FU-Q)
   50 CONTINUE
!
99998 FORMAT (3F7.4, 3I5, 4X, F7.4, 8X, 2F10.4)
99999 FORMAT (39X, '(IDX,IDY,IDZ)', /, 6X, 'X', 6X, 'Y', 6X,&
             'Z', 3X, 'IDX', 2X, 'IDY', 2X, 'IDZ', 2X, 'F          ',&
             '(X,Y,Z)', 3X, 'QD3DR', 5X, 'ERROR')
      END
!
      REAL FUNCTION FUNC (IX, IY, IZ, X, Y, Z)
      INTEGER    IX, IY, IZ
      REAL       X, Y, Z
!
      REAL       COS, SIN
      INTRINSIC  COS, SIN
!
      IF (IX.EQ.0 .AND. IY.EQ.0 .AND. IZ.EQ.0) THEN
!                                  Define (0,0,0) derivative
         FUNC = SIN(X+Y+Z)
      ELSE IF (IX.EQ.0 .AND. IY.EQ.0 .AND. IZ.EQ.1) THEN
!                                  Define (0,0,1) derivative
         FUNC = COS(X+Y+Z)
      ELSE IF (IX.EQ.0 .AND. IY.EQ.1 .AND. IZ.EQ.0) THEN
!                                  Define (0,1,0,) derivative
         FUNC = COS(X+Y+Z)
      ELSE IF (IX.EQ.0 .AND. IY.EQ.1 .AND. IZ.EQ.1) THEN
!                                  Define (0,1,1) derivative
         FUNC = -SIN(X+Y+Z)
      ELSE IF (IX.EQ.1 .AND. IY.EQ.0 .AND. IZ.EQ.0) THEN
!                                  Define (1,0,0) derivative
         FUNC = COS(X+Y+Z)
      ELSE IF (IX.EQ.1 .AND. IY.EQ.0 .AND. IZ.EQ.1) THEN
!                                  Define (1,0,1) derivative
         FUNC = -SIN(X+Y+Z)
```

```
      ELSE IF (IX.EQ.1 .AND. IY.EQ.1 .AND. IZ.EQ.0) THEN
!                                  Define (1,1,0) derivative
         FUNC = -SIN(X+Y+Z)
      ELSE IF (IX.EQ.1 .AND. IY.EQ.1 .AND. IZ.EQ.1) THEN
!                                  Define (1,1,1) derivative
         FUNC = -COS(X+Y+Z)
      ELSE
         FUNC = 0.0
      END IF
      RETURN
      END
```

Output

```
                                      (IDX,IDY,IDZ)
    X       Y       Z    IDX   IDY   IDZ  F           (X,Y,Z)   QD3DR     ERROR
 0.6283 0.6283 0.6283    0     0     0     0.9511             0.9511   -0.0001
 0.6283 0.6283 0.6283    0     0     1    -0.3090            -0.3080   -0.0010
 0.6283 0.6283 0.6283    0     1     0    -0.3090            -0.3088    0.0002
 0.6283 0.6283 0.6283    0     1     1    -0.9511            -0.9587    0.0077
 0.6283 0.6283 0.6283    1     0     0    -0.3090            -0.3078   -0.0012
 0.6283 0.6283 0.6283    1     0     1    -0.9511            -0.9348   -0.0162
 0.6283 0.6283 0.6283    1     1     0    -0.9511            -0.9613    0.0103
 0.6283 0.6283 0.6283    1     1     1     0.3090             0.0000    0.3090
```

SURF

more...

Computes a smooth bivariate interpolant to scattered data that is locally a quintic polynomial in two variables.

Required Arguments

XYDATA — A 2 by `NDATA` array containing the coordinates of the interpolation points. (Input)
These points must be distinct. The *x*-coordinate of the `I`-th data point is stored in `XYDATA`(1, `I`) and the *y*-coordinate of the `I`-th data point is stored in `XYDATA`(2, `I`).

FDATA — Array of length `NDATA` containing the interpolation values. (Input) `FDATA`(`I`) contains the value at (`XYDATA`(1, `I`), `XYDATA`(2, `I`)).

XOUT — Array of length `NXOUT` containing an increasing sequence of points. (Input)
These points are the *x*-coordinates of a grid on which the interpolated surface is to be evaluated.

YOUT — Array of length `NYOUT` containing an increasing sequence of points. (Input)
These points are the *y*-coordinates of a grid on which the interpolated surface is to be evaluated.

SUR — Matrix of size `NXOUT` by `NYOUT`. (Output)
This matrix contains the values of the surface on the `XOUT` by `YOUT` grid, i.e. `SUR`(`I`, `J`) contains the interpolated value at (`XOUT`(`I`), `YOUT`(`J`)).

Optional Arguments

NDATA — Number of data points. (Input)
`NDATA` must be at least four.
Default: `NDATA` = size (`FDATA`,1).

NXOUT — The number of elements in `XOUT`. (Input)
Default: `NXOUT` = size (`XOUT`,1).

NYOUT — The number of elements in `YOUT`. (Input)
Default: `NYOUT` = size (`YOUT`,1).

LDSUR — Leading dimension of SUR exactly as specified in the dimension statement of the calling program. (Input)
LDSUR must be at least as large as NXOUT.
Default: LDSUR = size (SUR,1).

FORTRAN 90 Interface

Generic: CALL SURF (XYDATA, FDATA, XOUT, YOUT, SUR [, …])

Specific: The specific interface names are S_SURF and D_SURF.

FORTRAN 77 Interface

Single: CALL SURF (NDATA, XYDATA, FDATA, NXOUT, NYOUT, XOUT, YOUT, SUR, LDSUR)

Double: The double precision name is DSURF.

Description

This routine is designed to compute a C^1 interpolant to scattered data in the plane. Given the data points

$$\left\{\left(x_i, y_i, f_i\right)\right\}_{i=1}^{N} \; in \; \mathbf{R}^3$$

SURF returns (in SUR, the user-specified grid) the values of the interpolant *s*. The computation of *s* is as follows: First the Delaunay triangulation of the points

$$\left\{\left(x_i, y_i\right)\right\}_{i=1}^{N}$$

is computed. On each triangle *T* in this triangulation, *s* has the form

$$s\left(x, y\right) = \sum_{m+n \le 5} c_{mn}^{T} x^m y^n \qquad \forall \; x, y \in T$$

Thus, *s* is a bivariate quintic polynomial on each triangle of the triangulation. In addition, we have

$$s(x_i, y_i) = f_i \;\text{ for } i = 1, \;\ldots, N$$

and *s* is continuously differentiable across the boundaries of neighboring triangles. These conditions do not exhaust the freedom implied by the above representation. This additional freedom is exploited in an attempt to produce an interpolant that is faithful to the global shape properties implied by the data. For more information on this routine, we refer the reader to the article by Akima (1978). The grid is specified by the two integer variables NXOUT, NYOUT that represent, respectively, the number of grid points in the first (second) variable and by two real vectors that represent, respectively, the first (second) coordinates of the grid.

Comments

1. Workspace may be explicitly provided, if desired, by use of S2RF/DS2RF. The reference is:

   CALL S2RF (NDATA, XYDATA, FDATA, NXOUT, NYOUT, XOUT, YOUT,
   SUR, LDSUR, IWK, WK)

   The additional arguments are as follows:

   IWK — Work array of length 31 * NDATA + 2*(NXOUT * NYOUT).

   WK — Work array of length 6 * NDATA.

2. Informational errors

Type	Code	Description
4	5	The data point values must be distinct.
4	6	The XOUT values must be strictly increasing.
4	7	The YOUT values must be strictly increasing.

3. This method of interpolation reproduces linear functions.

Example

In this example, the interpolant to the linear function 3 + 7*x* + 2*y* is computed from 20 data points equally spaced on the circle of radius 3. We then print the values on a 3 × 3 grid.

```
      USE IMSL_LIBRARIES

      IMPLICIT   NONE
      INTEGER    LDSUR, NDATA, NXOUT, NYOUT
      PARAMETER  (NDATA=20, NXOUT=3, NYOUT=3, LDSUR=NXOUT)
!
      INTEGER    I, J, NOUT
      REAL       ABS, COS, F, FDATA(NDATA), FLOAT, PI,&
                 SIN, SUR(LDSUR,NYOUT), X, XOUT(NXOUT),&
                 XYDATA(2,NDATA), Y, YOUT(NYOUT)
      INTRINSIC  ABS, COS, FLOAT, SIN
!                                  Define function
      F(X,Y) = 3.0 + 7.0*X + 2.0*Y
!                                  Get value for PI
      PI     = CONST('PI')
!                                  Set up X, Y, and F data on a circle
      DO 10  I=1, NDATA
         XYDATA(1,I) = 3.0*SIN(2.0*PI*FLOAT(I-1)/FLOAT(NDATA))
         XYDATA(2,I) = 3.0*COS(2.0*PI*FLOAT(I-1)/FLOAT(NDATA))
         FDATA(I)    = F(XYDATA(1,I),XYDATA(2,I))
   10 CONTINUE
!                                  Set up XOUT and YOUT data on [0,1] by
!                                  [0,1] grid.
      DO 20  I=1, NXOUT
         XOUT(I) = FLOAT(I-1)/FLOAT(NXOUT-1)
   20 CONTINUE
      DO 30  I=1, NYOUT
         YOUT(I) = FLOAT(I-1)/FLOAT(NYOUT-1)
```

```
   30 CONTINUE
!                                  Interpolate scattered data
      CALL SURF (XYDATA, FDATA, XOUT, YOUT, SUR)
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Write heading
      WRITE (NOUT,99998)
!                                  Print results
      DO 40  I=1, NYOUT
         DO 40  J=1, NXOUT
            WRITE (NOUT,99999) XOUT(J), YOUT(I), SUR(J,I),&
                                F(XOUT(J),YOUT(I)),&
                                ABS(SUR(J,I)-F(XOUT(J),YOUT(I)))
   40 CONTINUE
99998 FORMAT (' ', 10X, 'X', 11X, 'Y', 9X, 'SURF', 6X, 'F(X,Y)', 7X,&
             'ERROR', /)
99999 FORMAT (1X, 5F12.4)
      END
```

Output

```
     X           Y          SURF       F(X,Y)       ERROR

0.0000      0.0000      3.0000      3.0000      0.0000
0.5000      0.0000      6.5000      6.5000      0.0000
1.0000      0.0000     10.0000     10.0000      0.0000
0.0000      0.5000      4.0000      4.0000      0.0000
0.5000      0.5000      7.5000      7.5000      0.0000
1.0000      0.5000     11.0000     11.0000      0.0000
0.0000      1.0000      5.0000      5.0000      0.0000
0.5000      1.0000      8.5000      8.5000      0.0000
1.0000      1.0000     12.0000     12.0000      0.0000
```

SURFND

Performs multidimensional interpolation and differentiation for up to 7 dimensions.

The dimension, *n*, of the problem is determined by the rank of `FDATA`, and cannot be greater than seven. The number of gridpoints in the *i-th* direction, d_i, is determined by the corresponding dimension for `FDATA`.

Function Return Value

SURFND — Interpolated value of the function.

Required Arguments

X — Array of length *n* containing the point at which interpolation is to be done. (Input)
An interpolant is to be calculated at the point:

$$(\mathrm{X}_1, \mathrm{X}_2, \ldots, \mathrm{X}_n)$$

XDATA — Array of size *n* by *max*(d_1, ..., d_n) giving the gridpoint values for the function to be interpolated. (Input)
The gridpoints need not be uniformly spaced. For each row of XDATA, the specified gridpoint values must be either strictly increasing or strictly decreasing. See `FDATA` for more details.

FDATA — *n* dimensional array, dimensioned $d_1 \times d_2 \times \ldots \times d_n$ giving the values at the gridpoints of the function to be interpolated. (Input)
`FDATA`(*i*, *j*, *k*, ...) is the value of the function at

$$(\mathrm{XDATA}_{1,i}, \mathrm{XDATA}_{2,j}, \mathrm{XDATA}_{3,k}, \ldots)$$
$$\text{for } i = 1, \ldots, d_1,\ j = 1, \ldots, d_2, k = 1, \ldots, d_3, \ldots$$

Optional Arguments

NDEG — Array of length *n*, giving the degree of polynomial interpolation to be used in each dimension. (Input)
`NDEG`(*i*) must be less than or equal to 15.
Default: `NDEG`(*i*) = 5, `for` *i* = 1, ..., *n*.

NDERS — Maximum order of derivatives to be computed with respect to each variable. (Input)
`NDERS` cannot be larger than *max* (7- *n*, 2). See `DERIV` for more details.
Default: `NDERS` = 0.

DERIV — *n* dimensional array, dimensioned (NDERS+1) × (NDERS+1) ×... containing derivative estimates at the interpolation point. (Output)

DERIV (*i*, *j*, ...) will hold an estimate of the derivative with respect to X_1 *i* times, and with respect to X_2 *j* times, etc. where *i* = 0, ..., NDERS, *j* = 0, ..., NDERS, ... The 0-th derivative means the function value, thus, DERIV (0, 0, ...) = SURFND.

ERROR — Estimate of the error in SURFND. (Output)

FORTRAN 90 Interface

Generic: SURFND (X,XDATA,FDATA [, ...])

Specific: The specific interface names are S*n*_SURFND and D*n*_SURFND, where "*n*" indicates the dimension of the problem (*n* = 1, 2, 3, 4, 5, 6 or 7).

Description

The function SURFND interpolates a function of up to 7 variables, defined on a (possibly nonuniform) grid. It fits a polynomial of up to degree 15 in each variable through the grid points nearest the interpolation point. Approximations of partial derivatives are calculated, if requested. If derivatives are desired, high precision is strongly recommended. For more details, see Krogh (1970).

Comments

Informational errors

Type	Code	Description
3	1	NDERS is too large, it has been reset to *max*(7- *n*,2).
3	2	The interpolation point is outside the domain of the table, so extrapolation is used.
4	3	Too many derivatives requested for the polynomial degree used.
4	4	One of the polynomial degrees requested is too large for the number of gridlines in that direction.

Example

The 3D function $f(x, y, z) = exp(x + 2y + 3z)$, defined on a 20 by 30 by 40 uniform grid, is interpolated.

```
USE SURFND_INT
USE UMACH_INT
IMPLICIT NONE
```

```
      INTEGER, PARAMETER :: N=3, ND1=20, ND2=30, ND3=40, NDERS=1
      REAL          X(N),DEROUT(0:NDERS,0:NDERS,0:NDERS), &
                    XDATA(N,MAX(ND1,ND2,ND3)),FDATA(ND1,ND2,ND3), &
                    ERROR,XX,YY,ZZ,TRUE,RELERR,YOUT
      INTEGER       NDEG(N),I,J,K,NOUT
      CHARACTER*1   ORDER(3)
      INTRINSIC     EXP, MAX

!                              20 by 30 by 40 uniform grid used for
!                              interpolation of F(x,y,z) = exp(x+2*y+3*z)
      NDEG(1) =  8
      NDEG(2) =  7
      NDEG(3) =  9

      DO I=1,ND1
         XDATA(1,I) = 0.05*(I-1)
      END DO

      DO J=1,ND2
         XDATA(2,J) = 0.03*(J-1)
      END DO

      DO K=1,ND3
         XDATA(3,K) = 0.025*(K-1)
      END DO

      DO I=1,ND1
         DO J=1,ND2
            DO K=1,ND3
               XX = XDATA(1,I)
               YY = XDATA(2,J)
               ZZ = XDATA(3,K)
               FDATA(I,J,K) =  EXP(XX+2*YY+3*ZZ)
            END DO
         END DO
      END DO

!                              Interpolate at (0.18,0.43,0.35)
      X(1) =  0.18
      X(2) =  0.43
      X(3) =  0.35

!                              Call SURFND
      YOUT = SURFND(X,XDATA,FDATA,NDEG=NDEG,DERIV=DEROUT,ERROR=ERROR, &
        NDERS=NDERS)

!                              Output F,Fx,Fy,Fz,Fxy,Fxz,Fyz,Fxyz at
!                              interpolation point
      XX = X(1)
      YY = X(2)
      ZZ = X(3)
      CALL UMACH (2, NOUT)
      WRITE(NOUT, 10) YOUT,ERROR

      DO K=0,NDERS
         DO J=0,NDERS
            DO I=0,NDERS
               ORDER(1:3) = ' '
               IF (I.EQ.1) ORDER(1) = 'x'
               IF (J.EQ.1) ORDER(2) = 'y'
               IF (K.EQ.1) ORDER(3) = 'z'
               TRUE = 2**J*3**K*EXP(XX+2*YY+3*ZZ)
               RELERR = (DEROUT(I,J,K)-TRUE)/TRUE
               WRITE(NOUT, 20) ORDER,DEROUT(I,J,K),TRUE,RELERR
            END DO
         END DO
```

```
      END DO
   10 FORMAT (' EST. VALUE = ',F10.6,', EST. ERROR = ',E11.3,//, &
             11X,'Computed Der.',5X,'True Der.',4X,'Rel. Err')
   20 FORMAT (2X,'F',3A1,2F15.6,E15.3)
      END
```

Output

```
 EST. VALUE =   8.084915, EST. ERROR =   0.419E-05

           Computed Der.     True Der.    Rel. Err
   F          8.084915       8.084914      0.118E-06
   Fx         8.084907       8.084914     -0.944E-06
   F y       16.169882      16.169828      0.330E-05
   Fxy       16.171101      16.169828      0.787E-04
   F  z      24.254705      24.254742     -0.149E-05
   Fx z      24.255133      24.254742      0.161E-04
   F yz      48.505203      48.509483     -0.882E-04
   Fxyz      48.464718      48.509483     -0.923E-03
```

RLINE

Fits a line to a set of data points using least squares.

Required Arguments

XDATA — Vector of length `NOBS` containing the *x*-values. (Input)

YDATA — Vector of length `NOBS` containing the *y*-values. (Input)

B0 — Estimated intercept of the fitted line. (Output)

B1 — Estimated slope of the fitted line. (Output)

Optional Arguments

NOBS — Number of observations. (Input)
Default: `NOBS` = size (`XDATA`,1).

STAT — Vector of length 12 containing the statistics described below. (Output)

I	**STAT(I)**
1	Mean of `XDATA`
2	Mean of `YDATA`
3	Sample variance of `XDATA`
4	Sample variance of `YDATA`
5	Correlation
6	Estimated standard error of `B0`
7	Estimated standard error of `B1`
8	Degrees of freedom for regression
9	Sum of squares for regression
10	Degrees of freedom for error
11	Sum of squares for error
12	Number of (*x*, *y*) points containing NaN (not a number) as either the *x* or *y* value

FORTRAN 90 Interface

Generic: `CALL RLINE (XDATA, YDATA, B0, B1 [, …])`

Specific: The specific interface names are `S_RLINE` and `D_RLINE`.

FORTRAN 77 Interface

Single: `CALL RLINE (NOBS, XDATA, YDATA, B0, B1, STAT)`

Double: The double precision name is `DRLINE`.

Description

Routine `RLINE` fits a line to a set of (*x*, *y*) data points using the method of least squares. Draper and Smith (1981, pages 1 – 69) discuss the method. The fitted model is

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x$$

where $\hat{\beta}_0$ (stored in `B0`) is the estimated intercept and $\hat{\beta}_1$ (stored in `B1`) is the estimated slope. In addition to the fit, `RLINE` produces some summary statistics, including the means, sample variances, correlation, and the error (residual) sum of squares. The estimated standard errors of $\hat{\beta}_0$ and $\hat{\beta}_1$ are computed under the simple linear regression model. The errors in the model are assumed to be uncorrelated and with constant variance.

If the *x* values are all equal, the model is degenerate. In this case, `RLINE` sets $\hat{\beta}_1$ to zero and $\hat{\beta}_0$ to the mean of the *y* values.

Comments

Informational error

Type	Code	Description
4	1	Each (*x*, *y*) point contains NaN (not a number). There are no valid data.

Example

This example fits a line to a set of data discussed by Draper and Smith (1981, Table 1.1, pages 9-33). The response *y* is the amount of steam used per month (in pounds), and the independent variable *x* is the average atmospheric temperature (in degrees Fahrenheit).

```
      USE RLINE_INT
      USE UMACH_INT
      USE WRRRL_INT

      IMPLICIT   NONE
      INTEGER    NOBS
      PARAMETER  (NOBS=25)
!
      INTEGER    NOUT
      REAL       B0, B1, STAT(12), XDATA(NOBS), YDATA(NOBS)
      CHARACTER  CLABEL(13)*15, RLABEL(1)*4
!
      DATA XDATA/35.3, 29.7, 30.8, 58.8, 61.4, 71.3, 74.4, 76.7, 70.7,&
           57.5, 46.4, 28.9, 28.1, 39.1, 46.8, 48.5, 59.3, 70.0, 70.0,&
           74.5, 72.1, 58.1, 44.6, 33.4, 28.6/
      DATA YDATA/10.98, 11.13, 12.51, 8.4, 9.27, 8.73, 6.36, 8.5,&
           7.82, 9.14, 8.24, 12.19, 11.88, 9.57, 10.94, 9.58, 10.09,&
           8.11, 6.83, 8.88, 7.68, 8.47, 8.86, 10.36, 11.08/
      DATA RLABEL/'NONE'/, CLABEL/' ', 'Mean of X', 'Mean of Y',&
           'Variance X', 'Variance Y', 'Corr.', 'Std. Err. B0',&
           'Std. Err. B1', 'DF Reg.', 'SS Reg.', 'DF Error',&
           'SS Error', 'Pts. with NaN'/
!
      CALL RLINE (XDATA, YDATA, B0, B1, STAT=STAT)
!
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) B0, B1
99999 FORMAT (' B0 = ', F7.2, '  B1 = ', F9.5)
      CALL WRRRL ('%/STAT', STAT, RLABEL, CLABEL, 1, 12, 1, &
                  FMT = '(12W10.4)')
!
      END
```

Output

```
B0 =   13.62  B1 =  -0.07983

                                STAT
Mean of X   Mean of Y  Variance X  Variance Y       Corr.  Std. Err. B0
      52.6          9.424       298.1       2.659     -0.8452          0.5815

Std. Err. B1      DF Reg.     SS Reg.    DF Error     SS Error   Pts. with NaN
0.01052            1       45.59          23       18.22                0
```

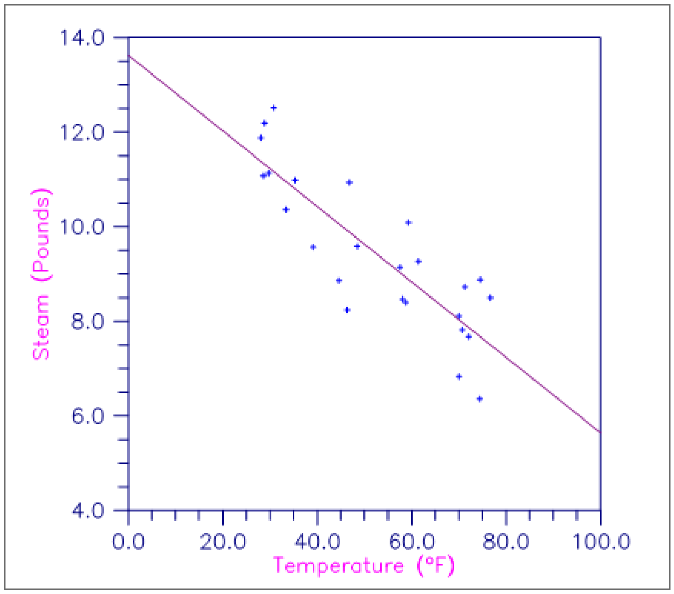


Figure 7, Plot of the Data and the Least Squares Line

RCURV

Fits a polynomial curve using least squares.

Required Arguments

XDATA — Vector of length NOBS containing the *x* values. (Input)

YDATA — Vector of length NOBS containing the *y* values. (Input)

B — Vector of length NDEG + 1 containing the coefficients $\hat{\beta}$. (Output)

The fitted polynomial is

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x + \hat{\beta}_2 x^2 + \cdots + \hat{\beta}_k x^k$$

Optional Arguments

NOBS — Number of observations. (Input)
Default: NOBS = size (XDATA,1).

NDEG — Degree of polynomial. (Input)
Default: NDEG = size (B,1) – 1.

SSPOLY — Vector of length NDEG + 1 containing the sequential sums of squares. (Output)
SSPOLY(1) contains the sum of squares due to the mean. For i = 1, 2, …, NDEG, SSPOLY(i + 1) contains the sum of squares due to x^i adjusted for the mean, x, x^2, …, and x^{i-1}.

STAT — Vector of length 10 containing statistics described below. (Output)

i	Statistics
1	Mean of *x*
2	Mean of *y*
3	Sample variance of *x*
4	Sample variance of *y*
5	R-squared (in percent)
6	Degrees of freedom for regression
7	Regression sum of squares
8	Degrees of freedom for error

i	Statistics
9	Error sum of squares
10	Number of data points (x, y) containing NaN (not a number) as a x or y value

FORTRAN 90 Interface

Generic: `CALL RCURV (XDATA, YDATA, B [, …])`

Specific: The specific interface names are `S_RCURV` and `D_RCURV`.

FORTRAN 77 Interface

Single: `CALL RCURV (NOBS, XDATA, YDATA, NDEG, B, SSPOLY, STAT)`

Double: The double precision name is `DRCURV`.

Description

Routine `RCURV` computes estimates of the regression coefficients in a polynomial (curvilinear) regression model. In addition to the computation of the fit, `RCURV` computes some summary statistics. Sequential sums of squares attributable to each power of the independent variable (stored in `SSPOLY`) are computed. These are useful in assessing the importance of the higher order powers in the fit. Draper and Smith (1981, pages 101– 102) and Neter and Wasserman (1974, pages 278–287) discuss the interpretation of the sequential sums of squares. The statistic R^2 (stored in `STAT(5)`) is the percentage of the sum of squares of y about its mean explained by the polynomial curve. Specifically,

$$R^2 = \frac{\sum_{i=1}^{n}\left(\hat{y}_i - \overline{y}\right)^2}{\sum_{i=1}^{n}\left(y_i - \overline{y}\right)^2} 100\%$$

where

$$\hat{y}_i$$

is the fitted y value at x_i and

$$\overline{y}$$

(stored in `STAT(2)`) is the mean of y. This statistic is useful in assessing the overall fit of the curve to the data. R^2 must be between 0% and 100%, inclusive. R^2 = 100% indicates a perfect fit to the data.

Routine RCURV computes estimates of the regression coefficients in a polynomial model using orthogonal polynomials as the regressor variables. This reparameterization of the polynomial model in terms of orthogonal polynomials has the advantage that the loss of accuracy resulting from forming powers of the *x*-values is avoided. All results are returned to the user for the original model.

The routine RCURV is based on the algorithm of Forsythe (1957). A modification to Forsythe's algorithm suggested by Shampine (1975) is used for computing the polynomial coefficients. A discussion of Forsythe's algorithm and Shampine's modification appears in Kennedy and Gentle (1980, pages 342−347).

Comments

1. Workspace may be explicitly provided, if desired, by use of R2URV/DR2URV. The reference is:

```
CALL R2URV (NOBS, XDATA, YDATA, NDEG, B, SSPOLY, STAT, WK,
   IWK)
```

The additional arguments are as follows:

WK — Work vector of length 11 * NOBS + 11 * NDEG + 5 + (NDEG + 1) * (NDEG + 3).

IWK — Work vector of length NOBS.

2. Informational errors

Type	Code	Description
4	3	Each (*x*, *y*) point contains NaN (not a number). There are no valid data.
4	7	The *x* values are constant. At least NDEG + 1 distinct *x* values are needed to fit a NDEG polynomial.
3	4	The *y* values are constant. A zero order polynomial is fit. High order coefficients are set to zero.
3	5	There are too few observations to fit the desired degree polynomial. High order coefficients are set to zero.
3	6	A perfect fit was obtained with a polynomial of degree less than NDEG. High order coefficients are set to zero.

3. If NDEG is greater than 10, the accuracy of the results may be questionable.

Example

A polynomial model is fitted to data discussed by Neter and Wasserman (1974, pages 279− 285). The data set contains the response variable *y* measuring coffee sales (in hundred gallons) and the number of self-service coffee dispensers. Responses for fourteen similar cafeterias are in the data set.

```
      USE RCURV_INT
```

```
      USE WRRRL_INT
      USE WRRRN_INT

      IMPLICIT   NONE
      INTEGER    NDEG, NOBS
      PARAMETER  (NDEG=2, NOBS=14)
!
      REAL       B(NDEG+1), SSPOLY(NDEG+1), STAT(10), XDATA(NOBS),&
                 YDATA(NOBS)
      CHARACTER  CLABEL(11)*15, RLABEL(1)*4
!
      DATA RLABEL/'NONE'/, CLABEL/' ', 'Mean of X', 'Mean of Y',&
                 'Variance X', 'Variance Y', 'R-squared',&
                 'DF Reg.', 'SS Reg.', 'DF Error', 'SS Error',&
                 'Pts. with NaN'/
      DATA XDATA/0., 0., 1., 1., 2., 2., 4., 4., 5., 5., 6., 6., 7.,&
           7./
      DATA YDATA/508.1, 498.4, 568.2, 577.3, 651.7, 657.0, 755.3,&
           758.9, 787.6, 792.1, 841.4, 831.8, 854.7, 871.4/
!
      CALL RCURV (XDATA, YDATA, B, SSPOLY=SSPOLY, STAT=STAT)
!
      CALL WRRRN ('B', B, 1, NDEG+1, 1)
      CALL WRRRN ('SSPOLY', SSPOLY, 1, NDEG+1, 1)

      CALL WRRRL ('%/STAT', STAT, RLABEL, CLABEL, 1, 10, 1, &
                  FMT='(2W10.4)')
      END
```

Output

```
           B
    1       2       3
503.3    78.9    -4.0

             SSPOLY
        1           2           3
7077152.0    220644.2      4387.7

                                 STAT
Mean of X   Mean of Y  Variance X  Variance Y   R-squared    DF Reg.
     3.571       711.0       6.418     17364.8       99.69           2

 SS Reg.    DF Error    SS Error  Pts. with NaN
225031.9          11       710.5              0
```

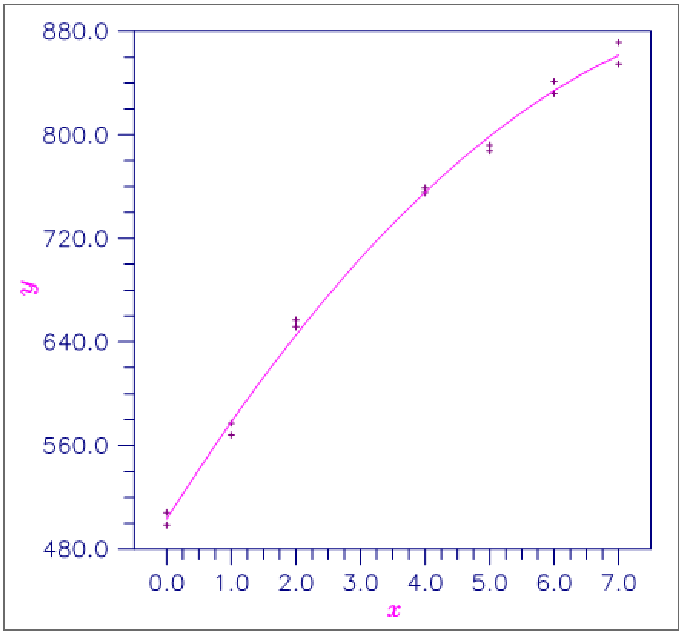


Figure 8, Plot of Data and Second Degree Polynomial Fit

FNLSQ

Computes a least-squares approximation with user-supplied basis functions.

Required Arguments

F — User-supplied function to evaluate basis functions. The form is F(K, X), where

K – Number of the basis function. (Input)

K may be equal to 1, 2, …, NBASIS.

X – Argument for evaluation of the *K*-th basis function. (Input)

F – The function value. (Output)

F must be declared EXTERNAL in the calling program. The data FDATA is approximated by A(1) * F(1, X) + A(2) * F(2, X) + … + A(NBASIS) * F(NBASIS, X) if INTCEP = 0 and is approximated by A(1) + A(2) * F(1, X) +…+ A(NBASIS + 1) * F(NBASIS, X) if INTCEP = 1.

XDATA — Array of length NDATA containing the abscissas of the data points. (Input)

FDATA — Array of length NDATA containing the ordinates of the data points. (Input)

A — Array of length INTCEP + NBASIS containing the coefficients of the approximation. (Output)
If INTCEP = 1, A(1) contains the intercept. A(INTCEP + I) contains the coefficient of the I-*th* basis function.

SSE — Sum of squares of the errors. (Output)

Optional Arguments

INTCEP — Intercept option. (Input)
Default: INTCEP = 0.

INTCEP	Action
0	No intercept is automatically included in the model.
1	An intercept is automatically included in the model.

NBASIS — Number of basis functions. (Input)
Default: NBASIS = size (A,1)

NDATA — Number of data points. (Input)
Default: NDATA = size (XDATA,1).

IWT — Weighting option. (Input)
Default: IWT = 0.

IWT	Action
0	Weights of one are assumed.
1	Weights are supplied in WEIGHT.

WEIGHT — Array of length NDATA containing the weights. (Input if IWT = 1)
If IWT = 0, WEIGHT is not referenced and may be dimensioned of length one.

FORTRAN 90 Interface

Generic: CALL FNLSQ (F, XDATA, FDATA, A, SSE [, …])

Specific: The specific interface names are S_FNLSQ and D_FNLSQ.

FORTRAN 77 Interface

Single: CALL FNLSQ (F, INTCEP, NBASIS, NDATA, XDATA, FDATA, IWT, WEIGHT, A, SSE)

Double: The double precision name is DFNLSQ.

Description

The routine FNLSQ computes a best least-squares approximation to given univariate data of the form

$$\left\{\left(x_i, f_i\right)\right\}_{i=1}^{N}$$

by *M* basis functions

$$\left\{F_j\right\}_{j=1}^{M}$$

(where *M* = NBASIS). In particular, if INTCEP = 0, this routine returns the error sum of squares SSE and the coefficients *a* which minimize

$$\sum_{i=1}^{N} w_i \left(f_i - \sum_{j=1}^{M} a_j F_j\left(x_i\right) \right)^2$$

where *w* = WEIGHT, *N* = NDATA, *x* = XDATA, and, *f* = FDATA.

If INTCEP = 1, then an intercept is placed in the model; and the coefficients *a*, returned by FNLSQ, minimize the error sum of squares as indicated below.

$$\sum_{i=1}^{N} w_i \left(f_i - a_1 - \sum_{j=1}^{M} a_{j+1} F_j(x_i) \right)^2$$

That is, the first element of the vector *a* is now the coefficient of the function that is identically 1 and the coefficients of the F_j's are now a_{j+1}.

One additional parameter in the calling sequence for FNLSQ is IWT. If IWT is set to 0, then $w_i = 1$ is assumed. If IWT is set to 1, then the user must supply the weights.

Comments

1. Workspace may be explicitly provided, if desired, by use of F2LSQ/DF2LSQ. The reference is:

```
CALL F2LSQ (F, INTCEP, NBASIS, NDATA, XDATA, FDATA, IWT,
   WEIGHT, A, SSE, WK)
```

   The additional argument is

   WK — Work vector of length (INTCEP + NBASIS)**2 + 4 * (INTCEP + NBASIS) + IWT + 1. On output, the first (INTCEP + NBASIS)**2 elements of WK contain the R matrix from a QR decomposition of the matrix containing a column of ones (if INTCEP = 1) and the evaluated basis functions in columns INTCEP + 1 through INTCEP + NBASIS.

2. Informational errors

Type	Code	Description
3	1	Linear dependence of the basis functions exists. One or more components of A are set to zero.
3	2	Linear dependence of the constant function and basis functions exists. One or more components of A are set to zero.
4	1	Negative weight encountered.

Example

In this example, we fit the following two functions (indexed by δ)

$$1 + \sin x + 7 \sin 3x + \delta\varepsilon$$

where ε is random uniform deviate over the range [−1, 1], and δ is 0 for the first function and 1 for the second. These functions are evaluated at 90 equally spaced points on the interval [0, 6]. We use 4 basis functions, sin *kx* for *k* = 1, …, 4, with and without the intercept.

```
      USE FNLSQ_INT
      USE RNSET_INT
      USE UMACH_INT
      USE RNUNF_INT

      IMPLICIT   NONE
      INTEGER    NBASIS, NDATA
      PARAMETER  (NBASIS=4, NDATA=90)
!
      INTEGER    I, INTCEP, NOUT
      REAL       A(NBASIS+1), F, FDATA(NDATA), FLOAT, G, RNOISE,&
                 SIN, SSE, X, XDATA(NDATA)
      INTRINSIC  FLOAT, SIN
      EXTERNAL   F
!
      G(X) = 1.0 + SIN(X) + 7.0*SIN(3.0*X)
!                                  Set random number seed
      CALL RNSET (1234579)
!                                  Set up data values
      DO 10  I=1, NDATA
         XDATA(I) = 6.0*(FLOAT(I-1)/FLOAT(NDATA-1))
         FDATA(I) = G(XDATA(I))
   10 CONTINUE

!                                  Compute least squares fit with no
!                                  intercept
      CALL FNLSQ (F, XDATA, FDATA, A, SSE, INTCEP=INTCEP, &
                  NBASIS=NBASIS)
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Write heading
      WRITE (NOUT,99996)
!                                  Write output
      WRITE (NOUT,99999) SSE, (A(I),I=1,NBASIS)
!
      INTCEP = 1
!                                  Compute least squares fit with
!                                  intercept
      CALL FNLSQ (F, XDATA, FDATA, A, SSE, INTCEP=INTCEP, &
                  NBASIS=NBASIS)
!                                  Write output
      WRITE (NOUT,99998) SSE, A(1), (A(I),I=2,NBASIS+1)
!                                  Introduce noise
      DO 20  I=1, NDATA
         RNOISE = RNUNF()
         RNOISE   = 2.0*RNOISE - 1.0
         FDATA(I) = FDATA(I) + RNOISE
   20 CONTINUE
      INTCEP = 0
!                                  Compute least squares fit with no
!                                  intercept
      CALL FNLSQ (F, XDATA, FDATA, A, SSE, INTCEP=INTCEP, &
                  NBASIS=NBASIS)
!                                  Write heading
      WRITE (NOUT,99997)
!                                  Write output
      WRITE (NOUT,99999) SSE, (A(I),I=1,NBASIS)
!
      INTCEP = 1
!                                  Compute least squares fit with
```

```
!                                  intercept
      CALL FNLSQ (F, XDATA, FDATA, A, SSE, INTCEP=INTCEP, &
                  NBASIS=NBASIS)
!                                  Write output
      WRITE (NOUT,99998) SSE, A(1), (A(I),I=2,NBASIS+1)
!
99996 FORMAT (//, ' Without error introduced we have :', /,&
             '    SSE          Intercept      Coefficients  ', /)
99997 FORMAT (//, ' With error introduced we have :', /, '    SSE      '&
             , '     Intercept      Coefficients  ', /)
99998 FORMAT (1X, F8.4, 5X, F9.4, 5X, 4F9.4, /)
99999 FORMAT (1X, F8.4, 14X, 5X, 4F9.4, /)
      END
      REAL FUNCTION F (K, X)
      INTEGER    K
      REAL       X
!
      REAL       SIN
      INTRINSIC  SIN
!
      F = SIN(K*X)
      RETURN
      END
```

Output

```
Without error introduced we have :
SSE          Intercept      Coefficients

89.8776                      1.0101    0.0199    7.0291    0.0374
 0.0000        1.0000        1.0000    0.0000    7.0000    0.0000

With error introduced we have :
SSE          Intercept      Coefficients

112.4662                     0.9963   -0.0675    6.9825    0.0133
 30.9831       0.9522        0.9867   -0.0864    6.9548   -0.0223
```

BSLSQ

Computes the least-squares spline approximation, and return the B-spline coefficients.

Required Arguments

XDATA — Array of length NDATA containing the data point abscissas. (Input)

FDATA — Array of length NDATA containing the data point ordinates. (Input)

KORDER — Order of the spline. (Input)
KORDER must be less than or equal to NDATA.

XKNOT — Array of length NCOEF + KORDER containing the knot sequence. (Input)
XKNOT must be nondecreasing.

NCOEF — Number of B-spline coefficients. (Input)
NCOEF cannot be greater than NDATA.

BSCOEF — Array of length NCOEF containing the B-spline coefficients. (Output)

Optional Arguments

NDATA — Number of data points. (Input)
Default: NDATA = size(XDATA, 1)

WEIGHT — Array of length NDATA containing the weights. (Input)
Default: WEIGHT = 1.0.

FORTRAN 90 Interface

Generic: CALL BSLSQ (XDATA, FDATA, KORDER, XKNOT, NCOEF, BSCOEF [, …])

Specific: The specific interface names are S_BSLSQ and D_BSLSQ.

FORTRAN 77 Interface

Single: CALL BSLSQ (NDATA, XDATA, FDATA, WEIGHT, KORDER, XKNOT, NCOEF, BSCOEF)

Double: The double precision name is DBSLSQ.

Description

The routine BSLSQ is based on the routine L2APPR by de Boor (1978, page 255). The IMSL routine BSLSQ computes a weighted discrete L_2 approximation from a spline subspace to a given data set (x_i, f_i) for $i = 1, \ldots, N$ (where N = NDATA). In other words, it finds B-spline coefficients,

a = BSCOEF, such that

$$\sum_{i=1}^{N} \left| f_i - \sum_{j=1}^{m} a_j B_j(x_i) \right|^2 w_i$$

is a minimum, where m = NCOEF and B_j denotes the j-th B-spline for the given order, KORDER, and knot sequence, XKNOT. This linear least squares problem is solved by computing and solving the normal equations. While the normal equations can sometimes cause numerical difficulties, their use here should not cause a problem because the B-spline basis generally leads to well-conditioned banded matrices.

The choice of weights depends on the problem. In some cases, there is a natural choice for the weights based on the relative importance of the data points. To approximate a continuous function (if the location of the data points can be chosen), then the use of Gauss quadrature weights and points is reasonable. This follows because BSLSQ is minimizing an approximation to the integral

$$\int | F - s |^2 dx$$

The Gauss quadrature weights and points can be obtained using the IMSL routine GQRUL (see *Chapter 4, "Integration and Differentiation"*).

Comments

1. Workspace may be explicitly provided, if desired, by use of B2LSQ/DB2LSQ. The reference is:

   ```
   CALL B2LSQ (NDATA, XDATA, FDATA, WEIGHT, KORDER, XKNOT,
      NCOEF, BSCOEF, WK1, WK2, WK3, WK4, IWK)
   ```

   The additional arguments are as follows:

   WK1 — Work array of length (3 + NCOEF) * KORDER.

   WK2 — Work array of length NDATA.

   WK3 — Work array of length NDATA.

   WK4 — Work array of length NDATA.

   IWK — Work array of length NDATA.

2. Informational errors

Type	Code	Description
4	5	Multiplicity of the knots cannot exceed the order of the spline.
4	6	The knots must be nondecreasing.
4	7	All weights must be greater than zero.
4	8	The smallest element of the data point array must be greater than or equal to the KORDth knot.
4	9	The largest element of the data point array must be less than or equal to the (NCOEF + 1)st knot.

3. The B-spline representation can be evaluated using BSVAL, and its derivative can be evaluated using BSDER.

Example

In this example, we try to recover a quadratic polynomial using a quadratic spline with one interior knot from two different data sets. The first data set is generated by evaluating the quadratic at 50 equally spaced points in the interval (0, 1) and then adding uniformly distributed noise to the data. The second data set includes the first data set, and, additionally, the values at 0 and at 1 with no noise added. Since the first and last data points are uncontaminated by noise, we have chosen weights equal to 10^5 for these two points in this second problem. The quadratic, the first approximation, and the second approximation are then evaluated at 11 equally spaced points. This example illustrates the use of the weights to enforce interpolation at certain of the data points.

```
      USE IMSL_LIBRARIES

      IMPLICIT   NONE
      INTEGER    KORDER, NCOEF
      PARAMETER  (KORDER=3, NCOEF=4)
!
      INTEGER    I, NDATA, NOUT
      REAL       ABS, BSCOF1(NCOEF), BSCOF2(NCOEF), F,&
                 FDATA1(50), FDATA2(52), FLOAT, RNOISE, S1,&
                 S2, WEIGHT(52), X, XDATA1(50), XDATA2(52),&
                 XKNOT(KORDER+NCOEF), XT, YT
      INTRINSIC  ABS, FLOAT
!
      DATA WEIGHT/52*1.0/
!                                  Define function
      F(X) = 8.0*X*(1.0-X)
!                                  Set random number seed
      CALL RNSET (12345679)
      NDATA = 50
!                                  Set up interior knots
      DO 10  I=1, NCOEF - KORDER + 2
         XKNOT(I+KORDER-1) = FLOAT(I-1)/FLOAT(NCOEF-KORDER+1)
   10 CONTINUE
!                                  Stack knots
      DO 20  I=1, KORDER - 1
         XKNOT(I) = XKNOT(KORDER)
         XKNOT(I+NCOEF+1) = XKNOT(NCOEF+1)
   20 CONTINUE
```

```
!                                   Set up data points excluding
!                                   the endpoints 0 and 1.
!                                   The function values have noise
!                                   introduced.
      DO 30  I=1, NDATA
         XDATA1(I) = FLOAT(I)/51.0
         RNOISE    = RNUNF()
         RNOISE    = RNOISE - 0.5
         FDATA1(I) = F(XDATA1(I)) + RNOISE
   30 CONTINUE
!                                   Compute least squares B-spline
!                                   representation.
      CALL BSLSQ (XDATA1, FDATA1, KORDER, XKNOT, NCOEF, BSCOF1)
!                                   Now use same XDATA values but with
!                                   the endpoints included.  These
!                                   points will have large weights.
      NDATA = 52
      CALL SCOPY (50, XDATA1, 1, XDATA2(2:), 1)
      CALL SCOPY (50, FDATA1, 1, FDATA2(2:), 1)
!
      WEIGHT(1) = 1.0E5
      XDATA2(1) = 0.0
      FDATA2(1) = F(XDATA2(1))
      WEIGHT(NDATA) = 1.0E5
      XDATA2(NDATA) = 1.0
      FDATA2(NDATA) = F(XDATA2(NDATA))
!                                   Compute least squares B-spline
!                                   representation.
      CALL BSLSQ (XDATA2, FDATA2, KORDER, XKNOT, NCOEF, BSCOF2, &
                  WEIGHT=WEIGHT)
!                                   Get output unit number
      CALL UMACH (2, NOUT)
!                                   Write heading
      WRITE (NOUT,99998)
!                                   Print the two interpolants
!                                   at 11 points.
      DO 40  I=1, 11
         XT = FLOAT(I-1)/10.0
         YT = F(XT)
!                                   Evaluate splines
         S1 = BSVAL(XT,KORDER,XKNOT,NCOEF,BSCOF1)
         S2 = BSVAL(XT,KORDER,XKNOT,NCOEF,BSCOF2)
         WRITE (NOUT,99999) XT, YT, S1, S2, (S1-YT), (S2-YT)
   40 CONTINUE
!
99998 FORMAT (7X, 'X', 9X, 'F(X)', 6X, 'S1(X)', 5X, 'S2(X)', 7X,&
             'F(X)-S1(X)', 7X, 'F(X)-S2(X)')
99999 FORMAT (' ', 4F10.4, 4X, F10.4, 7X, F10.4)
      END
```

Output

```
X          F(X)       S1(X)      S2(X)        F(X)-S1(X)        F(X)-S2(X)
0.0000     0.0000     0.0515     0.0000        0.0515            0.0000
0.1000     0.7200     0.7594     0.7490        0.0394            0.0290
0.2000     1.2800     1.3142     1.3277          0.0342          0.0477
0.3000     1.6800     1.7158     1.7362        0.0358            0.0562
0.4000     1.9200     1.9641     1.9744        0.0441            0.0544
0.5000     2.0000     2.0593     2.0423        0.0593            0.0423
0.6000     1.9200     1.9842     1.9468        0.0642            0.0268
0.7000     1.6800     1.7220     1.6948        0.0420            0.0148
0.8000     1.2800     1.2726     1.2863       -0.0074            0.0063
0.9000     0.7200     0.6360     0.7214       -0.0840            0.0014
1.0000     0.0000    -0.1878     0.0000       -0.1878            0.0000
```

BSVLS

Computes the variable knot B-spline least squares approximation to given data.

Required Arguments

XDATA — Array of length NDATA containing the data point abscissas. (Input)

FDATA — Array of length NDATA containing the data point ordinates. (Input)

KORDER — Order of the spline. (Input)
KORDER must be less than or equal to NDATA.

NCOEF — Number of B-spline coefficients. (Input)
NCOEF must be less than or equal to NDATA.

XGUESS — Array of length NCOEF + KORDER containing the initial guess of knots. (Input)
XGUESS must be nondecreasing.

XKNOT — Array of length NCOEF + KORDER containing the (nondecreasing) knot sequence. (Output)

BSCOEF — Array of length NCOEF containing the B-spline representation. (Output)

SSQ — The square root of the sum of the squares of the error. (Output)

Optional Arguments

NDATA — Number of data points. (Input)
NDATA must be at least 2.
Default: NDATA = size(XDATA, 1)

WEIGHT — Array of length NDATA containing the weights. (Input)
Default: WEIGHT = 1.0.

FORTRAN 90 Interface

Generic: CALL BSVLS (XDATA, FDATA, KORDER, NCOEF, XGUESS, XKNOT, BSCOEF, SSQ [, …])

Specific: The specific interface names are S_BSVLS and D_BSVLS.

FORTRAN 77 Interface

Single: `CALL BSVLS` (`NDATA`, `XDATA`, `FDATA`, `WEIGHT`, `KORDER`, `NCOEF`, `XGUESS`, `XKNOT`, `BSCOEF`, `SSQ`)

Double: The double precision name is `DBSVLS`.

Description

The routine `BSVLS` attempts to find the best placement of knots that will minimize the leastsquares error to given data by a spline of order k = `KORDER` with N = `NCOEF` coefficients. The user provides the order k of the spline and the number of coefficients N. For this problem to make sense, it is necessary that $N > k$. We then attempt to find the minimum of the functional

$$F(a,\mathbf{t}) = \sum_{i=1}^{M} w_i \left(f_i - \sum_{j=1}^{N} a_j B_{j,k,\mathbf{t}}(x_j) \right)^2$$

The user must provide the weights w = `WEIGHT`, the data x_i = `XDATA` and f_i = `FDATA`, and M = `NDATA`. The minimum is taken over all admissible knot sequences **t**.

The technique employed in `BSVLS` uses the fact that for a fixed knot sequence **t** the minimization in a is a linear least-squares problem that can be solved by calling the IMSL routine `BSLSQ`. Thus, we can think of our objective function F as a function of just **t** by setting

$$G(\mathbf{t}) = \min_a F(a,\mathbf{t})$$

A Gauss-Seidel (cyclic coordinate) method is then used to reduce the value of the new objective function G. In addition to this local method, there is a global heuristic built into the algorithm that will be useful if the data arise from a smooth function. This heuristic is based on the routine `NEWNOT` of de Boor (1978, pages 184 and 258–261).

The user must input an initial guess, $\mathbf{t}^g$ = `XGUESS`, for the knot sequence. This guess must be a *valid* knot sequence for the splines of order k with

$$\mathbf{t}_1^g \le \ldots \le \mathbf{t}_k^g \le x_i \le \mathbf{t}_{N+1}^g \le \ldots \le \mathbf{t}_{N+k}^g, \qquad i = 1, \ldots, M$$

with $\mathbf{t}^g$ nondecreasing, and

$$\mathbf{t}_1^g < \mathbf{t}_{i+k}^g \qquad i = 1, \ldots, N$$

The routine BSVLS returns the B-spline representation of the best fit found by the algorithm as well as the square root of the sum of squares error in SSQ. If this answer is unsatisfactory, you may reinitialize BSVLS with the return from BSVLS to see if an improvement will occur. We have found that this option does not usually (substantially) improve the result. In regard to execution speed, this routine can be several orders of magnitude slower than one call to the least-squares routine BSLSQ.

Comments

1. Workspace may be explicitly provided, if desired, by use of B2VLS/DB2VLS. The reference is:

```
CALL B2VLS (NDATA, XDATA, FDATA, WEIGHT, KORDER, NCOEF,
   XGUESS, XKNOT, BSCOEF, SSQ, IWK, WK)
```

   The additional arguments are as follows:

   IWK — Work array of length NDATA.

   WK — Work array of length NCOEF * (6 + 2 * KORDER) + KORDER * (7 − KORDER) + 3 * NDATA + 3.

2. Informational errors

Type	Code	Description
3	12	The knots found to be optimal are stacked more than KORDER. This indicates fewer knots will produce the same error sum of squares. The knots have been separated slightly.
4	9	The multiplicity of the knots in XGUESS cannot exceed the order of the spline.
4	10	XGUESS must be nondecreasing.

Example

In this example, we try to fit the function $|x - .33|$ evaluated at 100 equally spaced points on [0, 1]. We first use quadratic splines with 2 interior knots initially at .2 and .8. The eventual error should be zero since the function is a quadratic spline with two knots stacked at .33. As a second example, we try to fit the same data with cubic splines with three interior knots initially located at .1, .2, and, .5. Again, the theoretical error is zero when the three knots are stacked at .33.

We include a graph of the initial least-squares fit using the IMSL routine BSLSQ for the above quadratic spline example with knots at .2 and .8. This graph overlays the graph of the spline computed by BSVLS, which is indistinguishable from the data.

```
      USE BSVLS_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    KORD1, KORD2, NCOEF1, NCOEF2, NDATA
      PARAMETER  (KORD1=3, KORD2=4, NCOEF1=5, NCOEF2=7, NDATA=100)
!
      INTEGER    I, NOUT
      REAL       ABS, BSCOEF(NCOEF2), F, FDATA(NDATA), FLOAT, SSQ,&
                 WEIGHT(NDATA), X, XDATA(NDATA), XGUES1(NCOEF1+KORD1),&
                 XGUES2(KORD2+NCOEF2), XKNOT(NCOEF2+KORD2)
      INTRINSIC  ABS, FLOAT
!
      DATA XGUES1/3*0.0, .2, .8, 3*1.0001/
      DATA XGUES2/4*0.0, .1, .2, .5, 4*1.0001/
      DATA WEIGHT/NDATA*.01/
!                                  Define function
      F(X) = ABS(X-.33)
!                                  Set up data
      DO 10  I=1, NDATA
         XDATA(I) = FLOAT(I-1)/FLOAT(NDATA)
         FDATA(I) = F(XDATA(I))
   10 CONTINUE
!                                  Compute least squares B-spline
!                                  representation with KORD1, NCOEF1,
!                                  and XGUES1.
      CALL BSVLS (XDATA, FDATA, KORD1, NCOEF1, XGUES1,&
                  XKNOT, BSCOEF, SSQ, WEIGHT=WEIGHT)
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Print heading
      WRITE (NOUT,99998) 'quadratic'
!                                  Print SSQ and the knots
      WRITE (NOUT,99999) SSQ, (XKNOT(I),I=1,KORD1+NCOEF1)
!                                  Compute least squares B-spline
!                                  representation with KORD2, NCOEF2,
!                                  and XGUES2.
      CALL BSVLS (XDATA, FDATA, KORD2, NCOEF2, XGUES2,&
                  XKNOT, BSCOEF, SSQ, WEIGHT=WEIGHT)
!                                  Print SSQ and the knots
      WRITE (NOUT,99998) 'cubic'
      WRITE (NOUT,99999) SSQ, (XKNOT(I),I=1,KORD2+NCOEF2)
!
99998 FORMAT (' Piecewise ', A, /)
99999 FORMAT (' Square root of the sum of squares : ', F9.4, /,&
             ' Knot sequence : ', /, 1X, 11(F9.4,/,1X))
      END
```

Output

```
Piecewise quadratic

Square root of the sum of squares :    0.0008
Knot sequence :
   0.0000
   0.0000
   0.0000
   0.3137
   0.3464
   1.0001
   1.0001
   1.0001

Piecewise cubic
```

```
Square root of the sum of squares :    0.0005
Knot sequence :
   0.0000
   0.0000
   0.0000
   0.0000
   0.3167
   0.3273
   0.3464
   1.0001
   1.0001
   1.0001
   1.0001
```

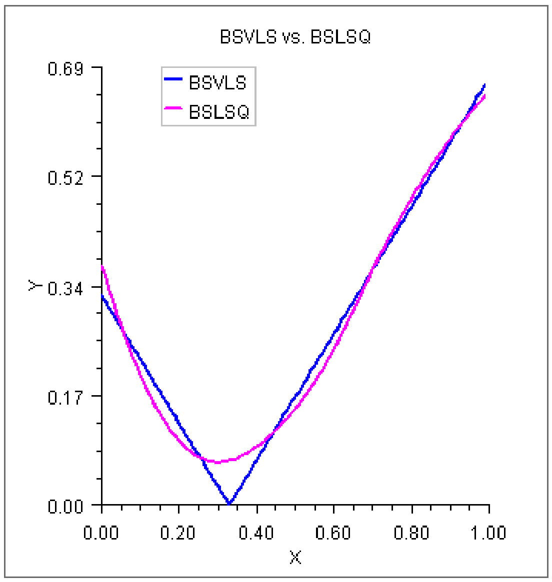


Figure 9, BSVLS vs. BSLSQ

CONFT

more...

Computes the least-squares constrained spline approximation, returning the B-spline coefficients.

Required Arguments

XDATA — Array of length `NDATA` containing the data point abscissas. (Input)

FDATA — Array of size `NDATA` containing the values to be approximated. (Input)
`FDATA(I)` contains the value at `XDATA(I)`.

XVAL — Array of length `NXVAL` containing the abscissas at which the fit is to be constrained. (Input)

NHARD — Number of entries of `XVAL` involved in the 'hard' constraints. (Input)
Note: (0 ≤ `NHARD` ≤ `NXVAL`). Setting `NHARD` to zero always results in a fit, while setting `NHARD` to `NXVAL` forces all constraints to be met. The 'hard' constraints must be satisfied or else the routine signals failure. The 'soft' constraints need not be satisfied, but there will be an attempt to satisfy the 'soft' constraints. The constraints must be ordered in terms of priority with the most important constraints first. Thus, all of the 'hard' constraints must preceed the 'soft' constraints. If infeasibility is detected among the soft constraints, we satisfy (in order) as many of the soft constraints as possible.

IDER — Array of length `NXVAL` containing the derivative value of the spline that is to be constrained. (Input)
If we want to constrain the integral of the spline over the closed interval (c, d), then we set `IDER(I)` = `IDER(I + 1)` = − 1 and `XVAL(I)` = c and `XVAL(I + 1)` = d. For consistency, we insist that `ITYPE(I)` = `ITYPE(I + 1)` .GE. 0 and c .LE. d. Note that every entry in `IDER` must be at least − 1.

ITYPE — Array of length `NXVAL` indicating the types of general constraints. (Input)

`ITYPE(I)`	I-th Constraint
1	$\mathrm{BL(I)} = f^{(d_i)}(x_i)$
2	$f^{(d_i)}(x_i) \le \mathrm{BU(I)}$
3	$f^{(d_i)}(x_i) \ge \mathrm{BL(I)}$
4	$\mathrm{BL(I)} \le f^{(d_i)}(x_i) \le \mathrm{BU(I)}$
$(d_i = -1)1$	$\mathrm{BL(I)} = \int_c^d f(t)dt$
$(d_i = -1)2$	$\int_c^d f(t)dt \le \mathrm{BU(I)}$
$(d_i = -1)3$	$\int_c^d f(t)dt \ge \mathrm{BL(I)}$
$(d_i = -1)4$	$\mathrm{BL(I)} \le \int_c^d f(t)dt \le \mathrm{BU(I)}$
10	periodic end conditions
99	disregard this constraint

In order to set two point constraints, we must have `ITYPE(I)` = `ITYPE(I` + 1) and `ITYPE(I)` must be negative.

`ITYPE(I)`	I-th Constraint
-1	$\mathrm{BL(I)} = f^{(d_i)}(x_i) - f^{(d_{i+1})}(x_{i+1})$
-2	$f^{(d_i)}(x_i) - f^{(d_{i+1})}(x_{i+1}) \le \mathrm{BU(I)}$
-3	$f^{(d_i)}(x_i) - f^{(d_{i+1})}(x_{i+1}) \ge \mathrm{BL(I)}$
-4	$\mathrm{BL(I)} \le f^{(d_i)}(x_i) - f^{(d_{i+1})}(x_{i+1}) \le \mathrm{BU(I)}$

BL — Array of length `NXVAL` containing the lower limit of the general constraints, if there is no lower limit on the `I`-*th* constraint, then `BL(I)` is not referenced. (Input)

BU — Array of length NXVAL containing the upper limit of the general constraints, if there is no upper limit on the I-*th* constraint, then BU(I) is not referenced; if there is no range constraint, BL and BU can share the same storage locations. (Input)
If the I-*th* constraint is an equality constraint, BU(I) is not referenced.

KORDER — Order of the spline. (Input)

XKNOT — Array of length NCOEF + KORDER containing the knot sequence. (Input)
The entries of XKNOT must be nondecreasing.

BSCOEF — Array of length NCOEF containing the B-spline coefficients. (Output)

Optional Arguments

NDATA — Number of data points. (Input)
Default: NDATA = size (XDATA,1).

WEIGHT — Array of length NDATA containing the weights. (Input)
Default: WEIGHT = 1.0.

NXVAL — Number of points in the vector XVAL. (Input)
Default: NXVAL = size (XVAL,1).

NCOEF — Number of B-spline coefficients. (Input)
Default: NCOEF = size (BSCOEF,1).

FORTRAN 90 Interface

Generic: CALL CONFT (XDATA, FDATA, XVAL, NHARD, IDER, ITYPE, BL, BU, KORDER, XKNOT, BSCOEF [, …])

Specific: The specific interface names are S_CONFT and D_CONFT.

FORTRAN 77 Interface

Single: CALL CONFT (NDATA, XDATA, FDATA, WEIGHT, NXVAL, XVAL, NHARD, IDER, ITYPE, BL, BU, KORDER, XKNOT, NCOEF, BSCOEF)

Double: The double precision name is DCONFT.

Description

The routine CONFT produces a constrained, weighted least-squares fit to data from a spline subspace. Constraints involving one point, two points, or integrals over an interval are allowed. The types of constraints supported by the routine are of four types.

$$
\begin{aligned}
E_p[f] \quad & = f^{(j_p)}(y_p) \\
\text{or} \quad & = f^{(j_p)}(y_p) - f^{(j_{p+1})}(y_{p+1}) \\
\text{or} \quad & = \int_{y_p}^{y_{p+1}} f(t)\,dt \\
\text{or} \quad & = \text{periodic end conditions}
\end{aligned}
$$

An interval, I_p, (which may be a point, a finite interval , or semi-infinite interval) is associated with each of these constraints.

The input for this routine consists of several items, first, the data set (x_i, f_i) for $i = 1, \ldots, N$ (where N = NDATA), that is the data which is to be fit. Second, we have the weights to be used in the least squares fit (w = WEIGHT). The vector XVAL of length NXVAL contains the abscissas of the points involved in specifying the constraints. The algorithm tries to satisfy all the constraints, but if the constraints are inconsistent then it will drop constraints, in the reverse order specified, until either a consistent set of constraints is found or the "hard" constraints are determined to be inconsistent (the "hard" constraints are those involving XVAL(1), …, XVAL(NHARD)). Thus, the algorithm satisfies as many constraints as possible in the order specified by the user. In the case when constraints are dropped, the user will receive a message explaining how many constraints had to be dropped to obtain the fit. The next several arguments are related to the type of constraint and the constraint interval. The last four arguments determine the spline solution. The user chooses the spline subspace (KORDER, XKNOT, and NCOEF), and the routine returns the B-spline coefficients in BSCOEF.

Let n_f denote the number of feasible constraints as described above. Then, the routine solves the problem.

$$
\sum_{i=1}^{N} \left| f_i - \sum_{j=1}^{m} a_j B_j(x_i) \right|^2 w_i
$$

$$
\text{subject to} \quad E_p\left[\sum_{j=1}^{m} a_j B_j\right] \in I_p \quad p = 1, \ldots, n_f
$$

This linearly constrained least-squares problem is treated as a quadratic program and is solved by invoking the IMSL routine QPROG (see *Chapter 8, "Optimization"*).

The choice of weights depends on the data uncertainty in the problem. In some cases, there is a natural choice for the weights based on the estimates of errors in the data points.

Determining feasibility of linear constraints is a numerically sensitive task. If you encounter difficulties, a quick fix would be to widen the constraint intervals I_p.

Comments

1. Workspace may be explicitly provided, if desired, by use of C2NFT/DC2NFT. The reference is:

```
CALL C2NFT (NDATA, XDATA, FDATA, WEIGHT, NXVAL, XVAL, NHARD,
   IDER, ITYPE, BL, BU, KORDER, XKNOT, NCOEF, BSCOEF, H, G,
   A, RHS, WK, IPERM, IWK)
```

The additional arguments are as follows:

H — Work array of size NCOEF by NCOEF. Upon output, H contains the Hessian matrix of the objective function used in the call to QPROG (see *Chapter 8, "Optimization"*).

G — Work array of size NCOEF. Upon output, G contains the coefficients of the linear term used in the call to QPROG.

A — Work array of size (2 * NXVAL + KORDER) by (NCOEF + 1). Upon output, A contains the constraint matrix used in the call QPROG. The last column of A is used to keep record of the original order of the constraints.

RHS — Work array of size 2 * NXVAL + KORDER . Upon output, RHS contains the right hand side of the constraint matrix *A* used in the call to QPROG.

WK — Work array of size (KORDER + 1) * (2 * KORDER + 1) + (3 * NCOEF * NCOEF + 13 * NCOEF)/2 + (2 * NXVAL + KORDER +30)*(2*NXVAL + KORDER) + NDATA + 1.

IPERM — Work array of size NXVAL. Upon output, IPERM contains the permutation of the original constraints used to generate the matrix A.

IWK — Work array of size NDATA + 30 * (2 * NXVAL + KORDER) + 4 * NCOEF.

2. Informational errors

Type	Code	Description
3	11	Soft constraints had to be removed in order to get a fit.
4	12	Multiplicity of the knots cannot exceed the order of the spline.
4	13	The knots must be nondecreasing.
4	14	The smallest element of the data point array must be greater than or equal to the KORD-th knot.
4	15	The largest element of the data point array must be less than or equal to the (NCOEF + 1)st knot.
4	16	All weights must be greater than zero.
4	17	The hard constraints could not be met.

Type	Code	Description
4	18	The abscissas of the constrained points must lie within knot interval.
4	19	The upperbound must be greater than or equal to the lowerbound for a range constaint.
4	20	The upper limit of integration must be greater than the lower limit of integration for constraints involving the integral of the approximation.

Examples

Example 1

This is a simple application of CONFT. We generate data from the function

$$\frac{x}{2} + \sin\left(\frac{x}{2}\right)$$

contaminated with random noise and fit it with cubic splines. The function is increasing so we would hope that our least-squares fit would also be increasing. This is not the case for the unconstrained least squares fit generated by BSLSQ. We then force the derivative to be greater than 0 at NXVAL = 15 equally spaced points and call CONFT. The resulting curve is monotone. We print the error for the two fits averaged over 100 equally spaced points.

```
      USE IMSL_LIBRARIES

      IMPLICIT   NONE
      INTEGER    KORDER, NCOEF, NDATA, NXVAL
      PARAMETER  (KORDER=4, NCOEF=8, NDATA=15, NXVAL=15)
!
      INTEGER    I, IDER(NXVAL), ITYPE(NXVAL), NHARD, NOUT
      REAL       ABS, BL(NXVAL), BSCLSQ(NDATA), BSCNFT(NDATA), &
                 BU(NXVAL), ERRLSQ, ERRNFT, F1, FDATA(NDATA), FLOAT,&
                 GRDSIZ, SIN, WEIGHT(NDATA), X, XDATA(NDATA),&
                 XKNOT(KORDER+NDATA), XVAL(NXVAL)
      INTRINSIC  ABS, FLOAT, SIN
!
      F1(X) = .5*X + SIN(.5*X)
!                                  Initialize random number generator
!                                  and get output unit number.
      CALL RNSET (234579)
      CALL UMACH (2, NOUT)
!                                  Use default weights of one.
!
!                                  Compute original XDATA and FDATA
!                                  with random noise.
      GRDSIZ = 10.0
      DO 10  I=1, NDATA
         XDATA(I) = GRDSIZ*((FLOAT(I-1)/FLOAT(NDATA-1)))
         FDATA(I) = RNUNF()
         FDATA(I) = F1(XDATA(I)) + (FDATA(I)-.5)
   10 CONTINUE
!                                  Compute knots
      DO 20  I=1, NCOEF - KORDER + 2
         XKNOT(I+KORDER-1) = GRDSIZ*((FLOAT(I-1)/FLOAT(NCOEF-KORDER+1))&
```

```
                               )
   20 CONTINUE
      DO 30  I=1, KORDER - 1
         XKNOT(I) = XKNOT(KORDER)
         XKNOT(I+NCOEF+1) = XKNOT(NCOEF+1)
   30 CONTINUE
!
!                                  Compute BSLSQ fit.
      CALL BSLSQ (XDATA, FDATA, KORDER, XKNOT, NCOEF, BSCLSQ)
!                                  Construct the constraints for
!                                  CONFT.
      DO 40  I=1, NXVAL
         XVAL(I)  = GRDSIZ*FLOAT(I-1)/FLOAT(NXVAL-1)
         ITYPE(I) = 3
         IDER(I)  = 1
         BL(I)    = 0.0
   40 CONTINUE
!                                  Call CONFT
      NHARD = 0
      CALL CONFT (XDATA, FDATA, XVAL, NHARD, IDER, ITYPE, BL, BU, KORDER,&
                  XKNOT, BSCNFT, NCOEF=NCOEF)
!                                  Compute the average error
!                                  of 100 points in the interval.
      ERRLSQ = 0.0
      ERRNFT = 0.0
      DO 50  I=1, 100
         X      = GRDSIZ*FLOAT(I-1)/99.0
         ERRNFT = ERRNFT + ABS(F1(X)-BSVAL(X,KORDER,XKNOT,NCOEF,BSCNFT)&
                  )
         ERRLSQ = ERRLSQ + ABS(F1(X)-BSVAL(X,KORDER,XKNOT,NCOEF,BSCLSQ)&
                  )
   50 CONTINUE
!                                  Print results
      WRITE (NOUT,99998) ERRLSQ/100.0
      WRITE (NOUT,99999) ERRNFT/100.0
!
99998 FORMAT (' Average error with BSLSQ fit:  ', F8.5)
99999 FORMAT (' Average error with CONFT fit:  ', F8.5)
      END
```

Output

```
Average error with BSLSQ fit:   0.20250
Average error with CONFT fit:   0.14334
```

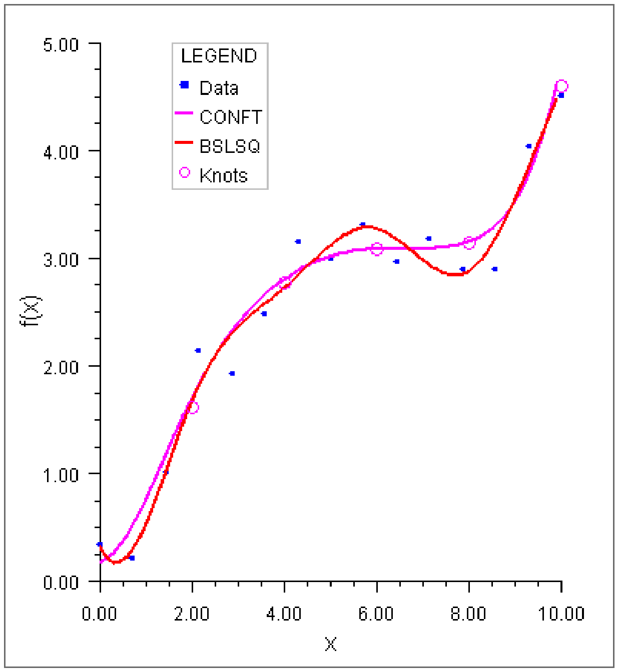


Figure 10, CONFT vs. BSLSQ Forcing Monotonicity

Example 2

We now try to recover the function

$$\frac{1}{1+x^4}$$

from noisy data. We first try the unconstrained least-squares fit using BSLSQ. Finding that fit somewhat unsatisfactory, we apply several constraints using CONFT. First, notice that the unconstrained fit oscillates through the true function at both ends of the interval. This is common for flat data. To remove this oscillation, we constrain the cubic spline to have zero second derivative at the first and last four knots. This forces the cubic spline to reduce to a linear polynomial on the first and last three knot intervals. In addition, we constrain the fit (which we will call *s*) as follows:

$$\begin{aligned} s(-7) &\geq 0 \\ \int_{-7}^{7} s(x)\,dx &\leq 2.3 \\ s(-7) &= s(7) \end{aligned}$$

Notice that the last constraint was generated using the periodic option (requiring only the zeroeth derivative to be periodic). We print the error for the two fits averaged over 100 equally spaced points.

```
      USE IMSL_LIBRARIES

      IMPLICIT   NONE
      INTEGER    KORDER, NCOEF, NDATA, NXVAL
      PARAMETER  (KORDER=4, NCOEF=13, NDATA=51, NXVAL=12)
!
      INTEGER    I, IDER(NXVAL), ITYPE(NXVAL), NHARPT, NOUT
      REAL       ABS, BL(NXVAL), BSCLSQ(NDATA), BSCNFT(NDATA),&
                 BU(NXVAL), ERRLSQ, ERRNFT, F1, FDATA(NDATA), FLOAT,&
                 GRDSIZ, WEIGHT(NDATA), X, XDATA(NDATA),&
                 XKNOT(KORDER+NDATA), XVAL(NXVAL)
      INTRINSIC  ABS, FLOAT
!
      F1(X) = 1.0/(1.0+X**4)
!                                  Initialize random number generator
!                                  and get output unit number.
      CALL UMACH (2, NOUT)
      CALL RNSET (234579)
!                                  Use deafult weights of one.
!
!                                  Compute original XDATA and FDATA
!                                  with random noise.
      GRDSIZ = 14.0
      DO 10  I=1, NDATA
         XDATA(I) = GRDSIZ*((FLOAT(I-1)/FLOAT(NDATA-1))) - GRDSIZ/2.0
         FDATA(I) = RNUNF()
         FDATA(I) = F1(XDATA(I)) + 0.125*(FDATA(I)-.5)
   10 CONTINUE
!                                  Compute KNOTS
      DO 20  I=1, NCOEF - KORDER + 2
         XKNOT(I+KORDER-1) = GRDSIZ*((FLOAT(I-1)/FLOAT(NCOEF-KORDER+1))&
                             ) - GRDSIZ/2.0
   20 CONTINUE
      DO 30  I=1, KORDER - 1
         XKNOT(I) = XKNOT(KORDER)
         XKNOT(I+NCOEF+1) = XKNOT(NCOEF+1)
   30 CONTINUE
!                                  Compute BSLSQ fit
      CALL BSLSQ (XDATA, FDATA, KORDER, XKNOT, NCOEF, BSCLSQ)
!                                  Construct the constraints for
!                                  CONFT
      DO 40  I=1, 4
         XVAL(I)     = XKNOT(KORDER+I-1)
         XVAL(I+4)   = XKNOT(NCOEF-3+I)
         ITYPE(I)    = 1
         ITYPE(I+4)  = 1
         IDER(I)     = 2
         IDER(I+4)   = 2
         BL(I)       = 0.0
         BL(I+4)     = 0.0
   40 CONTINUE
!
      XVAL(9)   = -7.0
      ITYPE(9)  = 3
      IDER(9)   = 0
      BL(9)     = 0.0
!
      XVAL(10)  = -7.0
      ITYPE(10) = 2
      IDER(10)  = -1
      BU(10)    = 2.3
!
      XVAL(11)  = 7.0
      ITYPE(11) = 2
      IDER(11)  = -1
```

```
      BU(11)    = 2.3
!
      XVAL(12)  = -7.0
      ITYPE(12) = 10
      IDER(12)  = 0
!                                   Call CONFT
      CALL CONFT (XDATA, FDATA, XVAL, NHARPT, IDER, ITYPE, BL, BU,&
                  KORDER, XKNOT, BSCNFT, NCOEF=NCOEF)
!                                   Compute the average error
!                                   of 100 points in the interval.
      ERRLSQ = 0.0
      ERRNFT = 0.0
      DO 50  I=1, 100
         X      = GRDSIZ*FLOAT(I-1)/99.0 - GRDSIZ/2.0
         ERRNFT = ERRNFT + ABS(F1(X)-BSVAL(X,KORDER,XKNOT,NCOEF,BSCNFT)&
                  )
         ERRLSQ = ERRLSQ + ABS(F1(X)-BSVAL(X,KORDER,XKNOT,NCOEF,BSCLSQ)&
                  )
   50 CONTINUE
!                                   Print results
      WRITE (NOUT,99998) ERRLSQ/100.0
      WRITE (NOUT,99999) ERRNFT/100.0
!
99998 FORMAT (' Average error with BSLSQ fit:   ', F8.5)
99999 FORMAT (' Average error with CONFT fit:   ', F8.5)
      END
```

Output

```
Average error with BSLSQ fit:   0.01783
Average error with CONFT fit:   0.01339
```

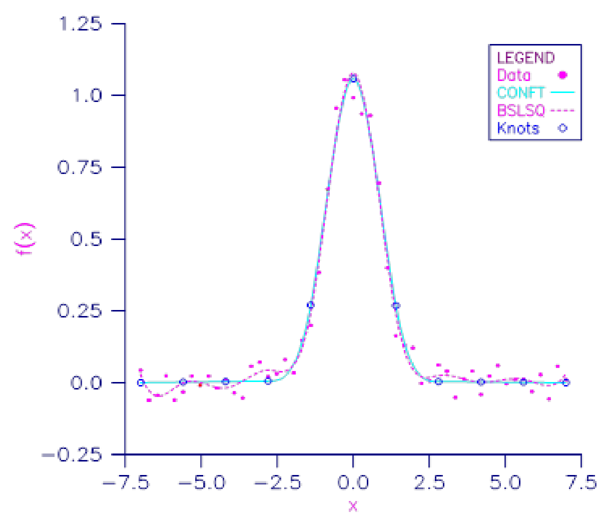


Figure 11, CONFT vs. BSLSQ Approximating 1/(1 + x4)

BSLS2

Computes a two-dimensional tensor-product spline approximant using least squares, returning the tensor-product B-spline coefficients.

Required Arguments

XDATA — Array of length NXDATA containing the data points in the X-direction. (Input)
XDATA must be nondecreasing.

YDATA — Array of length NYDATA containing the data points in the Y-direction. (Input)
YDATA must be nondecreasing.

FDATA — Array of size NXDATA by NYDATA containing the values on the X − Y grid to be interpolated. (Input)
FDATA(I, J) contains the value at (XDATA(I), YDATA(I)).

KXORD — Order of the spline in the X-direction. (Input)

KYORD — Order of the spline in the Y-direction. (Input)

XKNOT — Array of length KXORD + NXCOEF containing the knots in the X-direction. (Input)
XKNOT must be nondecreasing.

YKNOT — Array of length KYORD + NYCOEF containing the knots in the Y-direction. (Input)
YKNOT must be nondecreasing.

BSCOEF — Array of length NXCOEF * NYCOEF that contains the tensor product B-spline coefficients. (Output)
BSCOEF is treated internally as an array of size NXCOEF by NYCOEF.

Optional Arguments

NXDATA — Number of data points in the X-direction. (Input)
Default: NXDATA = size (XDATA,1).

NYDATA — Number of data points in the Y-direction. (Input)
Default: NYDATA = size (YDATA,1).

LDF — Leading dimension of FDATA exactly as specified in the dimension statement of calling program. (Input)
Default: LDF = size (FDATA,1).

NXCOEF — Number of B-spline coefficients in the X-direction. (Input)
Default: NXCOEF = size (XKNOT,1) – KXORD.

NYCOEF — Number of B-spline coefficients in the Y-direction. (Input)
Default: NYCOEF = size (YKNOT,1) – KYORD.

XWEIGH — Array of length NXDATA containing the positive weights of XDATA. (Input)
Default: XWEIGH = 1.0.

YWEIGH — Array of length NYDATA containing the positive weights of YDATA. (Input)
Default: YWEIGH = 1.0.

FORTRAN 90 Interface

Generic: CALL BSLS2 (XDATA, YDATA, FDATA, KXORD, KYORD, XKNOT, YKNOT, BSCOEF [, …])

Specific: The specific interface names are S_BSLS2 and D_BSLS2.

FORTRAN 77 Interface

Single: CALL BSLS2 (NXDATA, XDATA, NYDATA, YDATA, FDATA, LDF, KXORD, KYORD, XKNOT, YKNOT, NXCOEF, NYCOEF, XWEIGH, YWEIGH, BSCOEF)

Double: The double precision name is DBSLS2.

Description

The routine BSLS2 computes the coefficients of a tensor-product spline least-squares approximation to weighted tensor-product data. The input for this subroutine consists of data vectors to specify the tensor-product grid for the data, two vectors with the weights, the values of the surface on the grid, and the specification for the tensor-product spline. The grid is specified by the two vectors x = XDATA and y = YDATA of length n = NXDATA and m = NYDATA, respectively. A two-dimensional array f = FDATA contains the data values that are to be fit. The two vectors w_x = XWEIGH and w_y = YWEIGH contain the weights for the weighted least-squares problem. The information for the approximating tensor-product spline must also be provided. This information is contained in k_x = KXORD, $\mathbf{t}_x$ = XKNOT, and N = NXCOEF for the spline in the first variable, and in k_y = KYORD, $\mathbf{t}_y$ = YKNOT and M = NYCOEF for the spline in the second variable. The coefficients of the resulting tensor-product spline are returned in c = BSCOEF, which is an $N * M$ array. The procedure computes coefficients by solving the normal equations in tensor-product form as discussed in de Boor (1978, Chapter 17). The interested reader might also want to study the paper by E. Grosse (1980).

The final result produces coefficients c minimizing

$$\sum_{i=1}^{n}\sum_{j=1}^{m} w_x(i) w_y(j) \left[\sum_{k=1}^{N}\sum_{l=1}^{M} c_{kl} B_{kl}(x_i, y_j) - f_{ij} \right]^2$$

where the function B_{kl} is the tensor-product of two B-splines of order k_x and k_y. Specifically, we have

$$B_{kl}(x,y) = B_{k,k_x,\mathbf{t}_x}(x) B_{l,k_y,\mathbf{t}_y}(y)$$

The spline

$$\sum_{k=1}^{N}\sum_{l=1}^{M} c_{kl} B_{kl}$$

can be evaluated using BS2VL and its partial derivatives can be evaluated using BS2DR.

Comments

1. Workspace may be explicitly provided, if desired, by use of B2LS2/DB2LS2. The reference is:

```
CALL B2LS2 (NXDATA, XDATA, NYDATA, YDATA, FDATA, LDF, KXORD,
   KYORD, XKNOT, YKNOT, NXCOEF, NYCOEF, XWEIGH, YWEIGH,
   BSCOEF, WK)
```

   The additional argument is:

   WK — Work array of length (NXCOEF + 1) * NYDATA + KXORD * NXCOEF + KYORD * NYCOEF + 3 * MAX(KXORD, KYORD).

2. Informational errors

Type	Code	Description
3	14	There may be less than one digit of accuracy in the least squares fit. Try using higher precision if possible.
4	5	Multiplicity of the knots cannot exceed the order of the spline.
4	6	The knots must be nondecreasing.
4	7	All weights must be greater than zero.
4	9	The data point abscissae must be nondecreasing.

Type	Code	Description
4	10	The smallest element of the data point array must be greater than or equal to the K_ORDth knot.
4	11	The largest element of the data point array must be less than or equal to the (N_COEF + 1)st knot.

Example

The data for this example arise from the function $e^x \sin(x + y) + \varepsilon$ on the rectangle $[0, 3] \times [0, 5]$. Here, ε is a uniform random variable with range $[-1, 1]$. We sample this function on a 100×50 grid and then try to recover it by using cubic splines in the *x* variable and quadratic splines in the *y* variable. We print out the values of the function $e^x \sin(x + y)$ on a 3×5 grid and compare these values with the values of the tensor-product spline that was computed using the IMSL routine BSLS2.

```
      USE IMSL_LIBRARIES

      IMPLICIT   NONE
      INTEGER    KXORD, KYORD, LDF, NXCOEF, NXDATA, NXVEC, NYCOEF,&
                 NYDATA, NYVEC
      PARAMETER  (KXORD=4, KYORD=3, NXCOEF=15, NXDATA=100, NXVEC=4,&
                 NYCOEF=7, NYDATA=50, NYVEC=6, LDF=NXDATA)
!
      INTEGER    I, J, NOUT
      REAL       BSCOEF(NXCOEF,NYCOEF), EXP, F, FDATA(NXDATA,NYDATA),&
                 FLOAT, RNOISE, SIN, VALUE(NXVEC,NYVEC), X,&
                 XDATA(NXDATA), XKNOT(NXCOEF+KXORD), XVEC(NXVEC),&
                 XWEIGH(NXDATA), Y, YDATA(NYDATA),&
                 YKNOT(NYCOEF+KYORD), YVEC(NYVEC), YWEIGH(NYDATA)
      INTRINSIC  EXP, FLOAT, SIN
!                                  Define function
      F(X,Y) = EXP(X)*SIN(X+Y)
!                                  Set random number seed
      CALL RNSET (1234579)
!                                  Set up X knot sequence.
      DO 10  I=1, NXCOEF - KXORD + 2
         XKNOT(I+KXORD-1) = 3.0*(FLOAT(I-1)/FLOAT(NXCOEF-KXORD+1))
   10 CONTINUE
      XKNOT(NXCOEF+1) = XKNOT(NXCOEF+1) + 0.001
!                                  Stack knots.
      DO 20  I=1, KXORD - 1
         XKNOT(I) = XKNOT(KXORD)
         XKNOT(I+NXCOEF+1) = XKNOT(NXCOEF+1)
   20 CONTINUE
!                                  Set up Y knot sequence.
      DO 30  I=1, NYCOEF - KYORD + 2
         YKNOT(I+KYORD-1) = 5.0*(FLOAT(I-1)/FLOAT(NYCOEF-KYORD+1))
   30 CONTINUE
      YKNOT(NYCOEF+1) = YKNOT(NYCOEF+1) + 0.001
!                                  Stack knots.
      DO 40  I=1, KYORD - 1
         YKNOT(I) = YKNOT(KYORD)
         YKNOT(I+NYCOEF+1) = YKNOT(NYCOEF+1)
   40 CONTINUE
!                                  Set up X-grid.
      DO 50  I=1, NXDATA
         XDATA(I) = 3.0*(FLOAT(I-1)/FLOAT(NXDATA-1))
```

```
   50 CONTINUE
!                                  Set up Y-grid.
      DO 60  I=1, NYDATA
         YDATA(I) = 5.0*(FLOAT(I-1)/FLOAT(NYDATA-1))
   60 CONTINUE
!                                  Evaluate function on grid and
!                                  introduce random noise in [1,-1].
      DO 70  I=1, NYDATA
         DO 70  J=1, NXDATA
            RNOISE     = RNUNF()
            RNOISE     = 2.0*RNOISE - 1.0
            FDATA(J,I) = F(XDATA(J),YDATA(I)) + RNOISE
   70 CONTINUE
!                                  Use default weights equal to 1.
!
!                                  Compute least squares approximation.
      CALL BSLS2 (XDATA, YDATA, FDATA, KXORD, KYORD, &
                  XKNOT, YKNOT, BSCOEF)
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Write heading
      WRITE (NOUT,99999)
!                                  Print interpolated values
!                                  on [0,3] x [0,5].
      DO 80  I=1, NXVEC
         XVEC(I) = FLOAT(I-1)
   80 CONTINUE
      DO 90  I=1, NYVEC
         YVEC(I) = FLOAT(I-1)
   90 CONTINUE
!                                  Evaluate spline
      CALL BS2GD (0, 0, XVEC, YVEC, KXORD, KYORD, XKNOT,&
                  YKNOT, BSCOEF, VALUE)
      DO 110  I=1, NXVEC
         DO 100  J=1, NYVEC
            WRITE (NOUT,'(5F15.4)') XVEC(I), YVEC(J),&
                                   F(XVEC(I),YVEC(J)), VALUE(I,J),&
                                   (F(XVEC(I),YVEC(J))-VALUE(I,J))
  100    CONTINUE
  110 CONTINUE
99999 FORMAT (13X, 'X', 14X, 'Y', 10X, 'F(X,Y)', 9X, 'S(X,Y)', 10X,&
             'Error')
      END
```

Output

```
     X              Y            F(X,Y)         S(X,Y)          Error
0.0000         0.0000         0.0000         0.2782        -0.2782
0.0000         1.0000         0.8415         0.7762         0.0653
0.0000         2.0000         0.9093         0.8203         0.0890
0.0000         3.0000         0.1411         0.1391         0.0020
0.0000         4.0000        -0.7568        -0.5705        -0.1863
0.0000         5.0000        -0.9589        -1.0290         0.0701
1.0000         0.0000         2.2874         2.2678         0.0196
1.0000         1.0000         2.4717         2.4490         0.0227
1.0000         2.0000         0.3836         0.4947        -0.1111
1.0000         3.0000        -2.0572        -2.0378        -0.0195
1.0000         4.0000        -2.6066        -2.6218         0.0151
1.0000         5.0000        -0.7595        -0.7274        -0.0321
2.0000         0.0000         6.7188         6.6923         0.0265
2.0000         1.0000         1.0427         0.8492         0.1935
2.0000         2.0000        -5.5921        -5.5885        -0.0035
2.0000         3.0000        -7.0855        -7.0955         0.0099
```

```
 2.0000          4.0000          -2.0646          -2.1588          0.0942
 2.0000          5.0000           4.8545           4.7339          0.1206
 3.0000          0.0000           2.8345           2.5971          0.2373
 3.0000          1.0000         -15.2008         -15.1079         -0.0929
 3.0000          2.0000         -19.2605         -19.1698         -0.0907
 3.0000          3.0000          -5.6122          -5.5820         -0.0302
 3.0000          4.0000          13.1959          12.6659          0.5300
 3.0000          5.0000          19.8718          20.5170         -0.6452
```

BSLS3

Computes a three-dimensional tensor-product spline approximant using least squares, returning the tensor-product B-spline coefficients.

Required Arguments

XDATA — Array of length NXDATA containing the data points in the *x*-direction. (Input)
XDATA must be nondecreasing.

YDATA — Array of length NYDATA containing the data points in the *y*-direction. (Input)
YDATA must be nondecreasing.

ZDATA — Array of length NZDATA containing the data points in the *z*-direction. (Input)
ZDATA must be nondecreasing.

FDATA — Array of size NXDATA by NYDATA by NZDATA containing the values to be interpolated. (Input)
FDATA(I, J, K) contains the value at (XDATA(I), YDATA(J), ZDATA(K)).

KXORD — Order of the spline in the *x*-direction. (Input)

KYORD — Order of the spline in the *y*-direction. (Input)

KZORD — Order of the spline in the *z*-direction. (Input)

XKNOT — Array of length KXORD + NXCOEF containing the knots in the *x*-direction. (Input)
XKNOT must be nondecreasing.

YKNOT — Array of length KYORD + NYCOEF containing the knots in the *y*-direction. (Input)
YKNOT must be nondecreasing.

ZKNOT — Array of length KZORD + NZCOEF containing the knots in the *z*-direction. (Input)
ZKNOT must be nondecreasing.

BSCOEF — Array of length NXCOEF*NYCOEF*NZCOEF that contains the tensor product B-spline coefficients. (Output)

Optional Arguments

NXDATA — Number of data points in the *x*−direction. (Input)
NXDATA must be greater than or equal to NXCOEF.
Default: NXDATA = size (XDATA,1).

NYDATA — Number of data points in the *y*-direction. (Input)
NYDATA must be greater than or equal to NYCOEF.
Default: NYDATA = size (YDATA,1).

NZDATA — Number of data points in the *z*-direction. (Input)
NZDATA must be greater than or equal to NZCOEF.
Default: NZDATA = size (ZDATA,1).

LDFDAT — Leading dimension of FDATA exactly as specified in the dimension statement of the calling program. (Input)
Default: LDFDAT = size (FDATA,1).

MDFDAT — Second dimension of FDATA exactly as specified in the dimension statement of the calling program. (Input)
Default: MDFDAT = size (FDATA,2).

NXCOEF — Number of B-spline coefficients in the *x*-direction. (Input)
Default: NXCOEF = size (XKNOT,1) – KXORD.

NYCOEF — Number of B-spline coefficients in the *y*-direction. (Input)
Default: NYCOEF = size (YKNOT,1) – KYORD.

NZCOEF — Number of B-spline coefficients in the *z*-direction. (Input)
Default: NZCOEF = size (ZKNOT,1) – KZORD.

XWEIGH — Array of length NXDATA containing the positive weights of XDATA. (Input)
Default: XWEIGH = 1.0.

YWEIGH — Array of length NYDATA containing the positive weights of YDATA. (Input)
Default: YWEIGH = 1.0.

ZWEIGH — Array of length NZDATA containing the positive weights of ZDATA. (Input)
Default: ZWEIGH = 1.0.

FORTRAN 90 Interface

Generic: CALL BSLS3 (XDATA, YDATA, ZDATA, FDATA, KXORD, KYORD, KZORD, XKNOT, YKNOT, ZKNOT, BSCOEF [, …])

Specific: The specific interface names are S_BSLS3 and D_BSLS3.

FORTRAN 77 Interface

Single: CALL BSLS3 (NXDATA, XDATA, NYDATA, YDATA, NZDATA, ZDATA, FDATA, LDFDAT, MDFDAT, KXORD, KYORD, KZORD, XKNOT, YKNOT, ZKNOT, NXCOEF, NYCOEF, NZCOEF, XWEIGH, YWEIGH, ZWEIGH, BSCOEF)

Double: The double precision name is DBSLS3.

Description

The routine BSLS3 computes the coefficients of a tensor-product spline least-squares approximation to weighted tensor-product data. The input for this subroutine consists of data vectors to specify the tensor-product grid for the data, three vectors with the weights, the values of the surface on the grid, and the specification for the tensor-product spline. The grid is specified by the three vectors x = XDATA, y = YDATA, and z = ZDATA of length k = NXDATA, l = NYDATA , and m = NZDATA, respectively. A three-dimensional array f = FDATA contains the data values which are to be fit. The three vectors $w_{\boldsymbol{x}}$ = XWEIGH, $w_{\boldsymbol{y}}$ = YWEIGH, and $w_{\boldsymbol{z}}$ = ZWEIGH contain the weights for the weighted least-squares problem. The information for the approximating tensor-product spline must also be provided. This information is contained in $k_{\boldsymbol{x}}$ = KXORD, $\mathbf{t}_{\boldsymbol{x}}$ = XKNOT, and K = NXCOEF for the spline in the first variable, in $k_{\boldsymbol{y}}$ = KYORD, $\mathbf{t}_{\boldsymbol{y}}$ = YKNOT and L = NYCOEF for the spline in the second variable, and in $k_{\boldsymbol{z}}$ = KZORD, $\mathbf{t}_{\boldsymbol{z}}$ = ZKNOT and M = NZCOEF for the spline in the third variable.

The coefficients of the resulting tensor product spline are returned in c = BSCOEF, which is an $K \times L \times M$ array. The procedure computes coefficients by solving the normal equations in tensor-product form as discussed in de Boor (1978, Chapter 17). The interested reader might also want to study the paper by E. Grosse (1980).

The final result produces coefficients c minimizing

$$\sum_{i=l}^{k}\sum_{j=1}^{l}\sum_{p=1}^{m} w_x(i)\,w_y(j)\,w_z(p)\left[\sum_{s=1}^{K}\sum_{t=1}^{L}\sum_{u=1}^{M} c_{stu}B_{stu}\left(x_i,y_j,z_p\right)-f_{ijp}\right]^2$$

where the function $B_{\boldsymbol{stu}}$ is the tensor-product of three B-splines of order $k_{\boldsymbol{x}}$, $k_{\boldsymbol{y}}$, and $k_{\boldsymbol{z}}$. Specifically, we have

$$B_{stu}\left(x,y,z\right)=B_{s,k_x,\mathbf{t}_x}\left(x\right)B_{t,k_y,\mathbf{t}_y}\left(y\right)B_{u,k_z,\mathbf{t}_z}\left(z\right)$$

The spline

$$\sum_{s=1}^{K}\sum_{t=1}^{L}\sum_{u=1}^{M} c_{stu} B_{stu}$$

can be evaluated at one point using BS3VL and its partial derivatives can be evaluated using BS3DR. If the values on a grid are desired then we recommend BS3GD.

Comments

1. Workspace may be explicitly provided, if desired, by use of B2LS3/DB2LS3. The reference is:

```
CALL B2LS3 (NXDATA, XDATA, NYDATA, NZDATA, ZDATA, YDATA,
   FDATA, LDFDAT, KXORD, KYORD, KZORD, XKNOT, YKNOT, ZKNOT,
   NXCOEF, NYCOEF, NZCOEF, XWEIGH, YWEIGH, ZWEIGH, BSCOEF,
   WK)
```

The additional argument is:

WK — Work array of length NYCOEF * (NZDATA + KYORD + NZCOEF) + NZDATA * (1 + NYDATA) + NXCOEF * (KXORD + NYDATA * NZDATA) + KZORD * NZCOEF + 3 * MAX0(KXORD, KYORD, KZORD).

2. Informational errors

Type	**Code**	**Description**
3	13	There may be less than one digit of accuracy in the least squares fit. Try using higher precision if possible.
4	7	Multiplicity of knots cannot exceed the order of the spline.
4	8	The knots must be nondecreasing.
4	9	All weights must be greater than zero.
4	10	The data point abscissae must be nondecreasing.
4	11	The smallest element of the data point array must be greater than or equal to the K_ORDth knot.
4	12	The largest element of the data point array must be less than or equal to the (N_COEF + 1)st knot.

Example

The data for this example arise from the function $e^{(y-z)}\sin(x+y)+\varepsilon$ on the rectangle $[0, 3] \times [0, 2] \times [0, 1]$. Here, ε is a uniform random variable with range $[-.5, .5]$. We sample this function on a $4 \times 3 \times 2$ grid and then try to recover it by using tensor-product cubic splines in all variables. We print out the values of the function $e^{(y-z)}\sin(x+y)$ on a $4 \times 3 \times 2$ grid and compare these values with the values of the tensor-product spline that was computed using the IMSL routine BSLS3.

```
      USE BSLS3_INT
      USE RNSET_INT
      USE RNUNF_INT
      USE UMACH_INT
      USE BS3GD_INT

      IMPLICIT   NONE
      INTEGER    KXORD, KYORD, KZORD, LDFDAT, MDFDAT, NXCOEF, NXDATA,&
                 NXVAL, NYCOEF, NYDATA, NYVAL, NZCOEF, NZDATA, NZVAL
      PARAMETER  (KXORD=4, KYORD=4, KZORD=4, NXCOEF=8, NXDATA=15,&
                 NXVAL=4, NYCOEF=8, NYDATA=15, NYVAL=3, NZCOEF=8,&
                 NZDATA=15, NZVAL=2, LDFDAT=NXDATA, MDFDAT=NYDATA)
!
      INTEGER    I, J, K, NOUT
      REAL       BSCOEF(NXCOEF,NYCOEF,NZCOEF), EXP, F,&
                 FDATA(NXDATA,NYDATA,NZDATA), FLOAT, RNOISE,&
                 SIN, SPXYZ(NXVAL,NYVAL,NZVAL), X, XDATA(NXDATA),&
                 XKNOT(NXCOEF+KXORD), XVAL(NXVAL), XWEIGH(NXDATA), Y,&
                 YDATA(NYDATA), YKNOT(NYCOEF+KYORD), YVAL(NYVAL),&
                 YWEIGH(NYDATA), Z, ZDATA(NZDATA),&
                 ZKNOT(NZCOEF+KZORD), ZVAL(NZVAL), ZWEIGH(NZDATA)
      INTRINSIC  EXP, FLOAT, SIN
!                                  Define a function
      F(X,Y,Z) = EXP(Y-Z)*SIN(X+Y)
!
      CALL RNSET (1234579)
      CALL UMACH (2, NOUT)
!                                  Set up knot sequences
!                                  X-knots
      DO 10  I=1, NXCOEF - KXORD + 2
         XKNOT(I+KXORD-1) = 3.0*(FLOAT(I-1)/FLOAT(NXCOEF-KXORD+1))
   10 CONTINUE
      DO 20  I=1, KXORD - 1
         XKNOT(I) = XKNOT(KXORD)
         XKNOT(I+NXCOEF+1) = XKNOT(NXCOEF+1)
   20 CONTINUE
!                                  Y-knots
      DO 30  I=1, NYCOEF - KYORD + 2
         YKNOT(I+KYORD-1) = 2.0*(FLOAT(I-1)/FLOAT(NYCOEF-KYORD+1))
   30 CONTINUE
      DO 40  I=1, KYORD - 1
         YKNOT(I) = YKNOT(KYORD)
         YKNOT(I+NYCOEF+1) = YKNOT(NYCOEF+1)
   40 CONTINUE
!                                  Z-knots
      DO 50  I=1, NZCOEF - KZORD + 2
         ZKNOT(I+KZORD-1) = 1.0*(FLOAT(I-1)/FLOAT(NZCOEF-KZORD+1))
   50 CONTINUE
      DO 60  I=1, KZORD - 1
         ZKNOT(I) = ZKNOT(KZORD)
         ZKNOT(I+NZCOEF+1) = ZKNOT(NZCOEF+1)
   60 CONTINUE
!                                  Set up X-grid.
      DO 70  I=1, NXDATA
         XDATA(I) = 3.0*(FLOAT(I-1)/FLOAT(NXDATA-1))
   70 CONTINUE
!                                  Set up Y-grid.
      DO 80  I=1, NYDATA
         YDATA(I) = 2.0*(FLOAT(I-1)/FLOAT(NYDATA-1))
   80 CONTINUE
!                                  Set up Z-grid
      DO 90  I=1, NZDATA
         ZDATA(I) = 1.0*(FLOAT(I-1)/FLOAT(NZDATA-1))
   90 CONTINUE
!                                  Evaluate the function on the grid
```

```
!                                   and add noise.
      DO 100  I=1, NXDATA
         DO 100  J=1, NYDATA
            DO 100  K=1, NZDATA
               RNOISE = RNUNF()
               RNOISE = RNOISE - 0.5
               FDATA(I,J,K) = F(XDATA(I),YDATA(J),ZDATA(K)) + RNOISE
  100 CONTINUE
!                                   Use default weights equal to 1.0
!
!                                   Compute least-squares
      CALL BSLS3 (XDATA, YDATA, ZDATA, FDATA, KXORD, KYORD, KZORD, XKNOT, &
                  YKNOT, ZKNOT, BSCOEF)
!                                   Set up grid for evaluation.
      DO 110  I=1, NXVAL
         XVAL(I) = FLOAT(I-1)
  110 CONTINUE
      DO 120  I=1, NYVAL
         YVAL(I) = FLOAT(I-1)
  120 CONTINUE
      DO 130  I=1, NZVAL
         ZVAL(I) = FLOAT(I-1)
  130 CONTINUE
!                                   Evaluate on the grid.
      CALL BS3GD (0, 0, 0, XVAL, YVAL, ZVAL, KXORD, KYORD, KZORD, XKNOT, &
                  YKNOT, ZKNOT, BSCOEF, SPXYZ)
!                                   Print results.
      WRITE (NOUT,99998)
      DO 140  I=1, NXVAL
         DO 140  J=1, NYVAL
            DO 140  K=1, NZVAL
               WRITE (NOUT,99999) XVAL(I), YVAL(J), ZVAL(K),&
                                  F(XVAL(I),YVAL(J),ZVAL(K)),&
                                  SPXYZ(I,J,K), F(XVAL(I),YVAL(J),ZVAL(K)&
                                  ) - SPXYZ(I,J,K)
  140 CONTINUE
99998 FORMAT (8X, 'X', 9X, 'Y', 9X, 'Z', 6X, 'F(X,Y,Z)', 3X,&
             'S(X,Y,Z)', 4X, 'Error')
99999 FORMAT (' ', 3F10.3, 3F11.4)
      END
```

Output

```
    X         Y         Z      F(X,Y,Z)   S(X,Y,Z)    Error
  0.000     0.000     0.000     0.0000     0.1987    -0.1987
  0.000     0.000     1.000     0.0000     0.1447    -0.1447
  0.000     1.000     0.000     2.2874     2.2854     0.0019
  0.000     1.000     1.000     0.8415     1.0557    -0.2142
  0.000     2.000     0.000     6.7188     6.4704     0.2484
  0.000     2.000     1.000     2.4717     2.2054     0.2664
  1.000     0.000     0.000     0.8415     0.8779    -0.0365
  1.000     0.000     1.000     0.3096     0.2571     0.0524
  1.000     1.000     0.000     2.4717     2.4015     0.0703
  1.000     1.000     1.000     0.9093     0.8995     0.0098
  1.000     2.000     0.000     1.0427     1.1330    -0.0902
  1.000     2.000     1.000     0.3836     0.4951    -0.1115
  2.000     0.000     0.000     0.9093     0.8269     0.0824
  2.000     0.000     1.000     0.3345     0.3258     0.0087
  2.000     1.000     0.000     0.3836     0.3564     0.0272
  2.000     1.000     1.000     0.1411     0.1905    -0.0494
  2.000     2.000     0.000    -5.5921    -5.5362    -0.0559
  2.000     2.000     1.000    -2.0572    -1.9659    -0.0913
  3.000     0.000     0.000     0.1411     0.4841    -0.3430
  3.000     0.000     1.000     0.0519    -0.4257     0.4776
  3.000     1.000     0.000    -2.0572    -1.9710    -0.0862
```

```
  3.000      1.000      1.000     -0.7568     -0.8479      0.0911
  3.000      2.000      0.000     -7.0855     -7.0957      0.0101
  3.000      2.000      1.000     -2.6066     -2.1650     -0.4416
```

CSSED

Smooths one-dimensional data by error detection.

Required Arguments

XDATA — Array of length NDATA containing the abscissas of the data points. (Input)

FDATA — Array of length NDATA containing the ordinates (function values) of the data points. (Input)

DIS — Proportion of the distance the ordinate in error is moved to its interpolating curve. (Input)
It must be in the range 0.0 to 1.0. A suggested value for DIS is one.

SC — Stopping criterion. (Input)
SC should be greater than or equal to zero. A suggested value for SC is zero.

MAXIT — Maximum number of iterations allowed. (Input)

SDATA — Array of length NDATA containing the smoothed data. (Output)

Optional Arguments

NDATA — Number of data points. (Input)
Default: NDATA = size (XDATA,1).

FORTRAN 90 Interface

Generic: CALL CSSED (XDATA, FDATA, DIS, SC, MAXIT, SDATA [, …])

Specific: The specific interface names are S_CSSED and D_CSSED.

FORTRAN 77 Interface

Single: CALL CSSED (NDATA, XDATA, FDATA, DIS, SC, MAXIT, SDATA)

Double: The double precision name is DCSSED.

Description

The routine CSSED is designed to smooth a data set that is mildly contaminated with isolated errors. In general, the routine will not work well if more than 25% of the data points are in error. The routine CSSED is based on an algorithm of Guerra and Tapia (1974).

Setting NDATA = n, FDATA = f, SDATA = s and XDATA = x, the algorithm proceeds as follows. Although the user need not input an ordered XDATA sequence, we will assume that x is increasing for simplicity. The algorithm first sorts the XDATA values into an increasing sequence and then continues. A cubic spline interpolant is computed for each of the 6-point data sets (initially setting $s = f$)

$$(x_j, s_j) \qquad j = i - 3, \ldots, i + 3 \qquad j \neq i,$$

where $i = 4, \ldots, n - 3$ using CSAKM. For each i the interpolant, which we will call S_i, is compared with the current value of s_i, and a 'point energy' is computed as

$$pe_i = S_i(x_i) - s_i$$

Setting $sc = SC$, the algorithm terminates either if MAXIT iterations have taken place or if

$$|pe_i| \leq sc(x_{i+3} - x_{i-3})/6 \qquad i = 4, \ldots, n - 3$$

If the above inequality is violated for any i, then we update the i-th element of s by setting $s_i = s_i + d(pe_i)$, where d = DIS. Note that neither the first three nor the last three data points are changed. Thus, if these points are inaccurate, care must be taken to interpret the results.

The choice of the parameters d, sc and MAXIT are crucial to the successful usage of this subroutine. If the user has specific information about the extent of the contamination, then he should choose the parameters as follows: $d = 1$, $sc = 0$ and MAXIT to be the number of data points in error. On the other hand, if no such specific information is available, then choose $d = .5$, MAXIT $\leq 2n$, and

$$sc = .5\frac{\max s - \min s}{\left(x_n - x_1\right)}$$

In any case, we would encourage the user to experiment with these values.

Comments

1. Workspace may be explicitly provided, if desired, by use of C2SED/DC2SED. The reference is:

   ```
   CALL C2SED (NDATA, XDATA, FDATA, DIS, SC, MAXIT, DATA, WK,
      IWK)
   ```

   The additional arguments are as follows:

WK — Work array of length 4 * `NDATA` + 30.

IWK — Work array of length 2 * `NDATA`.

2. Informational error

Type	Code	Description
3	1	The maximum number of iterations allowed has been reached.

3. The arrays `FDATA` and `SDATA` may the same.

Example

We take 91 uniform samples from the function 5 + (5 + t^2 sin *t*)/*t* on the interval [1, 10]. Then, we contaminate 10 of the samples and try to recover the original function values.

```
      USE CSSED_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    NDATA
      PARAMETER  (NDATA=91)
!
      INTEGER    I, MAXIT, NOUT, ISB(10)
      REAL       DIS, F, FDATA(91), SC, SDATA(91), SIN, X, XDATA(91),&
                 RNOISE(10)
      INTRINSIC  SIN
!
      DATA ISB/6, 17, 26, 34, 42, 49, 56, 62, 75, 83/
      DATA RNOISE/2.5, -3.0, -2.0, 2.5, 3.0, -2.0, -2.5, 2.0, -2.0, 3.0/
!
      F(X) = (X*X*SIN(X)+5.0)/X + 5.0
!                                  EX. #1; No specific information
!                                  available
      DIS   = 0.5
      SC    = 0.56
      MAXIT = 182
!                                  Set values for XDATA and FDATA
      XDATA(1) = 1.0
      FDATA(1) = F(XDATA(1))
      DO 10  I=2, NDATA
         XDATA(I) = XDATA(I-1) + .1
         FDATA(I) = F(XDATA(I))
   10 CONTINUE
!                                  Contaminate the data
      DO 20 I=1, 10
         FDATA(ISB(I)) = FDATA(ISB(I)) + RNOISE(I)
   20 CONTINUE
!                                  Smooth data
      CALL CSSED (XDATA, FDATA, DIS, SC, MAXIT, SDATA)
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Write heading
      WRITE (NOUT,99997)
!                                  Write data
      DO 30 I=1, 10
         WRITE (NOUT,99999) F(XDATA(ISB(I))), FDATA(ISB(I)),&
                            SDATA(ISB(I))
```

```
   30 CONTINUE
!                                   EX. #2; Specific information
!                                   available
      DIS   = 1.0
      SC    = 0.0
      MAXIT = 10
!                                   A warning message is produced
!                                   because the maximum number of
!                                   iterations is reached.
!
!                                   Smooth data
      CALL CSSED (XDATA, FDATA, DIS, SC, MAXIT, SDATA)
!                                   Write heading
      WRITE (NOUT,99998)
!                                   Write data
      DO 40 I=1, 10
         WRITE (NOUT,99999) F(XDATA(ISB(I))), FDATA(ISB(I)),&
                            SDATA(ISB(I))
   40 CONTINUE
!
99997 FORMAT (' Case A - No specific information available', /,&
             '    F(X)       F(X)+NOISE         SDATA(X)', /)
99998 FORMAT (' Case B - Specific information available', /,&
             '    F(X)       F(X)+NOISE         SDATA(X)', /)
99999 FORMAT (' ', F7.3, 8X, F7.3, 11X, F7.3)
      END
```

Output

```
Case A - No specific information available
 F(X)        F(X)+NOISE          SDATA(X)

 9.830        12.330              9.870
 8.263         5.263              8.215
 5.201         3.201              5.168
 2.223         4.723              2.264
 1.259         4.259              1.308
 3.167         1.167              3.138
 7.167         4.667              7.131
10.880        12.880             10.909
12.774        10.774             12.708
 7.594        10.594              7.639

 *** WARNING  ERROR 1 from CSSED.  Maximum number of iterations limit MAXIT
 ***          =10 exceeded.  The best answer found is returned.
Case B - Specific information available
 F(X)        F(X)+NOISE          SDATA(X)

 9.830        12.330              9.831
 8.263         5.263              8.262
 5.201         3.201              5.199
 2.223         4.723              2.225
 1.259         4.259              1.261
 3.167         1.167              3.170
 7.167         4.667              7.170
10.880        12.880             10.878
12.774        10.774             12.770
 7.594        10.594              7.592
```

CSSMH

Computes a smooth cubic spline approximation to noisy data.

Required Arguments

XDATA — Array of length NDATA containing the data point abscissas. (Input)
XDATA must be distinct.

FDATA — Array of length NDATA containing the data point ordinates. (Input)

SMPAR — A nonnegative number which controls the smoothing. (Input)
The spline function S returned is such that
the sum from I = 1 to NDATA of ((S(XDATA(I)) - FDATA(I)) / WEIGHT(I))**2
is less than or equal to SMPAR. It is recommended that SMPAR lie in the confidence interval of this sum, i.e., NDATA − SQRT(2 * NDATA).LE. SMPAR.LE. NDATA + SQRT(2 * NDATA).

BREAK — Array of length NDATA containing the breakpoints for the piecewise cubic representation. (Output)

CSCOEF — Matrix of size 4 by NDATA containing the local coefficients of the cubic pieces. (Output)

Optional Arguments

NDATA — Number of data points. (Input)
NDATA must be at least 2.
Default: NDATA = size (XDATA,1).

WEIGHT — Array of length NDATA containing estimates of the standard deviations of FDATA. (Input)
All elements of WEIGHT must be positive.
Default: WEIGHT = 1.0.

FORTRAN 90 Interface

Generic: CALL CSSMH (XDATA, FDATA, SMPAR, BREAK, CSCOEF [, …])

Specific: The specific interface names are S_CSSMH and D_CSSMH.

FORTRAN 77 Interface

Single: CALL CSSMH (NDATA, XDATA, FDATA, WEIGHT, SMPAR, BREAK, CSCOEF)

Double: The double precision name is DCSSMH.

Description

The routine CSSMH is designed to produce a C^2 cubic spline approximation to a data set in which the function values are noisy. This spline is called a *smoothing spline*. It is a natural cubic spline with knots at all the data abscissas x = XDATA, but it does *not* interpolate the data (x_i, f_i). The smoothing spline S is the unique C^2 function which minimizes

$$\int_a^b S''(x)^2 dx$$

subject to the constraint

$$\sum_{i=1}^{N} \left| \frac{S(x_i) - f_i}{w_i} \right|^2 \leq \sigma$$

where w_i = WEIGHT(I), σ = SMPAR is the smoothing parameter, and N = NDATA.

Recommended values for σ depend on the weights w_i. If an estimate for the standard deviation of the error in the value f_i is available, then w_i should be set to this value and the smoothing parameter σ should be chosen in the confidence interval corresponding to the left side of the above inequality. That is,

$$N - \sqrt{2N} \leq \sigma \leq N + \sqrt{2N}$$

The routine CSSMH is based on an algorithm of Reinsch (1967). This algorithm is also discussed in de Boor (1978, pages 235– 243).

Comments

1. Workspace may be explicitly provided, if desired, by use of C2SMH/DC2SMH. The reference is:

```
CALL C2SMH (NDATA, XDATA, FDATA, WEIGHT, SMPAR, BREAK,
   CSCOEF, WK, IWK)
```

   The additional arguments are as follows:

   WK — Work array of length 8 * NDATA + 5.

   IWK — Work array of length NDATA.

2. Informational errors

Type	Code	Description
3	1	The maximum number of iterations has been reached. The best approximation is returned.
4	3	All weights must be greater than zero.

3. The cubic spline can be evaluated using CSVAL; its derivative can be evaluated using CSDER.

Example

In this example, function values are contaminated by adding a small “random” amount to the correct values. The routine CSSMH is used to approximate the original, uncontaminated data.

```
      USE IMSL_LIBRARIES

      IMPLICIT   NONE
      INTEGER    NDATA
      PARAMETER  (NDATA=300)
!
      INTEGER    I, NOUT
      REAL       BREAK(NDATA), CSCOEF(4,NDATA), ERROR, F,&
                 FDATA(NDATA), FLOAT, FVAL, SDEV, SMPAR, SQRT,&
                 SVAL, WEIGHT(NDATA), X, XDATA(NDATA), XT, RN
      INTRINSIC  FLOAT, SQRT
!
      F(X) = 1.0/(.1+(3.0*(X-1.0))**4)
!                                 Set up a grid
      DO 10  I=1, NDATA
         XDATA(I) = 3.0*(FLOAT(I-1)/FLOAT(NDATA-1))
         FDATA(I) = F(XDATA(I))
   10 CONTINUE
!                                 Set the random number seed
      CALL RNSET (1234579)
!                                 Contaminate the data
      DO 20  I=1, NDATA
         RN = RNUNF()
         FDATA(I) = FDATA(I) + 2.0*RN - 1.0
   20 CONTINUE
!                                 Set the WEIGHT vector
      SDEV = 1.0/SQRT(3.0)
      CALL SSET (NDATA, SDEV, WEIGHT, 1)
      SMPAR = NDATA
!                                 Smooth the data
      CALL CSSMH (XDATA, FDATA, SMPAR, BREAK, CSCOEF, WEIGHT=WEIGHT)
!                                 Get output unit number
      CALL UMACH (2, NOUT)
!                                 Write heading
      WRITE (NOUT,99999)
!                                 Print 10 values of the function.
      DO 30  I=1, 10
         XT    = 90.0*(FLOAT(I-1)/FLOAT(NDATA-1))
!                                 Evaluate the spline
         SVAL  = CSVAL(XT,BREAK,CSCOEF)
         FVAL  = F(XT)
         ERROR = SVAL - FVAL
         WRITE (NOUT,'(4F15.4)') XT, FVAL, SVAL, ERROR
   30 CONTINUE
```

```
!
99999 FORMAT (12X, 'X', 9X, 'Function', 7X, 'Smoothed', 10X,&
             'Error')
      END
```

Output

```
       X          Function        Smoothed          Error
  0.0000           0.0123          0.1118          0.0995
  0.3010           0.0514          0.0646          0.0131
  0.6020           0.4690          0.2972         -0.1718
  0.9030           9.3312          8.7022         -0.6289
  1.2040           4.1611          4.7887          0.6276
  1.5050           0.1863          0.2718          0.0856
  1.8060           0.0292          0.1408          0.1116
  2.1070           0.0082          0.0826          0.0743
  2.4080           0.0031          0.0076          0.0045
  2.7090           0.0014         -0.1789         -0.1803
```

CSSCV

Computes a smooth cubic spline approximation to noisy data using cross-validation to estimate the smoothing parameter.

Required Arguments

XDATA — Array of length NDATA containing the data point abscissas. (Input) XDATA must be distinct.

FDATA — Array of length NDATA containing the data point ordinates. (Input)

IEQUAL — A flag alerting the subroutine that the data is equally spaced. (Input)

BREAK — Array of length NDATA containing the breakpoints for the piecewise cubic representation. (Output)

CSCOEF — Matrix of size 4 by NDATA containing the local coefficients of the cubic pieces. (Output)

Optional Arguments

NDATA — Number of data points. (Input)
NDATA must be at least 3.
Default: NDATA = size (XDATA,1).

FORTRAN 90 Interface

Generic: CALL CSSCV (XDATA, FDATA, IEQUAL, BREAK, CSCOEF [, …])

Specific: The specific interface names are S_CSSCV and D_CSSCV.

FORTRAN 77 Interface

Single: CALL CSSCV (NDATA, XDATA, FDATA, IEQUAL, BREAK, CSCOEF)

Double: The double precision name is DCSSCV.

Description

The routine CSSCV is designed to produce a C^2 cubic spline approximation to a data set in which the function values are noisy. This spline is called a *smoothing spline*. It is a natural cubic spline with knots at all the data abscissas x = XDATA, but it does *not* interpolate the data (x_i, f_i). The smoothing spline S_σ is the unique C^2 function that minimizes

$$\int_a^b S_\sigma''(x)^2 dx$$

subject to the constraint

$$\sum_{i=1}^{N} \left| S_\sigma(x_i) - f_i \right|^2 \le \sigma$$

where σ is the smoothing parameter and N = NDATA. The reader should consult Reinsch (1967) for more information concerning smoothing splines. The IMSL subroutine CSSMH solves the above problem when the user provides the smoothing parameter σ. This routine attempts to find the 'optimal' smoothing parameter using the statistical technique known as cross-validation. This means that (in a very rough sense) one chooses the value of σ so that the smoothing spline (S_σ) best approximates the value of the data at x_i, if it is computed using all the data *except* the i-th; this is true for all $i = 1, \ldots, N$. For more information on this topic, we refer the reader to Craven and Wahba (1979).

Comments

1. Workspace may be explicitly provided, if desired, by use of C2SCV/DC2SCV. The reference is:

```
CALL C2SCV (NDATA, XDATA, FDATA, IEQUAL, BREAK, CSCOEF, WK,
   SDWK, IPVT)
```

   The additional arguments are as follows:

   WK — Work array of length 7 * (NDATA + 2).

   SDWK — Work array of length 2 * NDATA.

   IPVT — Work array of length NDATA.

2. Informational error

Type	Code	Description
4	2	Points in the data point abscissas array, XDATA, must be distinct.

Example

In this example, function values are computed and are contaminated by adding a small "random" amount. The routine CSSCV is used to try to reproduce the original, uncontaminated data.

```
      USE IMSL_LIBRARIES

      IMPLICIT   NONE
      INTEGER    NDATA
      PARAMETER  (NDATA=300)
!
      INTEGER    I, IEQUAL, NOUT
      REAL       BREAK(NDATA), CSCOEF(4,NDATA), ERROR, F,&
                 FDATA(NDATA), FLOAT, FVAL, SVAL, X,&
                 XDATA(NDATA), XT, RN
      INTRINSIC  FLOAT
!
      F(X) = 1.0/(.1+(3.0*(X-1.0))**4)
!
      CALL UMACH (2, NOUT)
!                                 Set up a grid
      DO 10  I=1, NDATA
         XDATA(I) = 3.0*(FLOAT(I-1)/FLOAT(NDATA-1))
         FDATA(I) = F(XDATA(I))
   10 CONTINUE
!                                 Introduce noise on [-.5,.5]
!                                 Contaminate the data
      CALL RNSET (1234579)
      DO 20  I=1, NDATA
         RN = RNUNF ()
         FDATA(I) = FDATA(I) + 2.0*RN - 1.0
   20 CONTINUE
!
!                                 Set IEQUAL=1 for equally spaced data
      IEQUAL = 1
!                                 Smooth data
      CALL CSSCV (XDATA, FDATA, IEQUAL, BREAK, CSCOEF)
!                                 Print results
      WRITE (NOUT,99999)
      DO 30  I=1, 10
         XT    = 90.0*(FLOAT(I-1)/FLOAT(NDATA-1))
         SVAL  = CSVAL(XT,BREAK,CSCOEF)
         FVAL  = F(XT)
         ERROR = SVAL - FVAL
         WRITE (NOUT,'(4F15.4)') XT, FVAL, SVAL, ERROR
   30 CONTINUE
99999 FORMAT (12X, 'X', 9X, 'Function', 7X, 'Smoothed', 10X,&
              'Error')
      END
```

Output

```
      X         Function        Smoothed           Error
  0.0000          0.0123          0.2528          0.2405
  0.3010          0.0514          0.1054          0.0540
  0.6020          0.4690          0.3117         -0.1572
  0.9030          9.3312          8.9461         -0.3850
  1.2040          4.1611          4.6847          0.5235
  1.5050          0.1863          0.3819          0.1956
  1.8060          0.0292          0.1168          0.0877
  2.1070          0.0082          0.0658          0.0575
  2.4080          0.0031          0.0395          0.0364
```

```
  2.7090          0.0014         -0.2155         -0.2169
```

RATCH

more...

Computes a rational weighted Chebyshev approximation to a continuous function on an interval.

Required Arguments

F — User-supplied FUNCTION to be approximated. The form is F(X), where

X – Independent variable. (Input)

F – The function value. (Output)

F must be declared EXTERNAL in the calling program.

PHI — User-supplied FUNCTION to supply the variable transformation which must be continuous and monotonic. The form is PHI(X), where

X – Independent variable. (Input)

PHI – The function value. (Output)

PHI must be declared EXTERNAL in the calling program.

WEIGHT — User-supplied FUNCTION to scale the maximum error. It must be continuous and nonvanishing on the closed interval (A, B). The form is WEIGHT(X), where

X – Independent variable. (Input)

WEIGHT – The function value. (Output)

WEIGHT must be declared EXTERNAL in the calling program.

A — Lower end of the interval on which the approximation is desired. (Input)

B — Upper end of the interval on which the approximation is desired. (Input)

P — Vector of length N + 1 containing the coefficients of the numerator polynomial. (Output)

Q — Vector of length M + 1 containing the coefficients of the denominator polynomial. (Output)

ERROR — Min-max error of approximation. (Output)

Optional Arguments

N — The degree of the numerator. (Input)
Default: `N` = size (`P`,1) – 1.

M — The degree of the denominator. (Input)
Default: `M` = size (`Q`,1) – 1.

FORTRAN 90 Interface

Generic: `CALL RATCH (F, PHI, WEIGHT, A, B, P, Q, ERROR [, …])`

Specific: The specific interface names are `S_RATCH` and `D_RATCH`.

FORTRAN 77 Interface

Single: `CALL RATCH (F, PHI, WEIGHT, A, B, N, M, P, Q, ERROR)`

Double: The double precision name is `DRATCH`.

Description

The routine `RATCH` is designed to compute the best weighted L_∞ (Chebyshev) approximant to a given function. Specifically, given a weight function *w* = `WEIGHT`, a monotone function ϕ = `PHI`, and a function *f* to be approximated on the interval [*a*, *b*], the subroutine `RATCH` returns the coefficients (in *P* and *Q*) for a rational approximation to *f* on [*a*, *b*]. The user must supply the degree of the numerator *N* and the degree of the denominator *M* of the rational function

$$R_M^N$$

The goal is to produce coefficients which minimize the expression

$$\left\| \frac{f - R_M^N}{w} \right\| := \max_{x \in [a,b]} \frac{\left| f(x) - \frac{\sum_{i=1}^{N+1} P_i \phi^{i-1}(x)}{\sum_{i=1}^{M+1} Q_i \phi^{i-1}(x)} \right|}{w(x)}$$

Notice that setting $\phi(x) = x$ yields ordinary rational approximation. A typical use of the function ϕ occurs when one wants to approximate an even function on a symmetric interval, say [−*a*, *a*] using ordinary rational functions. In this case, it is known that the answer must be an even function. Hence, one can set $\phi(x) = x^2$, only approximate on [0, *a*], and decrease by one half the degrees in the numerator and denominator.

The algorithm implemented in this subroutine is designed for fast execution. It assumes that the best approximant has precisely *N* + *M* + 2 equi-oscillations. That is, that there exist *N* + *M* + 2 points $\mathbf{t}_1 < \ldots < \mathbf{t}_{N+M+2}$ satisfying

$$e(\mathbf{t}_i) = \; -e(\mathbf{t}_{i+1}) = \; \pm\left\|\frac{f - R_M^N}{w}\right\|$$

Such points are called alternants. Unfortunately, there are many instances in which the best rational approximant to the given function has either fewer alternants or more alternants. In this case, it is not expected that this subroutine will perform well. For more information on rational Chebyshev approximation, the reader can consult Cheney (1966). The subroutine is based on work of Cody, Fraser, and Hart (1968).

Comments

1. Workspace may be explicitly provided, if desired, by use of `R2TCH/DR2TCH`. The reference is:

```
CALL R2TCH (F, PHI, WEIGHT, A, B, N, M, P, Q, ERROR, ITMAX,
   IWK, WK)
```

The additional arguments are as follows:

ITMAX — Maximum number of iterations. (Input)
The default value is 20.

IWK — Workspace vector of length (`N` + `M` + 2). (Workspace)

WK — Workspace vector of length (`N` + `M` + 8) * (`N` + `M` + 2). (Workspace)

2. Informational errors

Type	Code	Description
3	1	The maximum number of iterations has been reached. The routine `R2TCH` may be called directly to set a larger value for `ITMAX`.
3	2	The error was reduced as far as numerically possible. A good approximation is returned in `P` and `Q`, but this does not necessarily give the Chebyshev approximation.
4	3	The linear system that defines `P` and `Q` was found to be algorithmically singular. This indicates the possibility of a degenerate approximation.
4	4	A sequence of critical points that was not monotonic generated. This indicates the possibility of a degenerate approximation.
4	5	The value of the error curve at some critical point is too large. This indicates the possibility of poles in the rational function.
4	6	The weight function cannot be zero on the closed interval (`A`, `B`).

Example

In this example, we compute the best rational approximation to the gamma function, Γ, on the interval [2, 3] with weight function $w = 1$ and $N = M = 2$. We display the maximum error and the coefficients. This problem is taken from the paper of Cody, Fraser, and Hart (1968). We compute in double precision due to the conditioning of this problem.

```
      USE RATCH_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    M, N
      PARAMETER  (M=2, N=2)
!
      INTEGER    NOUT
      DOUBLE PRECISION  A, B, ERROR, F, P(N+1), PHI, Q(M+1), WEIGHT
      EXTERNAL   F, PHI, WEIGHT
!
      A = 2.0D0
      B = 3.0D0
!                                  Compute double precision rational
!                                  approximation
      CALL RATCH (F, PHI, WEIGHT, A, B, P, Q, ERROR)
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Print P, Q and min-max error
      WRITE (NOUT,'(1X,A)') 'In double precision we have:'
      WRITE (NOUT,99999) 'P      = ', P
      WRITE (NOUT,99999) 'Q      = ', Q
      WRITE (NOUT,99999) 'ERROR  = ', ERROR
99999 FORMAT (' ', A, 5X, 3F20.12, /)
      END
! -----------------------------------------------------------------------
!
      DOUBLE PRECISION FUNCTION F (X)
      DOUBLE PRECISION X
!
      DOUBLE PRECISION DGAMMA
      EXTERNAL   DGAMMA
!
      F = DGAMMA(X)
      RETURN
      END
! -----------------------------------------------------------------------
!
      DOUBLE PRECISION FUNCTION PHI (X)
      DOUBLE PRECISION X
!
      PHI = X
      RETURN
      END
! -----------------------------------------------------------------------
!
      DOUBLE PRECISION FUNCTION WEIGHT (X)
      DOUBLE PRECISION X
!
      DOUBLE PRECISION DGAMMA
      EXTERNAL   DGAMMA
!
      WEIGHT = DGAMMA(X)
      RETURN
      END
```

Output

```
In double precision we have:
P      =            1.265583562487     -0.650585004466      0.197868699191

Q      =            1.000000000000     -0.064342721236     -0.028851461855

ERROR  =           -0.000026934190
```

Integration and Differentiation

Routines

Usage Notes

Univariate Quadrature

The first ten routines described in this chapter are designed to compute approximations to integrals of the form

$$\int_a^b f(x)w(x)dx$$

The weight function *w* is used to incorporate known singularities (either algebraic or logarithmic), to incorporate oscillations, or to indicate that a Cauchy principal value is desired. For general purpose integration, we recommend the use of `QDAGS` (even if no endpoint singularities are present). If more efficiency is desired, then the use of `QDAG` (or `QDAG*`) should be considered. These routines are organized as follows:

- w = 1
    - QDAGS
    - QDAG
    - QDAGP
    - QDAG1D
    - QDAGI
    - QDNG
- $w(x) = \sin \omega x$ or $w(x) = \cos \omega x$
    - `QDAWO` (for a finite interval)
    - `QDAWF` (for an infinite interval)
- $w(x) = (x - a)^{\alpha} (b - x)^{\beta} \ln(x - a) \ln(b - x)$, where the ln factors are optional
    - `QDAWS`
- $w(x) = 1/(x - c)$ Cauchy principal value
    - `QDAWC`

The calling sequences for these routines are very similar. The function to be integrated is always `F`; the lower and upper limits are, respectively, `A` and `B`. The requested absolute error ε is `ERRABS`, while the requested relative error ρ is `ERRREL`. These quadrature routines return two numbers of interest, namely, `RESULT` and `ERREST`, which are the approximate integral *R* and the error estimate *E*, respectively.

These numbers are related as follows:

$$|\int_a^b f(x)w(x)dx - R| \le E \le \max\left\{\varepsilon, \rho |\int_a^b f(x)w(x)dx|\right\}$$

The requested absolute and relative errors must be interpreted as 'tuning knobs.' The actual errors may be much larger than these values indicate if the sampling of the integrand function misses a peak. Coarse sampling of the integration interval occurs with larger values of ERRABS or ERRREL. We recommend experimenting with these values, starting with small positive values and then increasing them until the required accuracy is obtained.

One situation that occasionally arises in univariate quadrature concerns the approximation of integrals when only tabular data are given. The routines described above do not directly address this question. However, the standard method for handling this problem is first to interpolate the data and then to integrate the interpolant. This can be accomplished by using the IMSL spline interpolation routines described in *Chapter 3, "Interpolation and Approximation"*, with one of the integration routines CSINT, BSINT, or PPITG.

Multivariate Quadrature

Four routines are described in this chapter that are of use in approximating certain multivariate integrals. In particular, the routine TWODQ and QDAG2D return an approximation to an iterated two-dimensional integral of the form

$$\int_a^b \int_{g(x)}^{h(x)} f(x,y)\,dy\,dx$$

while QDAG3D returns an approximation to an iterated three-dimensional integral of the form

$$\int_a^b \int_{g(x)}^{h(x)} \int_{p(x,y)}^{q(x,y)} f(x,y,z)\,dz\,dy\,dx$$

The fourth routine QAND returns an approximation to the integral of a function of *n* variables over a hyper-rectangle

$$\int_{a_1}^{b_1} \cdots \int_{a_n}^{b_n} f(x_1, \cdots, x_n)\,dx_n \cdots dx_1$$

If one has two- or three-dimensional tensor-product tabular data, use the IMSL spline interpolation routines BS2IN or BS3IN, followed by the IMSL spline integration routines BS2IG and BS3IG that are described in *Chapter 3, "Interpolation and Approximation"*.

Gauss Rules and Three-Term Recurrences

The routines described in this section deal with the constellation of problems encountered in Gauss quadrature. These problems arise when quadrature formulas, which integrate polynomials of the highest degree possible, are computed. Once a member of a family of seven weight functions is specified, the routine GQRUL produces the points $\{x_i\}$ and weights $\{w_i\}$ for $i = 1, \ldots, N$ that satisfy

$$\int_a^b f(x)w(x)dx = \sum_{i=1}^{N} f(x_i)w_i$$

for all functions f that are polynomials of degree less than $2N$. The weight functions w may be selected from the following table:

w(x)	Interval	Name
1	(−1,1)	Legendre
$1/\sqrt{1-x^2}$	(−1,1)	Chebyshev 1st kind
$\sqrt{1-x^2}$	(−1,1)	Chebyshev 2nd kind
e^{-x^2}	$(-\infty,\infty)$	Hermite
$(1-x)^{\alpha}(1+x)^{\beta}$	(−1,1)	Jacobi
$e^{-x}x^{\alpha}$	$(0,\infty)$	Generalized Laguerre
$1/\cosh(x)$	$(-\infty,\infty)$	Hyperbolic Cosine

Where permissible, GQRUL will also compute Gauss-Radau and Gauss-Lobatto quadrature rules. The routine RECCF produces the three-term recurrence relation for the monic orthogonal polynomials with respect to the above weight functions.

Another routine, GQRCF, produces the Gauss, Gauss-Radau, or Gauss-Lobatto quadrature rule from the three-term recurrence relation. This means Gauss rules for general weight functions may be obtained if the three-term recursion for the orthogonal polynomials is known. The routine RECQR is an inverse to GQRCF in the sense that it produces the recurrence coefficients given the Gauss quadrature formula.

The last routine described in this section, FQRUL, generates the Fejér quadrature rules for the following family of weights:

$$
\begin{aligned}
w(x) &= 1 \\
w(x) &= 1/(x-\alpha) \\
w(x) &= (b-x)^{\alpha}(x-a)^{\beta} \\
w(x) &= (b-x)^{\alpha}(x-a)^{\beta}\ln(x-a) \\
w(x) &= (b-x)^{\alpha}(x-a)^{\beta}\ln(b-x)
\end{aligned}
$$

Numerical Differentiation

We provide one routine, `DERIV`, for numerical differentiation. This routine provides an estimate for the first, second, or third derivative of a user-supplied function.

QDAGS

Integrates a function (which may have endpoint singularities).

Required Arguments

F — User-supplied FUNCTION to be integrated. The form is F(X), where

X –Independent variable. (Input)

F – The function value. (Output)

F must be declared EXTERNAL in the calling program.

A — Lower limit of integration. (Input)

B — Upper limit of integration. (Input)

RESULT — Estimate of the integral from A to B of F. (Output)

Optional Required Arguments

ERRABS — Absolute accuracy desired. (Input)
Default: ERRABS = 1.e-3 for single precision and 1.d-8 for double precision.

ERRREL — Relative accuracy desired. (Input)
Default: ERRREL = 1.e-3 for single precision and 1.d-8 for double precision.

ERREST — Estimate of the absolute value of the error. (Output)

FORTRAN 90 Interface

Generic: CALL QDAGS (F, A, B, RESULT [, …])

Specific: The specific interface names are S_QDAGS and D_QDAGS.

FORTRAN 77 Interface

Single: CALL QDAGS (F, A, B, ERRABS, ERRREL, RESULT, ERREST)

Double: The double precision name is DQDAGS.

Description

The routine QDAGS is a general-purpose integrator that uses a globally adaptive scheme to reduce the absolute error. It subdivides the interval [*A*, *B*] and uses a 21-point Gauss-Kronrod rule to estimate the integral over each subinterval. The error for each subinterval is estimated by comparison with the 10-point Gauss quadrature rule. This routine is designed to handle functions with endpoint singularities. However, the performance on functions, which are well-behaved at the endpoints, is quite good also. In addition to the general strategy described in QDAG, this routine uses an extrapolation procedure known as the ε-algorithm. The routine QDAGS is an implementation of the routine QAGS, which is fully documented by Piessens et al. (1983). Should QDAGS fail to produce acceptable results, then either IMSL routines QDAG or QDAG* may be appropriate. These routines are documented in this chapter.

Comments

1. Workspace may be explicitly provided, if desired, by use of Q2AGS/DQ2AGS. The reference is

   CALL Q2AGS (F, A, B, ERRABS, ERREL, RESULT, ERREST, MAXSUB, NEVAL, NSUBIN, ALIST, BLIST, RLIST, ELIST, IORD)

   The additional arguments are as follows:

   MAXSUB — Number of subintervals allowed. (Input)
   A value of 500 is used by QDAGS.

   NEVAL — Number of evaluations of F. (Output)

   NSUBIN — Number of subintervals generated. (Output)

   ALIST — Array of length MAXSUB containing a list of the NSUBIN left endpoints. (Output)

   BLIST — Array of length MAXSUB containing a list of the NSUBIN right endpoints. (Output)

   RLIST — Array of length MAXSUB containing approximations to the NSUBIN integrals over the intervals defined by ALIST, BLIST. (Output)

   ELIST — Array of length MAXSUB containing the error estimates of the NSUBIN values in RLIST. (Output)

   IORD — Array of length MAXSUB. (Output)
   Let *k* be
   NSUBIN if NSUBIN ≤ (MAXSUB/2 + 2);
   MAXSUB + 1 − NSUBIN otherwise.
   The first *k* locations contain pointers to the error estimates over the subintervals such that ELIST (IORD(1)), …, ELIST(IORD(*k*)) form a decreasing sequence.

2. Informational errors

Type	Code	Description
4	1	The maximum number of subintervals allowed has been reached.
3	2	Roundoff error, preventing the requested tolerance from being achieved, has been detected.
3	3	A degradation in precision has been detected.
3	4	Roundoff error in the extrapolation table, preventing the requested tolerance from being achieved, has been detected.
4	5	Integral is probably divergent or slowly convergent.

3. If EXACT is the exact value, QDAGS attempts to find RESULT such that |EXACT − RESULT| ≤ max(ERRABS, ERRREL * |EXACT|). To specify only a relative error, set ERRABS to zero. Similarly, to specify only an absolute error, set ERRREL to zero.

Example

The value of

$$\int_0^1 \ln(x) x^{-1/2} dx = -4$$

is estimated. The values of the actual and estimated error are machine dependent.

```
      USE QDAGS_INT
      USE UMACH_INT

      IMPLICIT NONE
      INTEGER    NOUT
      REAL       A, ABS, B, ERRABS, ERREST, ERROR, ERRREL, EXACT, F, &
                RESULT
      INTRINSIC  ABS
      EXTERNAL   F
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Set limits of integration
      A = 0.0
      B = 1.0
!                                  Set error tolerances
      ERRABS = 0.0
      CALL QDAGS (F, A, B, RESULT, ERRABS=ERRABS, ERREST=ERREST)
!                                  Print results
      EXACT = -4.0
      ERROR = ABS(RESULT-EXACT)
      WRITE (NOUT,99999) RESULT, EXACT, ERREST, ERROR
99999 FORMAT (' Computed =', F8.3, 13X, ' Exact =', F8.3, /, /, &
            ' Error estimate =', 1PE10.3, 6X, 'Error =', 1PE10.3)
      END
!
      REAL FUNCTION F (X)
      REAL       X
      REAL       ALOG, SQRT
      INTRINSIC  ALOG, SQRT
```

```
      F = ALOG(X)/SQRT(X)
      RETURN
      END
```

Output

```
Computed =  -4.000              Exact =  -4.000

Error estimate = 1.519E-04      Error = 2.098E-05
```

QDAG

Integrates a function using a globally adaptive scheme based on Gauss-Kronrod rules.

Required Arguments

F — User-supplied `FUNCTION` to be integrated. The form is
`F(X)`, where

`X` – Independent variable. (Input)

`F` – The function value. (Output)

`F` must be declared `EXTERNAL` in the calling program.

A — Lower limit of integration. (Input)

B — Upper limit of integration. (Input)

RESULT — Estimate of the integral from `A` to `B` of `F`. (Output)

Optional Arguments

ERRABS — Absolute accuracy desired. (Input)
Default: `ERRABS` = 1.e-3 for single precision and 1.d-8 for double precision.

ERRREL — Relative accuracy desired. (Input)
Default: `ERRREL` = 1.e-3 for single precision and 1.d-8 for double precision.

IRULE — Choice of quadrature rule. (Input)
Default: `IRULE` = 2.
The Gauss-Kronrod rule is used with the following points:

IRULE	Points
1	7-15
2	10-21
3	15-31
4	20-41
5	25-51
6	30-61

IRULE = 2 is recommended for most functions. If the function has a peak singularity, use IRULE = 1. If the function is oscillatory, use IRULE = 6.

ERREST — Estimate of the absolute value of the error. (Output)

FORTRAN 90 Interface

Generic: CALL QDAG (F, A, B, RESULT [, …])

Specific: The specific interface names are S_QDAG and D_QDAG.

FORTRAN 77 Interface

Single: CALL QDAG (F, A, B, ERRABS, ERRREL, IRULE, RESULT, ERREST)

Double: The double precision name is DQDAG.

Description

The routine QDAG is a general-purpose integrator that uses a globally adaptive scheme in order to reduce the absolute error. It subdivides the interval [*A*, *B*] and uses a (2*k* + 1)-point Gauss-Kronrod rule to estimate the integral over each subinterval. The error for each subinterval is estimated by comparison with the *k*-point Gauss quadrature rule. The subinterval with the largest estimated error is then bisected and the same procedure is applied to both halves. The bisection process is continued until either the error criterion is satisfied, roundoff error is detected, the subintervals become too small, or the maximum number of subintervals allowed is reached. The routine QDAG is based on the subroutine QAG by Piessens et al. (1983).

Should QDAG fail to produce acceptable results, then one of the IMSL routines QDAG* may be appropriate. These routines are documented in this chapter.

Comments

1. Workspace may be explicitly provided, if desired, by use of Q2AG/DQ2AG. The reference is:

   CALL Q2AG (F, A, B, ERRABS, ERRREL, IRULE, RESULT, ERREST, MAXSUB, NEVAL, NSUBIN, ALIST, BLIST, RLIST, ELIST, IORD)

   The additional arguments are as follows:

   MAXSUB — Number of subintervals allowed. (Input)
   A value of 500 is used by QDAG.

   NEVAL — Number of evaluations of F. (Output)

   NSUBIN — Number of subintervals generated. (Output)

ALIST — Array of length MAXSUB containing a list of the NSUBIN left endpoints. (Output)

BLIST — Array of length MAXSUB containing a list of the NSUBIN right endpoints. (Output)

RLIST — Array of length MAXSUB containing approximations to the NSUBIN integrals over the intervals defined by ALIST, BLIST. (Output)

ELIST — Array of length MAXSUB containing the error estimates of the NSUBIN values in RLIST. (Output)

IORD — Array of length MAXSUB. (Output)
Let K be NSUBIN if NSUBIN.LE.(MAXSUB/2 + 2), MAXSUB + 1 − NSUBIN otherwise. The first K locations contain pointers to the error estimates over the corresponding subintervals, such that ELIST(IORD(1)), …, ELIST(IORD(K)) form a decreasing sequence.

2. Informational errors

Type	Code	Description
4	1	The maximum number of subintervals allowed has been reached.
3	2	Roundoff error, preventing the requested tolerance from being achieved, has been detected.
3	3	A degradation in precision has been detected.

3. If EXACT is the exact value, QDAG attempts to find RESULT such that ABS(EXACT − RESULT).LE.MAX(ERRABS, ERRREL * ABS(EXACT)). To specify only a relative error, set ERRABS to zero. Similarly, to specify only an absolute error, set ERRREL to zero.

Example

The value of

$$\int_0^2 xe^x dx = e^2 + 1$$

is estimated. Since the integrand is not oscillatory, IRULE = 1 is used. The values of the actual and estimated error are machine dependent.

```
      USE QDAG_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    IRULE, NOUT
      REAL       A, ABS, B, ERRABS, ERREST, ERROR, EXACT, EXP, &
                 F, RESULT
      INTRINSIC  ABS, EXP
      EXTERNAL   F
!                                 Get output unit number
```

```
      CALL UMACH (2, NOUT)
!                                  Set limits of integration
      A = 0.0
      B = 2.0
!                                  Set error tolerances
      ERRABS = 0.0
!                                  Parameter for non-oscillatory
!                                  function
      IRULE = 1
      CALL QDAG (F, A, B, RESULT, ERRABS=ERRABS, IRULE=IRULE, ERREST=ERREST)
!                                  Print results
      EXACT = 1.0 + EXP(2.0)
      ERROR = ABS(RESULT-EXACT)
      WRITE (NOUT,99999) RESULT, EXACT, ERREST, ERROR
99999 FORMAT (' Computed =', F8.3, 13X, ' Exact =', F8.3, /, /, &
            ' Error estimate =', 1PE10.3, 6X, 'Error =', 1PE10.3)
      END
!
      REAL FUNCTION F (X)
      REAL       X
      REAL       EXP
      INTRINSIC  EXP
      F = X*EXP(X)
      RETURN
      END
```

Output

```
Computed =   8.389            Exact =   8.389
Error estimate = 5.000E-05      Error = 9.537E-07
```

QDAGP

Integrates a function with singularity points given.

Required Arguments

F — User-supplied FUNCTION to be integrated. The form is
F(X), where

X – Independent variable. (Input)

F – The function value. (Output)

F must be declared EXTERNAL in the calling program.

A — Lower limit of integration. (Input)

B — Upper limit of integration. (Input)

POINTS — Array of length NPTS containing breakpoints in the range of integration. (Input)
Usually these are points where the integrand has singularities.

RESULT — Estimate of the integral from A to B of F. (Output)

Optional Arguments

NPTS — Number of break points given. (Input)
Default: NPTS = size (POINTS,1).

ERRABS — Absolute accuracy desired. (Input)
Default: ERRABS = 1.e-3 for single precision and 1.d-8 for double precision.

ERRREL — Relative accuracy desired. (Input)
Default: ERRREL = 1.e-3 for single precision and 1.d-8 for double precision.

ERREST — Estimate of the absolute value of the error. (Output)

FORTRAN 90 Interface

Generic: CALL QDAGP (F, A, B, POINTS, RESULT [, …])

Specific: The specific interface names are S_QDAGP and D_QDAGP.

FORTRAN 77 Interface

Single: CALL QDAGP (F, A, B, NPTS, POINTS, ERRABS, ERRREL, RESULT, ERREST)

Double: The double precision name is DQDAGP.

Description

The routine QDAGP uses a globally adaptive scheme in order to reduce the absolute error. It initially subdivides the interval [A, B] into NPTS + 1 user-supplied subintervals and uses a 21-point Gauss-Kronrod rule to estimate the integral over each subinterval. The error for each subinterval is estimated by comparison with the 10-point Gauss quadrature rule. This routine is designed to handle endpoint as well as interior singularities. In addition to the general strategy described in the IMSL routine QDAG, this routine employs an extrapolation procedure known as the **ε**-algorithm. The routine QDAGP is an implementation of the subroutine QAGP, which is fully documented by Piessens et al. (1983).

Comments

1. Workspace may be explicitly provided, if desired, by use of Q2AGP/DQ2AGP. The reference is:

   CALL Q2AGP (F, A, B, NPTS, POINTS, ERRABS, ERRREL, RESULT, ERREST, MAXSUB, NEVAL, NSUBIN, ALIST, BLIST, RLIST, ELIST, IORD, LEVEL, WK, IWK)

   The additional arguments are as follows:

   MAXSUB — Number of subintervals allowed. (Input)
   A value of 450 is used by QDAGP.

   NEVAL — Number of evaluations of F. (Output)

   NSUBIN — Number of subintervals generated. (Output)

   ALIST — Array of length MAXSUB containing a list of the NSUBIN left endpoints. (Output)

   BLIST — Array of length MAXSUB containing a list of the NSUBIN right endpoints. (Output)

   RLIST — Array of length MAXSUB containing approximations to the NSUBIN integrals over the intervals defined by ALIST, BLIST. (Output)

   ELIST — Array of length MAXSUB containing the error estimates of the NSUBIN values in RLIST. (Output)

   IORD — Array of length MAXSUB. (Output)
   Let K be NSUBIN if NSUBIN.LE.(MAXSUB/2 + 2), MAXSUB + 1 − NSUBIN otherwise. The first K locations contain pointers to the error estimates over the subintervals, such that ELIST(IORD(1)), …, ELIST(IORD(K)) form a decreasing sequence.

LEVEL — Array of length `MAXSUB`, containing the subdivision levels of the subinterval. (Output)
That is, if (`AA`, `BB`) is a subinterval of (`P1`, `P2`) where `P1` as well as `P2` is a user-provided break point or integration limit, then (`AA`, `BB`) has level `L` if `ABS(BB - AA)` = `ABS(P2 - P1) * 2**(-L)`.

WK — Work array of length `NPTS` + 2.

IWK — Work array of length `NPTS` + 2.

2. Informational errors

Type	Code	Description
4	1	The maximum number of subintervals allowed has been reached.
3	2	Roundoff error, preventing the requested tolerance from being achieved, has been detected.
3	3	A degradation in precision has been detected.
3	4	Roundoff error in the extrapolation table, preventing the requested tolerance from being achieved, has been detected.
4	5	Integral is probably divergent or slowly convergent.

3. If `EXACT` is the exact value, `QDAGP` attempts to find `RESULT` such that `ABS(EXACT − RESULT).LE.MAX(ERRABS, ERRREL * ABS(EXACT))`. To specify only a relative error, set `ERRABS` to zero. Similarly, to specify only an absolute error, set `ERRREL` to zero.

Example

The value of

$$\int_0^3 x^3 \ln\left|\left(x^2-1\right)\left(x^2-2\right)\right| dx = 61\ln 2 + \frac{77}{4}\ln 7 - 27$$

is estimated. The values of the actual and estimated error are machine dependent. Note that this subroutine never evaluates the user-supplied function at the user-supplied breakpoints.

```
      USE QDAGP_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    NOUT, NPTS
      REAL       A, ABS, ALOG, B, ERRABS, ERREST, ERROR, ERRREL, &
                EXACT, F, POINTS(2), RESULT, SQRT
      INTRINSIC  ABS, ALOG, SQRT
      EXTERNAL   F
!                                 Get output unit number
      CALL UMACH (2, NOUT)
!                                 Set limits of integration
      A = 0.0
      B = 3.0
```

```
!                                  Set error tolerances
      ERRABS = 0.0
      ERRREL = 0.01
!                                  Set singularity parameters
      NPTS      = 2
      POINTS(1) = 1.0
      POINTS(2) = SQRT(2.0)
      CALL QDAGP (F, A, B, POINTS, RESULT, ERRABS=ERRABS, ERRREL=ERRREL, &
                  ERREST=ERREST)
!                                  Print results
      EXACT = 61.0*ALOG(2.0) + 77.0/4.0*ALOG(7.0) - 27.0
      ERROR = ABS(RESULT-EXACT)
      WRITE (NOUT,99999) RESULT, EXACT, ERREST, ERROR
99999 FORMAT (' Computed =', F8.3, 13X, ' Exact =', F8.3, /, /, &
            ' Error estimate =', 1PE10.3, 6X, 'Error =', 1PE10.3)
!
      END
!
      REAL FUNCTION F (X)
      REAL       X
      REAL       ABS, ALOG
      INTRINSIC  ABS, ALOG
      F = X**3*ALOG(ABS((X*X-1.0)*(X*X-2.0)))
      RETURN
      END
```

Output

```
Computed =   52.741                Exact =   52.741

Error estimate = 5.062E-01       Error = 6.104E-04
```

QDAG1D

Integrates a function with a possible internal or endpoint singularity.

Required Arguments

***F* —** User-supplied `FUNCTION` to be integrated. The form is `F(X [, …])`, where

Function Return Value

F — The function value. (Output)

Required Arguments

X — Independent variable. (Input)

Optional Arguments

FCN_DATA — A derived type, `s_fcn_data`, which may be used to pass additional information to/from the user-supplied function. For a detailed description of this argument see `FCN_DATA` below.

`F` must be declared `EXTERNAL` in the calling program.

A — Lower limit of integration. (Input)

B — Upper limit of integration. The relative values of `A` and `B` are interpreted properly. Thus if one exchanges `A` and `B`, the sign of the answer is changed. When the integrand is positive, the sign of the result is the same as the sign of `B` − `A`. (Input)

RESULT — Estimate of the integral from `A` to `B` of `F`. (Output)

Optional Arguments

ERRABS — Absolute error tolerance. See *Comment 1* for a discussion on the error tolerances. (Input)
Default: `ERRABS` = 0.0.

ERRFRAC — A fraction expressing the (number of correct digits of accuracy desired)/(number of digits of achievable precision). See *Comment 1* for a discussion on the error tolerances. (Input)
Default: `ERRFRAC` = 0.75.

ERRREL —The error tolerance relative to the value of the integral. See *Comment 1* for a discussion on the error tolerances. (Input)
Default: `ERRREL` = 0.0.

ERRPOST — An a posteriori estimate of the absolute value of the error committed while evaluating the integrand. This value may be computed during the evaluation of the integrand. When this optional argument is used, `FCN_DATA` must also be used as `FCN_DATA%RDATA(1)` will be used to pass the newly calculated value of `ERRPOST` back from the evaluator, `F`. In this case, the user should not use `FCN_DATA%RDATA(1)` for passing other data. (Input)
Default: `ERRPOST` = 0.0.

ERRPRIOR— An a priori estimate of the absolute value of the relative error expected to be committed while evaluating the integrand. Changes to this value are not detected during evaluation of the integral. (Input)
Default: `ERRPRIOR` = 1.19e-7 for single precision and 2.22d-16 for double precision.

MAXFCN —The maximum number of function values to use to compute the integral. (Input)
Default: The number of function values is not bounded.

SINGULARITY —The real part of the abscissa of a singularity or discontinuity in the integrand. If this option is used, `SINGULARITY_TYPE` must also be used. (Input)
Default: It is assumed that there is no singularity in the integrand so `SINGULARITY` is not set. It is an error to set `SINGULARITY` without also setting `SINGULARITY_TYPE`.

SINGULARITY_TYPE—A signed integer specifying the type of singularity which occurs in the integrand. If the singularity has a leading term of the form x^{α} where α is not an integer, if α is "large" or has the form $\alpha = (2n-1)/2$ where n is a nonnegative integer, or the singularity is well outside the interval, set `SINGULARITY_TYPE` to a positive integer. Otherwise, set `SINGULARITY_TYPE` to a negative integer. (Input)
Default: It is assumed that there is no singularity in the integrand so `SINGULARITY_TYPE` is not set. It is an error to set `SINGULARITY_TYPE` without also setting `SINGULARITY`.

FCN_DATA — A derived type, `s_fcn_data`, which may be used to pass additional information to/from the user-supplied function. The derived type,
`s _fcn_data`, is defined as:

```
type s_fcn_data
   real(kind(1e0)), pointer, dimension(:) :: rdata
   integer, pointer, dimension(:) :: idata
end type
```

in module `mp_types`. The double precision counterpart to `s_fcn_data` is named `d_fcn_data`. The user must include a `use mp_types` statement in the calling program to define this derived type. Note that if this optional argument is used then this argument must also be used in the user-supplied function. (Input/Output)

NEVAL — Number of function evaluations used to calculate the integral. (Output)

ERREST — An estimate of the upper bound of the magnitude of the difference between `RESULT` and the true value of the integral. (Output)

ISTATUS — A status flag indicating the error criteria which was satisfied on exit.

ISTATUS = −1 indicates normal termination with either the absolute or relative error tolerance criteria satisfied.

ISTATUS = −2 indicates normal termination with neither the absolute nor the relative error tolerance criteria satisfied, but the error tolerance based on the locally achievable precision is satisfied.

ISTATUS = −3 indicates normal termination with none of the error tolerance criteria satisfied.

ISTATUS = any value other than the above indicates abnormal termination due to an error condition. (Output)

FORTRAN 90 Interface

Generic: CALL QDAG1D (F,A, B, RESULT [, …])

Specific: The specific interface names are S_QDAG1D and D_QDAG1D.

Description

QDAG1D is based on the JPL Library routine SINT1. The integral is estimated using quadrature formulae due to T. N. L. Patterson (1968). Patterson described a family of formulae in which the k^{th} formula used all the integrand values used in the $k{-}1^{st}$ formula, and added 2^{k-1} new integrand values in an optimal way. The first formula is the midpoint rule, the second is the three point Gauss formula, and the third is the seven point Kronrod formula. Formulae of this family of higher degree had not previously been described. This program uses formulae up to $k = 8$.

An error estimate is obtained by comparing the values of the integral estimated by two adjacent formulae, examining differences up to the fifteenth order, integrating round-off error, integrating error declared to have been committed during computation of the integrand, integrating a first order estimate of the effect round-off error in the abscissa has on integrand values, and including errors in the limits. The latter four methods are also used to derive a bound on the achievable precision.

If the integral over an interval cannot be estimated with sufficient accuracy, the interval is subdivided. The difference table is used to discover whether the integral is difficult to compute because the integrand is too complex or has singular behavior. In the former case, the estimated error, requested error tolerance, and difference table are used to choose a step size.

In the latter case, the difference table is used in a search algorithm to find the abscissa of the singular behavior. If the singular behavior is discovered on the end of an interval, a change of independent variable is applied to reduce the strength of the singularity.

The program also uses the difference table to detect nonintegrable singularities, jump discontinuities, and computational noise.

Comments

1. The user provides the absolute error tolerance through optional argument ERRABS. Optional argument ERRFRAC represents the ratio of the (number of correct digits of accuracy desired) to (number of digits of achievable precision). Optional argument ERRREL represents the error tolerance relative to the value of the integral. The internal value for ERRFRAC is bounded between .5 and 1. By default, ERRABS and ERRREL are set to 0.0 and ERRFRAC is set to .75. These default values usually provide all the accuracy that can be obtained efficiently.

   The error tolerance relative to the value of the integral is applied globally (over the entire region of integration) rather than locally (one step at a time). This policy provides true control of error relative to the value of the integral when the integrand is not sign definite, as well as when the integrand is sign definite. To apply the criterion of error tolerance relative to the value of the integral, the value of the integral over the entire region, estimated without refinement of the region, is used to derive an absolute error tolerance that may be applied locally. If the preliminary estimate of the value of the integral is significantly in error, and the least restrictive error tolerance is relative to the value of the integral, the cost of computing the integral will be larger than the cost of computing the integral to the same degree of accuracy using appropriate values of either of the other tolerance criteria. The preliminary estimate of the integral may be significantly in error if the integrand is not sign definite or has large variation.

2. Optional arguments SINGULARITY and SINGULARITY_TYPE provide the user with a means to give the routine information about the location and type of any known singularity of the integrand. When an integrand appears to have singular behavior at the end of the interval, a transformation of the variable of integration is applied to reduce the strength of the singularity. When an integrand appears to have singular behavior inside the interval, the abscissa of the singularity is determined as precisely as necessary, depending on the error tolerance, and the interval is subdivided. The discovery of singular behavior and determination of the abscissa of singular behavior are expensive. If the user knows of the existence of a singularity, the efficiency of computation of the integral may be improved by requesting an immediate transformation of the independent variable or subdivision of the interval. It is recommended that the user select these optional arguments for all singularities, even those outside [A, B]. If the singularity has a leading term of the form x^{α} where α is not an integer, if α is "large" or has the form α = (2n-1)/2 where n is a nonnegative integer, or the singularity is well outside the interval, set SINGULARITY_TYPE to a positive value. Otherwise, set SINGULARITY_TYPE to a negative value. The meaning of "large" depends on the rest of the integrand and the length of the interval. For the typical case, a value of about 2 is considered "large". For a singularity of the form $x^{\alpha}\log x$ use the above rule, even if α is an integer. For other types of singularities make a reasonable guess based on the above. If several similar integrals are to be computed, some experimentation may be useful.

When SINGULARITY_TYPE is positive, a transformation of the form $T = TA + (X - TA)^2 / (TB - TA)$ is applied, where *TA* is the abscissa of the singularity and *TB* is the end of the interval. If *TA* is outside the interval, *TB* will be the end of the interval farthest from *TA*. If *TA* is inside the interval, the interval will immediately be subdivided at *TA*, and both parts will be separately integrated with *TB* equal to each end of the original interval, respectively. When SINGULARITY_TYPE is negative, a transformation of the form $T = TA + (X - TA)^4 / (TB - TA)^3$ is applied, with *TA* and *TB* as above.

If the integrand has singularities at more than one abscissa within the region, or more than one pole near the real axis such that the real parts are within the region of integration, then the interval should be subdivided at the abscissa of the singularities or the real parts of the poles, and the integrals should be computed as separate problems, with the results summed.

Examples

Example

The value of

$$\int_0^1 \ln(x)\left(x^{-1/2}\right)dx = -4$$

is estimated. Note that the optional arguments SINGULARITY and SINGULARITY_TYPE are used.

```
      USE QDAG1D_INT
      USE UMACH_INT

      IMPLICIT NONE
!                                  Declare variables
      INTEGER    NOUT, SINGULARITY_TYPE

      REAL    A, B, ERREST, F, RESULT, SINGULARITY

      EXTERNAL      F
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Set limits of integration
      A = 0.0
      B = 1.0
!                              Set singularity value and type
      SINGULARITY = 0.0
      SINGULARITY_TYPE = -1
      CALL QDAG1D ( F, A, B, RESULT, SINGULARITY=SINGULARITY, &
      SINGULARITY_TYPE=SINGULARITY_TYPE, ERREST=ERREST)
!                              Print the results
      WRITE(NOUT,*)'Result = ', RESULT
      WRITE(NOUT,9999) ERREST
 9999 FORMAT('Error Estimate = ', 1PE9.1)
      END

      REAL FUNCTION F (X)
      REAL       X
      REAL       ALOG, SQRT
```

```
      INTRINSIC  ALOG, SQRT
      F = ALOG(X)/SQRT(X)
      RETURN
      END
```

Output

```
Result = -4.0
Error Estimate = 6.0E-07
```

Example 2

The value of

$$\int_1^2 \left(2x + kx\right) dx = 6$$

is estimated. Note that the optional argument `FCN_DATA` is used to set the value of $k = 2$ in the user-supplied function, `F`.

```
      USE QDAG1D_INT
      USE UMACH_INT
      USE MP_TYPES

      IMPLICIT NONE
!                                  Declare variables
      INTEGER             NOUT

      REAL             A, B, ERREST, F, RESULT
      REAL, TARGET ::        RDATA(1)

      TYPE (S_FCN_DATA) USER_DATA

      EXTERNAL      F
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Set limits of integration
      A = 1.0
      B = 2.0
!                                  Set IPARAM
      RDATA(1) = 2.0
      USER_DATA%RDATA=>RDATA
      CALL QDAG1D ( F, A, B, RESULT, FCN_DATA=USER_DATA, ERREST=ERREST)
!                              Print the results
      WRITE(NOUT,*)'Result = ', RESULT
      WRITE(NOUT,9999) ERREST
 9999 FORMAT('Error Estimate = ', 1PE9.1)
      END

      REAL FUNCTION F (X, FCN_DATA)
      USE MP_TYPES
      TYPE (S_FCN_DATA) FCN_DATA
      REAL       X
      F = 2.0 * X + FCN_DATA%RDATA(1) * X
      RETURN
      END
```

Output

```
Result = 6.0
Error Estimate = 1.2E-06
```

QDAGI

Integrates a function over an infinite or semi-infinite interval.

Required Arguments

F — User-supplied FUNCTION to be integrated. The form is
F(X), where

X – Independent variable. (Input)

F – The function value. (Output)

F must be declared EXTERNAL in the calling program.

BOUND — Finite bound of the integration range. (Input)
Ignored if INTERV = 2.

INTERV — Flag indicating integration interval. (Input)

INTERV	Interval
−1	(−∞, BOUND)
1	(BOUND, + ∞)
2	(−∞, + ∞)

RESULT — Estimate of the integral from A to B of F. (Output)

Optional Arguments

ERRABS — Absolute accuracy desired. (Input)
Default: ERRABS = 1.e-3 for single precision and 1.d-8 for double precision.

ERRREL — Relative accuracy desired. (Input)
Default: ERRREL = 1.e-3 for single precision and 1.d-8 for double precision.

ERREST — Estimate of the absolute value of the error. (Output)

FORTRAN 90 Interface

Generic: CALL QDAGI (F, BOUND, INTERV, RESULT [, …])

Specific: The specific interface names are S_QDAGI and D_QDAGI.

FORTRAN 77 Interface

Single: CALL QDAGI (F, BOUND, INTERV, ERRABS, ERRREL, RESULT, ERREST)

Double: The double precision name is DQDAGI.

Description

The routine QDAGI uses a globally adaptive scheme in an attempt to reduce the absolute error. It initially transforms an infinite or semi-infinite interval into the finite interval [0, 1]. Then, QDAGI uses a 21-point Gauss-Kronrod rule to estimate the integral and the error. It bisects any interval with an unacceptable error estimate and continues this process until termination. This routine is designed to handle endpoint singularities. In addition to the general strategy described in QDAG, this subroutine employs an extrapolation procedure known as the ε-algorithm. The routine QDAGI is an implementation of the subroutine QAGI, which is fully documented by Piessens et al. (1983).

Comments

1. Workspace may be explicitly provided, if desired, by use of Q2AGI/DQ2AGI. The reference is

   CALL Q2AGI (F, BOUND, INTERV, ERRABS, ERRREL, RESULT, ERREST, MAXSUB, NEVAL, NSUBIN, ALIST, BLIST, RLIST, ELIST, IORD)

   The additional arguments are as follows:

   MAXSUB — Number of subintervals allowed. (Input)
   A value of 500 is used by QDAGI.

   NEVAL — Number of evaluations of F. (Output)

   NSUBIN — Number of subintervals generated. (Output)

   ALIST — Array of length MAXSUB containing a list of the NSUBIN left endpoints. (Output)

   BLIST — Array of length MAXSUB containing a list of the NSUBIN right endpoints. (Output)

   RLIST — Array of length MAXSUB containing approximations to the NSUBIN integrals over the intervals defined by ALIST, BLIST. (Output)

   ELIST — Array of length MAXSUB containing the error estimates of the NSUBIN values in RLIST. (Output)

   IORD — Array of length MAXSUB. (Output)
   Let K be NSUBIN if NSUBIN .LE.(MAXSUB/2 + 2), MAXSUB + 1 − NSUBIN otherwise. The first K locations contain pointers to the error estimates over the subintervals, such that ELIST(IORD(1)), …, ELIST(IORD(K)) form a decreasing sequence.

2. Informational errors

Type	Code	Description
4	1	The maximum number of subintervals allowed has been reached.
3	2	Roundoff error, preventing the requested tolerance from being achieved, has been detected.
3	3	A degradation in precision has been detected.
3	4	Roundoff error in the extrapolation table, preventing the requested tolerance from being achieved, has been detected.
4	5	Integral is divergent or slowly convergent.

3. If EXACT is the exact value, QDAGI attempts to find RESULT such that ABS(EXACT − RESULT).LE.MAX(ERRABS, ERRREL * ABS(EXACT)). To specify only a relative error, set ERRABS to zero. Similarly, to specify only an absolute error, set ERRREL to zero.

4. Since QDAGI makes a transformation of the original interval into the finite interval [0,1] the resulting function values can be extremely small and the resulting function might have "spikes". In some cases QDAGI "overlooks" these spikes. The user can try adjusting the absolute and relative error tolerances to remedy this or, alternatively, try using IMSL routine QDAG1D.

Example

The value of

$$\int_0^{\infty} \frac{\ln(x)}{1+(10x)^2} dx = \frac{-\pi \ln(10)}{20}$$

is estimated. The values of the actual and estimated error are machine dependent. Note that we have requested an absolute error of 0 and a relative error of .001. The effect of these requests, as documented in Comment 3 above, is to ignore the absolute error requirement.

```
      USE QDAGI_INT
      USE UMACH_INT
      USE CONST_INT

      IMPLICIT   NONE
      INTEGER    INTERV, NOUT
      REAL       ABS, ALOG, BOUND, ERRABS, ERREST, ERROR, &
                ERRREL, EXACT, F, PI, RESULT
      INTRINSIC  ABS, ALOG
      EXTERNAL   F
!                                 Get output unit number
      CALL UMACH (2, NOUT)
!                                 Set limits of integration
      BOUND  = 0.0
      INTERV = 1
!                                 Set error tolerances
      ERRABS = 0.0
      CALL QDAGI (F, BOUND, INTERV, RESULT, ERRABS=ERRABS,  &
```

```
                  ERREST=ERREST)
!                                  Print results
      PI    = CONST('PI')
      EXACT = -PI*ALOG(10.)/20.
      ERROR = ABS(RESULT-EXACT)
      WRITE (NOUT,99999) RESULT, EXACT, ERREST, ERROR
99999 FORMAT (' Computed =', F8.3, 13X, ' Exact =', F8.3//' Error ', &
            'estimate =', 1PE10.3, 6X, 'Error =', 1PE10.3)
      END
!
      REAL FUNCTION F (X)
      REAL       X
      REAL       ALOG
      INTRINSIC  ALOG
      F = ALOG(X)/(1.+(10.*X)**2)
      RETURN
      END
```

Output

```
Computed =  -0.362              Exact =  -0.362
Error estimate = 2.652E-06      Error = 5.960E-08
```

QDAWO

Integrates a function containing a sine or a cosine.

Required Arguments

F — User-supplied function to be integrated. The form is
F(X), where

X – Independent variable. (Input)

F – The function value. (Output)

F must be declared EXTERNAL in the calling program.

A — Lower limit of integration. (Input)

B — Upper limit of integration. (Input)

IWEIGH — Type of weight function used. (Input)

IWEIGH	Weight
1	COS(OMEGA * X)
2	SIN(OMEGA * X)

OMEGA — Parameter in the weight function. (Input)

RESULT — Estimate of the integral from A to B of F * WEIGHT. (Output)

Optional Arguments

ERRABS — Absolute accuracy desired. (Input)
Default: ERRABS = 1.e-3 for single precision and 1.d-8 for double precision.

ERRREL — Relative accuracy desired. (Input)
Default: ERRREL = 1.e-3 for single precision and 1.d-8 for double precision.

ERREST — Estimate of the absolute value of the error. (Output)

FORTRAN 90 Interface

Generic: CALL QDAWO (F, A, B, IWEIGH, OMEGA, RESULT [, …])

Specific: The specific interface names are S_QDAWO and D_QDAWO.

FORTRAN 77 Interface

Single: CALL QDAWO (F, A, B, IWEIGH, OMEGA, ERRABS, ERREL, RESULT, ERREST)

Double: The double precision name is DQDAWO.

Description

The routine QDAWO uses a globally adaptive scheme in an attempt to reduce the absolute error. This routine computes integrals whose integrands have the special form $w(x) f(x)$, where $w(x)$ is either $\cos \omega x$ or $\sin \omega x$. Depending on the length of the subinterval in relation to the size of ω, either a modified Clenshaw-Curtis procedure or a Gauss-Kronrod 7/15 rule is employed to approximate the integral on a subinterval. In addition to the general strategy described for the IMSL routine QDAG, this subroutine uses an extrapolation procedure known as the ε-algorithm. The routine QDAWO is an implementation of the subroutine QAWO, which is fully documented by Piessens et al. (1983).

Comments

1. Workspace may be explicitly provided, if desired, by use of Q2AWO/DQ2AWO. The reference is:

   CALL Q2AWO (F, A, B, IWEIGH, OMEGA, ERRABS, ERREL, RESULT, ERREST, MAXSUB, MAXCBY, NEVAL, NSUBIN, ALIST, BLIST, RLIST, ELIST, IORD, NNLOG, WK)

   The additional arguments are as follows:

   MAXSUB — Maximum number of subintervals allowed. (Input)
   A value of 390 is used by QDAWO.

   MAXCBY — Upper bound on the number of Chebyshev moments which can be stored. That is, for the intervals of lengths ABS (B − A) * 2**(−L), L = 0, 1, …, MAXCBY − 2, MAXCBY.GE.1. The routine QDAWO uses 21. (Input)

   NEVAL — Number of evaluations of F. (Output)

   NSUBIN — Number of subintervals generated. (Output)

   ALIST — Array of length MAXSUB containing a list of the NSUBIN left endpoints. (Output)

   BLIST — Array of length MAXSUB containing a list of the NSUBIN right endpoints. (Output)

   RLIST — Array of length MAXSUB containing approximations to the NSUBIN integrals over the intervals defined by ALIST, BLIST. (Output)

   ELIST — Array of length MAXSUB containing the error estimates of the NSUBIN values in RLIST. (Output)

IORD — Array of length MAXSUB. Let K be NSUBIN if .NSUBIN.LE. (MAXSUB/2 + 2), MAXSUB + 1 – NSUBIN otherwise. The first K locations contain pointers to the error estimates over the subintervals, such that ELIST(IORD(1)), …, ELIST(IORD(K)) form a decreasing sequence. (Output)

NNLOG — Array of length MAXSUB containing the subdivision levels of the subintervals, i.e. NNLOG(I) = L means that the subinterval numbered I is of length ABS (B – A) * (1 – L). (Output)

WK — Array of length 25 * MAXCBY. (Workspace)

2. Informational errors

Type	Code	Description
4	1	The maximum number of subintervals allowed has been reached.
3	2	Roundoff error, preventing the requested tolerance from being achieved, has been detected.
3	3	A degradation in precision has been detected.
3	4	Roundoff error in the extrapolation table, preventing the requested tolerances from being achieved, has been detected.

3. If EXACT is the exact value, QDAWO attempts to find RESULT such that ABS(EXACT – RESULT) .LE. MAX(ERRABS, ERRREL * ABS(EXACT)). To specify only a relative error, set ERRABS to zero. Similarly, to specify only an absolute error, set ERRREL to zero.

Example

The value of

$$\int_0^1 \ln(x)\sin(10\pi x)\,dx$$

is estimated. The values of the actual and estimated error are machine dependent. Notice that the log function is coded to protect for the singularity at zero.

```
      USE QDAWO_INT
      USE UMACH_INT
      USE CONST_INT

      IMPLICIT   NONE
      INTEGER    IWEIGH, NOUT
      REAL       A, ABS, B, ERRABS, ERREST, ERROR, &
                EXACT, F, OMEGA, PI, RESULT
      INTRINSIC  ABS
      EXTERNAL   F
!                                 Get output unit number
      CALL UMACH (2, NOUT)
!                                 Set limits of integration
```

```
      A = 0.0
      B = 1.0
!                                 Weight function = sin(10.*pi*x)
      IWEIGH = 2
      PI     = CONST('PI')
      OMEGA  = 10.*PI
!                                 Set error tolerances
      ERRABS = 0.0
      CALL QDAWO (F, A, B, IWEIGH, OMEGA, RESULT, ERRABS=ERRABS, &
                 ERREST=ERREST)
!                                 Print results
      EXACT = -0.1281316
      ERROR = ABS(RESULT-EXACT)
      WRITE (NOUT,99999) RESULT, EXACT, ERREST, ERROR
99999 FORMAT (' Computed =', F8.3, 13X, ' Exact =', F8.3, /, /, &
            ' Error estimate =', 1PE10.3, 6X, 'Error =', 1PE10.3)
      END
!
      REAL FUNCTION F (X)
      REAL       X
      REAL       ALOG
      INTRINSIC  ALOG
      IF (X .EQ. 0.) THEN
         F = 0.0
      ELSE
         F = ALOG(X)
      END IF
      RETURN
      END
```

Output

```
Computed =  -0.128              Exact =  -0.128

Error estimate = 7.504E-05      Error = 5.260E-06
```

QDAWF

Computes a Fourier integral.

Required Arguments

F — User-supplied FUNCTION to be integrated. The form is
F(X), where

X – Independent variable. (Input)

F – The function value. (Output)

F must be declared EXTERNAL in the calling program.

A — Lower limit of integration. (Input)

IWEIGH — Type of weight function used. (Input)

IWEIGH	Weight
1	COS(OMEGA * X)
2	SIN(OMEGA * X)

OMEGA — Parameter in the weight function. (Input)

RESULT — Estimate of the integral from A to infinity of F * WEIGHT. (Output)

Optional Arguments

ERRABS — Absolute accuracy desired. (Input)
Default: ERRABS = 1.e-3 for single precision and 1.d-8 for double precision.

ERREST — Estimate of the absolute value of the error. (Output)
Default: ERREST = 1.e-3 for single precision and 1.d-8 for double precision.

FORTRAN 90 Interface

Generic: CALL QDAWF (F, A, IWEIGH, OMEGA, RESULT [, …])

Specific: The specific interface names are S_QDAWF and D_QDAWF.

FORTRAN 77 Interface

Single: `CALL QDAWF (F, A, IWEIGH, OMEGA, ERRABS, RESULT, ERREST)`

Double: The double precision name is `DQDAWF`.

Description

The routine `QDAWF` uses a globally adaptive scheme in an attempt to reduce the absolute error. This routine computes integrals whose integrands have the special form $w(x) f(x)$, where $w(x)$ is either $\cos \omega x$ or $\sin \omega x$. The integration interval is always semi-infinite of the form $[A, \infty]$. These Fourier integrals are approximated by repeated calls to the IMSL routine `QDAWO` followed by extrapolation. The routine `QDAWF` is an implementation of the subroutine `QAWF`, which is fully documented by Piessens et al. (1983).

Comments

1. Workspace may be explicitly provided, if desired, by use of `Q2AWF`/`DQ2AWF`. The reference is:

   `CALL Q2AWF (F, A, IWEIGH, OMEGA, ERRABS, RESULT, ERREST, MAXCYL, MAXSUB, MAXCBY, NEVAL, NCYCLE, RSLIST, ERLIST, IERLST, NSUBIN, WK, IWK)`

   The additional arguments are as follows:

   MAXSUB — Maximum number of subintervals allowed. (Input)
   A value of 365 is used by `QDAWF`.

   MAXCYL — Maximum number of cycles allowed. (Input)
   `MAXCYL` must be at least 3. `QDAWF` uses 50.

   MAXCBY — Maximum number of Chebyshev moments allowed. (Input)
   `QDAWF` uses 21.

   NEVAL — Number of evaluations of `F`. (Output)

   NCYCLE — Number of cycles used. (Output)

   RSLIST — Array of length `MAXCYL` containing the contributions to the integral over the interval $(A + (k - 1) * C, A + k * C)$, for $k = 1, \ldots,$ `NCYCLE`. (Output)
   `C = (2 * INT(ABS(OMEGA)) + 1) * PI/ABS(OMEGA)`.

   ERLIST — Array of length `MAXCYL` containing the error estimates for the intervals defined in `RSLIST`. (Output)

   IERLST — Array of length `MAXCYL` containing error flags for the intervals defined in `RSLIST`. (Output)

IERLST(K)	Meaning
1	The maximum number of subdivisions (MAXSUB) has been achieved on the *k*-th cycle.
2	Roundoff error prevents the desired accuracy from being achieved on the *k*-th cycle.
3	Extremely bad integrand behavior occurs at some points of the *k*-th cycle.
4	Integration procedure does not converge (to the desired accuracy) due to roundoff in the extrapolation procedure on the *k*-th cycle. It is assumed that the result on this interval is the best that can be obtained.
5	Integral over the *k*-th cycle is divergent or slowly convergent.

NSUBIN — Number of subintervals generated. (Output)

WK — Work array of length 4 * MAXSUB + 25 * MAXCBY.

IWK — Work array of length 2 * MAXSUB.

2. Informational errors

Type	Code	Description
3	1	Bad integrand behavior occurred in one or more cycles.
4	2	Maximum number of cycles allowed has been reached.
3	3	Extrapolation table constructed for convergence acceleration of the series formed by the integral contributions of the cycles does not converge to the requested accuracy.

3. If EXACT is the exact value, QDAWF attempts to find RESULT such that ABS(EXACT – RESULT) .LE. ERRABS.

Example

The value of

$$\int_0^{\infty} x^{-1/2} \cos(\pi x / 2)\, dx = 1$$

is estimated. The values of the actual and estimated error are machine dependent. Notice that *F* is coded to protect for the singularity at zero.

```
USE QDAWF_INT
USE UMACH_INT
```

```
      USE CONST_INT

      IMPLICIT   NONE
      INTEGER    IWEIGH, NOUT
      REAL       A, ABS, ERRABS, ERREST, ERROR, EXACT, F, &
                OMEGA, PI, RESULT
      INTRINSIC  ABS
      EXTERNAL   F
!                                 Get output unit number
      CALL UMACH (2, NOUT)
!                                 Set lower limit of integration
      A = 0.0
!                                 Select weight W(X) = COS(PI*X/2)
      IWEIGH = 1
      PI     = CONST('PI')
      OMEGA  = PI/2.0
!                                 Set error tolerance
      CALL QDAWF (F, A, IWEIGH, OMEGA, RESULT, ERREST=ERREST)
!                                 Print results
      EXACT = 1.0
      ERROR = ABS(RESULT-EXACT)
      WRITE (NOUT,99999) RESULT, EXACT, ERREST, ERROR
99999 FORMAT (' Computed =', F8.3, 13X, ' Exact =', F8.3, /, /, &
            ' Error estimate =', 1PE10.3, 6X, 'Error =', 1PE10.3)
      END
!
      REAL FUNCTION F (X)
      REAL       X
      REAL       SQRT
      INTRINSIC  SQRT
      IF (X .GT. 0.0) THEN
         F = 1.0/SQRT(X)
      ELSE
         F = 0.0
      END IF
      RETURN
      END
```

Output

```
Computed =   1.000               Exact =   1.000

Error estimate = 6.267E-04      Error = 2.205E-06
```

QDAWS

Integrates a function with algebraic-logarithmic singularities.

Required Arguments

F — User-supplied FUNCTION to be integrated. The form is
F(X), where

X – Independent variable. (Input)

F – The function value. (Output)

F must be declared EXTERNAL in the calling program.

A — Lower limit of integration. (Input)

B — Upper limit of integration. (Input)
B must be greater than A

IWEIGH — Type of weight function used. (Input)

IWEIGH	Weight
1	(X – A)**ALPHA * (B – X)**BETAW
2	(X – A)**ALPHA * (B – X)**BETAW * LOG(X – A)
3	(X – A)**ALPHA * (B – X)**BETAW * LOG(B – X)
4	(X – A)**ALPHA * (B – X)**BETAW * LOG (X – A) * LOG (B – X)

ALPHA — Parameter in the weight function. (Input)
ALPHA must be greater than –1.0.

BETAW — Parameter in the weight function. (Input)
BETAW must be greater than –1.0.

RESULT — Estimate of the integral from A to B of F * WEIGHT. (Output)

Optional Arguments

ERRABS — Absolute accuracy desired. (Input)
Default: ERRABS = 1.e-3 for single precision and 1.d-8 for double precision.

ERRREL — Relative accuracy desired. (Input)
Default: `ERRREL` = 1.e-3 for single precision and 1.d-8 for double precision.

ERREST — Estimate of the absolute value of the error. (Output)

FORTRAN 90 Interface

Generic: `CALL QDAWS (F, A, B, IWEIGH, ALPHA, BETAW, RESULT [, …] )`

Specific: The specific interface names are `S_QDAWS` and `D_QDAWS`.

FORTRAN 77 Interface

Single: `CALL QDAWS (F, A, B, IWEIGH, ALPHA, BETAW, ERRABS, ERRREL, RESULT, ERREST)`

Double: The double precision name is `DQDAWS`.

Description

The routine `QDAWS` uses a globally adaptive scheme in an attempt to reduce the absolute error. This routine computes integrals whose integrands have the special form $w(x) f(x)$, where $w(x)$ is a weight function described above. A combination of modified Clenshaw-Curtis and Gauss-Kronrod formulas is employed. In addition to the general strategy described for the IMSL routine `QDAG`, this routine uses an extrapolation procedure known as the ε-algorithm. The routine `QDAWS` is an implementation of the routine `QAWS`, which is fully documented by Piessens et al. (1983).

Comments

1. Workspace may be explicitly provided, if desired, by use of `Q2AWS/DQ2AWS`. The reference is

   `CALL Q2AWS (F, A, B, IWEIGH, ALPHA, BETAW, ERRABS, ERRREL, RESULT, ERREST, MAXSUB, NEVAL, NSUBIN, ALIST, BLIST, RLIST, ELIST, IORD)`

   The additional arguments are as follows:

   MAXSUB — Maximum number of subintervals allowed. (Input)
   A value of 500 is used by `QDAWS`.

   NEVAL — Number of evaluations of *F*. (Output)

   NSUBIN — Number of subintervals generated. (Output)

   ALIST — Array of length `MAXSUB` containing a list of the `NSUBIN` left endpoints. (Output)

   BLIST — Array of length `MAXSUB` containing a list of the `NSUBIN` right endpoints. (Output)

RLIST — Array of length MAXSUB containing approximations to the NSUBIN integrals over the intervals defined by ALIST, BLIST. (Output)

ELIST — Array of length MAXSUB containing the error estimates of the NSUBIN values in RLIST. (Output)

IORD — Array of length MAXSUB. Let *k* be NSUBIN if NSUBIN .LE. (MAXSUB/2 + 2), MAXSUB + 1 – NSUBIN otherwise. The first *k* locations contain pointers to the error estimates over the subintervals, such that ELIST(IORD(1)), …, ELIST(IORD(*k*)) form a decreasing sequence. (Output)

2. Informational errors

Type	Code	Description
4	1	The maximum number of subintervals allowed has been reached.
3	2	Roundoff error, preventing the requested tolerance from being achieved, has been detected.
3	3	A degradation in precision has been detected.

3. If EXACT is the exact value, QDAWS attempts to find RESULT such that ABS(EXACT – RESULT).LE.MAX(ERRABS, ERRREL * ABS(EXACT)). To specify only a relative error, set ERRABS to zero. Similarly, to specify only an absolute error, set ERRREL to zero.

Example

The value of

$$\int_0^1 [\,(1+x)(1-x)\,]^{1/2} x \ln(x)\,dx = \frac{3\ln(2)-4}{9}$$

is estimated. The values of the actual and estimated error are machine dependent.

```
      USE QDAWS_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    IWEIGH, NOUT
      REAL       A, ABS, ALOG, ALPHA, B, BETAW, ERRABS, ERREST, ERROR, &
                EXACT, F, RESULT
      INTRINSIC  ABS, ALOG
      EXTERNAL   F
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Set limits of integration
      A = 0.0
      B = 1.0
!                                  Select weight
      ALPHA  = 1.0
      BETAW   = 0.5
      IWEIGH = 2
!                                  Set error tolerances
```

```
      ERRABS = 0.0
      CALL QDAWS (F, A, B, IWEIGH, ALPHA, BETAW, RESULT, &
                ERRABS=ERRABS, ERREST=ERREST)
!                                 Print results
      EXACT = (3.*ALOG(2.)-4.)/9.
      ERROR = ABS(RESULT-EXACT)
      WRITE (NOUT,99999) RESULT, EXACT, ERREST, ERROR
99999 FORMAT (' Computed =', F8.3, 13X, ' Exact =', F8.3, /, /, &
            ' Error estimate =', 1PE10.3, 6X, 'Error =', 1PE10.3)
      END
!
      REAL FUNCTION F (X)
      REAL       X
      REAL       SQRT
      INTRINSIC  SQRT
      F = SQRT(1.0+X)
      RETURN
      END
```

Output

```
Computed =  -0.213                Exact =  -0.213

Error estimate = 1.261E-08        Error = 2.980E-08
```

QDAWC

Integrates a function *f(x)/(x-c)* in the Cauchy principal value sense.

Required Arguments

F — User-supplied `FUNCTION` to be integrated. The form is
`F(X)`, where

`X` – Independent variable. (Input)

`F` – The function value. (Output)

`F` must be declared `EXTERNAL` in the calling program.

A — Lower limit of integration. (Input)

B — Upper limit of integration. (Input)

C — Singular point. (Input)
`C` must not equal `A` or `B`.

RESULT — Estimate of the integral from `A` to `B` of `F(X)/(X – C)`. (Output)

Optional Arguments

ERRABS — Absolute accuracy desired. (Input)
Default: `ERRABS` = 1.e-3 for single precision and 1.d-8 for double precision.

ERRREL — Relative accuracy desired. (Input)
Default: `ERREL` =1.e-3 for single precision and 1.d-8 for double precision.

ERREST — Estimate of the absolute value of the error. (Output)

FORTRAN 90 Interface

Generic: `CALL QDAWC (F, A, B, C, RESULT [, …])`

Specific: The specific interface names are `S_QDAWC` and `D_QDAWC`.

FORTRAN 77 Interface

Single: `CALL QDAWC (F, A, B, C, ERRABS, ERRREL, RESULT, ERREST)`

Double: The double precision name is DQDAWC.

Description

The routine QDAWC uses a globally adaptive scheme in an attempt to reduce the absolute error. This routine computes integrals whose integrands have the special form $w(x) f(x)$, where $w(x) = 1/(x - c)$. If c lies in the interval of integration, then the integral is interpreted as a Cauchy principal value. A combination of modified Clenshaw-Curtis and Gauss-Kronrod formulas are employed. In addition to the general strategy described for the IMSL routine QDAG, this routine uses an extrapolation procedure known as the ε-algorithm. The routine QDAWC is an implementation of the subroutine QAWC, which is fully documented by Piessens et al. (1983).

Comments

1. Workspace may be explicitly provided, if desired, by use of Q2AWC/DQ2AWC. The reference is:

   CALL Q2AWC (F, A, B, C, ERRABS, ERREL, RESULT, ERREST, MAXSUB, NEVAL, NSUBIN, ALIST, BLIST, RLIST, ELIST, IORD)

   The additional arguments are as follows:

   MAXSUB — Number of subintervals allowed. (Input)
   A value of 500 is used by QDAWC.

   NEVAL — Number of evaluations of F. (Output)

   NSUBIN — Number of subintervals generated. (Output)

   ALIST — Array of length MAXSUB containing a list of the NSUBIN left endpoints. (Output)

   BLIST — Array of length MAXSUB containing a list of the NSUBIN right endpoints. (Output)

   RLIST — Array of length MAXSUB containing approximations to the NSUBIN integrals over the intervals defined by ALIST, BLIST. (Output)

   ELIST — Array of length MAXSUB containing the error estimates of the NSUBIN values in RLIST. (Output)

   IORD — Array of length MAXSUB. (Output)
   Let k be NSUBIN if NSUBIN.LE.(MAXSUB/2 + 2), MAXSUB + 1 − NSUBIN otherwise. The first k locations contain pointers to the error estimates over the subintervals, such that ELIST(IORD(1)), …, ELIST(IORD(k)) form a decreasing sequence.

2. Informational errors

Type	Code	Description
4	1	The maximum number of subintervals allowed has been reached.
3	2	Roundoff error, preventing the requested tolerance from being achieved, has been detected.
3	3	A degradation in precision has been detected.

3. If EXACT is the exact value, QDAWC attempts to find RESULT such that ABS(EXACT − RESULT) .LE. MAX(ERRABS, ERRREL * ABS(EXACT)). To specify only a relative error, set ERRABS to zero. Similarly, to specify only an absolute error, set ERRREL to zero.

Example

The Cauchy principal value of

$$\int_{-1}^{5} \frac{1}{x\left(5x^3+6\right)} dx = \frac{\ln\left(125/631\right)}{18}$$

is estimated. The values of the actual and estimated error are machine dependent.

```
      USE QDAWC_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    NOUT
      REAL       A, ABS, ALOG, B, C, ERRABS, ERREST, ERROR, EXACT, &
                 F, RESULT
      INTRINSIC  ABS, ALOG
      EXTERNAL   F
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Set limits of integration and C
      A = -1.0
      B = 5.0
      C = 0.0
!                                  Set error tolerances
      ERRABS = 0.0
      CALL QDAWC (F, A, B, C, RESULT, ERRABS=ERRABS, ERREST=ERREST)
!                                  Print results
      EXACT = ALOG(125./631.)/18.
      ERROR = 2*ABS(RESULT-EXACT)
      WRITE (NOUT,99999) RESULT, EXACT, ERREST, ERROR
99999 FORMAT (' Computed =', F8.3, 13X, ' Exact =', F8.3, /, /, &
            ' Error estimate =', 1PE10.3, 6X, 'Error =', 1PE10.3)
      END
!
      REAL FUNCTION F (X)
      REAL       X
      F = 1.0/(5.*X**3+6.0)
      RETURN
      END
```

Output

```
Computed =  -0.090               Exact =  -0.090
Error estimate = 2.022E-06       Error = 2.980E-08
```

QDNG

Integrates a smooth function using a nonadaptive rule.

Required Arguments

F — User-supplied FUNCTION to be integrated. The form is
F(X), where

X – Independent variable. (Input)

F – The function value. (Output)

F must be declared EXTERNAL in the calling program.

A — Lower limit of integration. (Input)

B — Upper limit of integration. (Input)

RESULT — Estimate of the integral from A to B of F. (Output)

Optional Arguments

ERRABS — Absolute accuracy desired. (Input)
Default: ERRABS = 1.e-3 for single precision and 1.d-8 for double precision.

ERRREL — Relative accuracy desired. (Input)
Default: ERRREL = 1.e-3 for single precision and 1.d-8 for double precision.

ERREST — Estimate of the absolute value of the error. (Output)

FORTRAN 90 Interface

Generic:	CALL QDNG (F, A, B, RESULT [, …])
Specific:	The specific interface names are S_QDNG and D_QDNG.

FORTRAN 77 Interface

Single:	CALL QDNG (F, A, B, ERRABS, ERRREL, RESULT, ERREST)
Double:	The double precision name is DQDNG.

Description

The routine QDNG is designed to integrate smooth functions. This routine implements a nonadaptive quadrature procedure based on nested Paterson rules of order 10, 21, 43, and 87. These rules are positive quadrature rules with degree of accuracy 19, 31, 64, and 130, respectively. The routine QDNG applies these rules successively, estimating the error, until either the error estimate satisfies the user-supplied constraints or the last rule is applied. The routine QDNG is based on the routine QNG by Piessens et al. (1983).

This routine is not very robust, but for certain smooth functions it can be efficient. If QDNG should not perform well, we recommend the use of the IMSL routine QDAGS.

Comments

1. Informational error

Type	Code	Description
4	1	The maximum number of steps allowed have been taken. The integral is too difficult for QDNG.

2. If EXACT is the exact value, QDNG attempts to find RESULT such that ABS(EXACT − RESULT).LE.MAX(ERRABS, ERRREL * ABS(EXACT)). To specify only a relative error, set ERRABS to zero. Similarly, to specify only an absolute error, set ERRREL to zero.

3. This routine is designed for efficiency, not robustness. If the above error is encountered, try QDAGS.

Example

The value of

$$\int_0^2 xe^x dx = e^2 + 1$$

is estimated. The values of the actual and estimated error are machine dependent.

```
      USE QDNG_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    NOUT
      REAL       A, ABS, B, ERRABS, ERREST, ERROR, EXACT, EXP, &
                F, RESULT
      INTRINSIC  ABS, EXP
      EXTERNAL   F
!                                 Get output unit number
      CALL UMACH (2, NOUT)
!                                 Set limits of integration
```

```
      A = 0.0
      B = 2.0
!                                  Set error tolerances
      ERRABS = 0.0
      CALL QDNG (F, A, B, RESULT, ERRABS=ERRABS, ERREST=ERREST)
!                                  Print results
      EXACT = 1.0 + EXP(2.0)
      ERROR = ABS(RESULT-EXACT)
      WRITE (NOUT,99999) RESULT, EXACT, ERREST, ERROR
99999 FORMAT (' Computed =', F8.3, 13X, ' Exact =', F8.3, /, /, &
            ' Error estimate =', 1PE10.3, 6X, 'Error =', 1PE10.3)
      END
!
      REAL FUNCTION F (X)
      REAL       X
      REAL       EXP
      INTRINSIC  EXP
      F = X*EXP(X)
      RETURN
      END
```

Output

```
Computed =   8.389                Exact =   8.389

Error estimate = 5.000E-05      Error = 9.537E-07
```

TWODQ

Computes a two-dimensional iterated integral.

Required Arguments

F — User-supplied `FUNCTION` to be integrated. The form is
`F(X, Y)`, where

`X` – First argument of `F`. (Input)

`Y` – Second argument of `F`. (Input)

`F` – The function value. (Output)

`F` must be declared `EXTERNAL` in the calling program.

A — Lower limit of outer integral. (Input)

B — Upper limit of outer integral. (Input)

G — User-supplied `FUNCTION` to evaluate the lower limits of the inner integral. The form is `G(X)`, where

`X` – Only argument of `G`. (Input)

`G` – The function value. (Output)

`G` must be declared `EXTERNAL` in the calling program.

H — User-supplied `FUNCTION` to evaluate the upper limits of the inner integral. The form is `H(X)`, where

`X` – Only argument of `H`. (Input)

`H` – The func`tion value. (Output)

`H` must be declared `EXTERNAL` in the calling program.

RESULT — Estimate of the integral from `A` to `B` of `F`. (Output)

Optional Arguments

ERRABS — Absolute accuracy desired. (Input)
Default: `ERRABS` = 1.e-3 for single precision and 1.d-8 for double precision.

ERRREL — Relative accuracy desired. (Input)
Default: `ERRREL` = 1.e-3 for single precision and 1.d-8 for double precision.

IRULE --- Choice of quadrature rule. (Input)
Default: `IRULE` = 2.
The Gauss-Kronrod rule is used with the following points:

IRULE	Points
1	7-15
2	10-21
3	15-31
4	20-41
5	25-51
6	30-61

If the function has a peak singularity, use `IRULE` = 1. If the function is oscillatory, use `IRULE` = 6.

ERREST — Estimate of the absolute value of the error. (Output)

FORTRAN 90 Interface

Generic: `CALL TWODQ (F, A, B, G, H, RESULT [, …])`

Specific: The specific interface names are `S_TWODQ` and `D_TWODQ`.

FORTRAN 77 Interface

Single: `CALL TWODQ (F, A, B, G, H, ERRABS, ERRREL, IRULE, RESULT, ERREST)`

Double: The double precision name is `DTWODQ`.

Description

The routine `TWODQ` approximates the two-dimensional iterated integral

$$\int_a^b \int_{g(x)}^{h(x)} f(x,y)\, dy\, dx$$

with the approximation returned in `RESULT`. An estimate of the error is returned in `ERREST`. The approximation is achieved by iterated calls to `QDAG`. Thus, this algorithm will share many of the characteristics of the routine `QDAG`. As in `QDAG`, several options are available. The absolute and relative error must be specified, and in addition, the Gauss-Kronrod pair must be specified (`IRULE`). The lower-numbered rules are used for less smooth integrands while the higher-order rules are more efficient for smooth (oscillatory) integrands.

Comments

1. Workspace may be explicitly provided, if desired, by use of T2ODQ/DT2ODQ. The reference is:

   CALL T2ODQ (F, A, B, G, H, ERRABS, ERRREL, IRULE, RESULT, ERREST, MAXSUB, NEVAL, NSUBIN, ALIST, BLIST, RLIST, ELIST, IORD, WK, IWK)

   The additional arguments are as follows:

   MAXSUB — Number of subintervals allowed. (Input)
   A value of 250 is used by TWODQ.

   NEVAL — Number of evaluations of F. (Output)

   NSUBIN — Number of subintervals generated in the outer integral. (Output)

   ALIST — Array of length MAXSUB containing a list of the NSUBIN left endpoints for the outer integral. (Output)

   BLIST — Array of length MAXSUB containing a list of the NSUBIN right endpoints for the outer integral. (Output)

   RLIST — Array of length MAXSUB containing approximations to the NSUBIN integrals over the intervals defined by ALIST, BLIST, pertaining only to the outer integral. (Output)

   ELIST — Array of length MAXSUB containing the error estimates of the NSUBIN values in RLIST. (Output)

   IORD — Array of length MAXSUB. (Output)
   Let K be NSUBIN if NSUBIN.LE.(MAXSUB/2 + 2), MAXSUB + 1 − NSUBIN otherwise. Then the first K locations contain pointers to the error estimates over the corresponding subintervals, such that ELIST(IORD(1)), …, ELIST(IORD(K)) form a decreasing sequence.

   WK — Work array of length 4 * MAXSUB, needed to evaluate the inner integral.

   IWK — Work array of length MAXSUB, needed to evaluate the inner integral.

2. Informational errors

Type	Code	Description
4	1	The maximum number of subintervals allowed has been reached.
3	2	Roundoff error, preventing the requested tolerance from being achieved, has been detected.
3	3	A degradation in precision has been detected.

3. If EXACT is the exact value, TWODQ attempts to find RESULT such that ABS(EXACT − RESULT).LE.MAX(ERRABS, ERRREL * ABS(EXACT)). To specify only a relative error, set ERRABS to zero. Similarly, to specify only an absolute error, set ERRREL to zero.

Examples

Example 1

In this example, we approximate the integral

$$\int_0^1 \int_1^3 y\cos\left(x + y^2\right) dydx$$

The value of the error estimate is machine dependent.

```
      USE TWODQ_INT
      USE UMACH_INT
      IMPLICIT   NONE
      INTEGER    IRULE, NOUT
      REAL       A, B, ERRABS, ERREST, ERRREL, F, G, H, RESULT
      EXTERNAL   F, G, H
!                                 Get output unit number
      CALL UMACH (2, NOUT)
!                                 Set limits of integration
      A = 0.0
      B = 1.0
!                                 Set error tolerances
      ERRABS = 0.0
      ERRREL = 0.01
!                                 Parameter for oscillatory function
      IRULE = 6
      CALL TWODQ (F, A, B, G, H, RESULT, ERRABS, ERRREL, IRULE, errest)
!                                 Print results
      WRITE (NOUT,99999) RESULT, ERREST
99999 FORMAT (' Result =', F8.3, 13X, ' Error estimate = ', 1PE9.3)
      END
!
      REAL FUNCTION F (X, Y)
      REAL       X, Y
      REAL       COS
      INTRINSIC  COS
      F = Y*COS(X+Y*Y)
      RETURN
      END
!
      REAL FUNCTION G (X)
      REAL       X
      G = 1.0
      RETURN
      END
!
      REAL FUNCTION H (X)
      REAL       X
      H = 3.0
      RETURN
      END
```

Output

```
Result =  -0.514              Error estimate = 3.065E-06
```

Example 2

We modify the above example by assuming that the limits for the inner integral depend on *x* and, in particular, are $g(x) = -2x$ and $h(x) = 5x$. The integral now becomes

$$\int_0^1 \int_{-2x}^{5x} y\cos\left(x + y^2\right) dy\,dx$$

The value of the error estimate is machine dependent.

```
      USE TWODQ_INT
      USE UMACH_INT
!                                 Declare F, G, H
      INTEGER    IRULE, NOUT
      REAL       A, B, ERRABS, ERREST, ERRREL, F, G, H, RESULT
      EXTERNAL   F, G, H
!
      CALL UMACH (2, NOUT)
!                                   Set limits of integration
      A = 0.0
      B = 1.0
!                                   Set error tolerances
      ERRABS = 0.001
      ERRREL = 0.0
!                                   Parameter for oscillatory function
      IRULE = 6
      CALL TWODQ (F, A, B, G, H, RESULT, ERRABS, ERRREL, IRULE, ERREST)
!                                   Print results
      WRITE (NOUT,99999) RESULT, ERREST
99999 FORMAT (' Computed =', F8.3, 13X, ' Error estimate = ', 1PE9.3)
      END
      REAL FUNCTION F (X, Y)
      REAL       X, Y
!
      REAL       COS
      INTRINSIC  COS
!
      F = Y*COS(X+Y*Y)
      RETURN
      END
      REAL FUNCTION G (X)
      REAL       X
!
      G = -2.0*X
      RETURN
      END
      REAL FUNCTION H (X)
      REAL       X
!
      H = 5.0*X
      RETURN
      END
```

Output

```
Computed =   -0.083                Error estimate = 2.095E-06
```

QDAG2D

Integrates a function of two variables with a possible internal or end point singularity.

Required Arguments

F **—** User-supplied `FUNCTION` to be integrated. The form is `F(X, Y [, …])`, where

Function Return Value

F — The function value. (Output)

Required Arguments

X — Independent variable. (Input)

Y — Independent variable. (Input)

Optional Arguments

FCN_DATA — A derived type, `s_fcn_data`, which may be used to pass additional information to/from the user-supplied function. For a detailed description of this argument see `FCN_DATA` below.

`F` must be declared `EXTERNAL` in the calling program.

A — Lower limit of integration for outer dimension. (Input)

B — Upper limit of integration. The relative values of `A` and `B` are interpreted properly. Thus if one exchanges `A` and `B`, the sign of the answer is changed. When the integrand is positive, the sign of the result is the same as the sign of `B` − `A`. (Input)

G **—** User-supplied `FUNCTION` to compute the lower limit of integration for the inner dimension. The form is `G(X [, …])`, where

Function Return Value

G — The function value. (Output)

Required Arguments

X — Independent variable. (Input)

Optional Arguments

FCN_DATA — A derived type, `s_fcn_data`, which may be used to pass additional information to/from the user-supplied function. For a detailed description of this argument see `FCN_DATA` below.

`G` must be declared `EXTERNAL` in the calling program.

H **—** User-supplied `FUNCTION` to compute the upper limit of integration for the inner dimension. The form is `H(X [,])`, where

Function Return Value

H — The function value. (Output)

Required Arguments

X — Independent variable. (Input)

Optional Arguments

FCN_DATA — A derived type, `s_fcn_data`, which may be used to pass additional information to/from the user-supplied function. For a detailed description of this argument see `FCN_DATA` below.

`H` must be declared `EXTERNAL` in the calling program.

RESULT — Estimate of the integral from `A` to `B` of the integral from `G`(`X`) to `H`(`X`) of `G`(`X`,`Y`). (Output)

Optional Arguments

ERRABS — Absolute error tolerance. See *Comment 1* for a discussion of the error tolerances. (Input)
Default: `ERRABS` = 0.0.

ERRFRAC — A fraction expressing the (number of correct digits of accuracy desired)/(number of digits of achievable precision). See *Comment 1* for a discussion of the error tolerances. (Input)
Default: `ERRFRAC` = 0.75.

ERRREL— Relative error tolerance. See *Comment 1* for a discussion of the error tolerances. (Input)
Default: `ERRABS` = 0.0.

ERRPOST — An a posteriori estimate of the absolute value of the error committed while evaluating the integrand. This value may be computed during the evaluation of the integrand. When this optional argument is used, `FCN_DATA` must also be used as `FCN_DATA%RDATA(1)` will be used to pass the newly calculated value of `ERRPOST` back from the evaluator, `F`. In this case, the user should not use `FCN_DATA%RDATA(1)` for passing other data. (Input)
Default: `ERRPOST` = 0.0.

ERRPRIOR— An a priori estimate of the absolute value of the relative error expected to be committed while evaluating the integrand. Changes to this value are not detected during evaluation of the integral. (Input)
Default: `ERRPRIOR` = 1.19e-7 for single precision and 2.22d-16 for double precision.

MAXFCN — The maximum number of function values to use to compute the integral. (Input)
Default: The number of function values is not bounded.

SINGULARITY — The real part of the abscissa of a singularity or discontinuity in the innermost integrand. If this option is used, `SINGULARITY_TYPE` must also be used. (Input)
Default: It is assumed that there is no singularity in the innermost integrand so `SINGULARITY` is not set. It is an error to set `SINGULARITY` without also setting `SINGULARITY_TYPE`.

SINGULARITY_TYPE— A signed integer specifying the type of singularity which occurs in the innermost integrand. If the singularity has a leading term of the form x^{α} where α is not an integer, if α is "large" or has the form $\alpha = (2n-1)/2$ where n is a nonnegative integer, or the singularity is well outside the interval, set `SINGULARITY_TYPE` to a positive integer. Otherwise, set `SINGULARITY_TYPE` to a negative integer. (Input)
Default: It is assumed that there is no singularity in the innermost integrand so `SINGULARITY_TYPE` is not set. It is an error to set `SINGULARITY_TYPE` without also setting `SINGULARITY`.

FCN_DATA — A derived type, `s_fcn_data`, which may be used to pass additional information to/from the user-supplied function. The derived type, `s_fcn_data`, is defined as:

```
type s_fcn_data
   real(kind(1e0)), pointer, dimension(:) :: rdata
   integer, pointer, dimension(:) :: idata
end type
```

in module `mp_types`. The double precision counterpart to `s_fcn_data` is named `d_fcn_data`. The user must include a `use mp_types` statement in the calling program to define this derived type. (Input/Output)

NEVAL — Number of function evaluations used to calculate the integral. (Output)

ERREST — An estimate of the upper bound of the magnitude of the difference between `RESULT` and the true value of the integral. (Output)

ISTATUS — A status flag indicating the error criteria which was satisfied on exit.
`ISTATUS` = −1 indicates normal termination with either the absolute or relative error tolerance criteria satisfied.
`ISTATUS` = −2 indicates normal termination with neither the absolute nor the relative error tolerance criteria satisfied, but the error tolerance based on the locally achievable precision is satisfied.
`ISTATUS` = −3 indicates normal termination with none of the error tolerance criteria satisfied.
`ISTATUS` = any value other than the above indicates abnormal termination due to an error condition. (Output)

FORTRAN 90 Interface

Generic: `CALL QDAG2D (F, A, B, G, H, RESULT [, …])`

Specific: The specific interface names are `S_QDAG2D` and `D_QDAG2D`.

Description

QDAG2D, based on the JPL Library routine SINTM, approximates an iterated two-dimensional integral of the form

$$\int_a^b \int_{g(x)}^{h(x)} f(x,y)\,dy\,dx$$

The integral over two dimensions is computed by repeated integration over one dimension. The integration over one dimension is estimated using quadrature formulae due to T. N. L. Patterson (1968). Patterson described a family of formulae in which the k^{th} formula used all the integrand values used in the $k-1^{st}$ formula, and added 2^{k-1} new integrand values in an optimal way. The first formula is the midpoint rule, the second is the three point Gauss formula, and the third is the seven point Kronrod formula. Formulae of this family of higher degree had not previously been described. This program uses formulae up to $k = 8$.

An error estimate is obtained by comparing the values of the integral estimated by two adjacent formulae, examining differences up to the fifteenth order, integrating round-off error, integrating error declared to have been committed during computation of the integrand, integrating a first order estimate of the effect round-off error in the abscissa has on integrand values, and including errors in the limits. The latter four methods are also used to derive a bound on the achievable precision.

If the integral over an interval cannot be estimated with sufficient accuracy, the interval is subdivided. The difference table is used to discover whether the integral is difficult to compute because the integrand is too complex or has singular behavior. In the former case, the estimated error, requested error tolerance, and difference table are used to choose a step size.

In the latter case, the difference table is used in a search algorithm to find the abscissa of the singular behavior. If the singular behavior is discovered on the end of an interval, a change of independent variable is applied to reduce the strength of the singularity.

The program also uses the difference table to detect nonintegrable singularities, jump discontinuities, and computational noise.

Comments

1. The user provides the absolute error tolerance through optional argument ERRABS. Optional argument ERRFRAC represents the ratio of the (number of correct digits of accuracy desired) to (number of digits of achievable precision). The internal value for ERRFRAC is bounded between .5 and 1.The error tolerance relative to the value of the integral is specified via optional argument ERRREL. By default, ERRABS and ERRREL are set to 0.0 and ERRFRAC is set to .75. These default values usually provide all the accuracy that can be obtained efficiently.

The error tolerance relative to the value of the integral is applied globally (over the entire region of integration) rather than locally (one step at a time). This policy provides true control of error relative to the value of the integral when the integrand is not sign definite, as well as when the integrand is sign definite. To apply the criterion of error tolerance relative to the value of the integral, the value of the integral over the entire region, estimated without refinement of the region, is used to derive an absolute error tolerance that may be applied locally. If the preliminary estimate of the value of the integral is significantly in error, and the least restrictive error tolerance is relative to the value of the integral, the cost of computing the integral will be larger than the cost of computing the integral to the same degree of accuracy using appropriate values of either of the other tolerance criteria. The preliminary estimate of the integral may be significantly in error if the integrand is not sign definite or has large variation.

2. Optional arguments `SINGULARITY` and `SINGULARITY_TYPE` provide the user with a means to give the routine information about the location and type of any known singularity of the innermost integrand. When an integrand appears to have singular behavior at the end of the interval, a transformation of the variable of integration is applied to reduce the strength of the singularity. When an integrand appears to have singular behavior inside the interval, the abscissa of the singularity is determined as precisely as necessary, depending on the error tolerance, and the interval is subdivided. The discovery of singular behavior and determination of the abscissa of singular behavior are expensive. If the user knows of the existence of a singularity, the efficiency of computation of the integral may be improved by requesting an immediate transformation of the independent variable or subdivision of the interval. It is recommended that the user select these optional arguments for all singularities, even those outside `[A, B]`. If the singularity has a leading term of the form x^{α} where α is not an integer, if α is "large" or has the form $\alpha = (2n-1)/2$ where n is a nonnegative integer, or the singularity is well outside the interval, set `SINGULARITY_TYPE` to a positive value. Otherwise, set `SINGULARITY_TYPE` to a negative value. The meaning of "large" depends on the rest of the integrand and the length of the interval. For the typical case, a value of about 2 is considered "large". For a singularity of the form $x^{\alpha} \log x$ use the above rule, even if α is an integer. For other types of singularities make a reasonable guess based on the above. If several similar integrals are to be computed, some experimentation may be useful.

When `SINGULARITY_TYPE` is positive, a transformation of the form $T = TA + (X - TA)^2 / (TB - TA)$ is applied, where *TA* is the abscissa of the singularity and *TB* is the end of the interval. If *TA* is outside the interval, *TB* will be the end of the interval farthest from *TA*. If *TA* is inside the interval, the interval will immediately be subdivided at *TA*, and both parts will be separately integrated with *TB* equal to each end of the original interval, respectively. When `SINGULARITY_TYPE` is negative, a transformation of the form $T = TA + (X - TA)^4 / (TB - TA)^3$ is applied, with *TA* and *TB* as above.

If the integrand has singularities at more than one abscissa within the region, or more than one pole near the real axis such that the real parts are within the region of integration, then the interval should be subdivided at the abscissa of the singularities or the real parts of the poles, and the integrals should be computed as separate problems, with the results summed.

Example

The value of

$$\int_0^1 \int_1^3 y\cos\left(x + y^2\right) dydx$$

is estimated.

```
      USE QDAG2D_INT
      USE UMACH_INT

      IMPLICIT NONE
!                                  Declare variables
      REAL    A, B, ERREST, F, G, H, RESULT

      EXTERNAL      F, G, H
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Set limits of integration
      A = 0.0
      B = 1.0
!                              Set singularity value and type
      CALL QDAG2D ( F, A, B, G, H, RESULT, ERREST=ERREST)
!                              Print the results
      WRITE(NOUT,*)'Result = ', RESULT
      WRITE(NOUT,9999) ERREST
 9999 FORMAT('Error Estimate = ', 1PE9.1)

      END

      REAL FUNCTION F (X, Y)
      REAL       X, Y
      REAL       COS
      INTRINSIC  COS
      F = Y*COS(X+Y*Y)
      RETURN
      END

      REAL FUNCTION G (X)
      REAL       X
      G = 1.0
      RETURN
      END

      REAL FUNCTION H (X)
      REAL       X
      H = 3.0
      RETURN
      END
```

Output

```
RESULT = -0.51425
Error Estimate = 5.3-06
```

QDAG3D

Integrates a function of three variables with a possible internal or endpoint singularity.

Required Arguments

F **—** User-supplied `FUNCTION` to be integrated. The form is `F(X, Y, Z [, …])`, where

Function Return Value

F — The function value. (Output)

Required Arguments

X — Independent variable. (Input)

Y — Independent variable. (Input)

Z — Independent variable. (Input)

Optional Arguments

FCN_DATA — A derived type, `s_fcn_data`, which may be used to pass additional information to/from the user-supplied function. For a detailed description of this argument see `FCN_DATA` below.

`F` must be declared `EXTERNAL` in the calling program.

A — Lower limit of integration for outer dimension. (Input)

B — Upper limit of integration for outer dimension. The relative values of `A` and `B` are interpreted properly. Thus if one exchanges `A` and `B`, the sign of the answer is changed. When the integrand is positive, the sign of the result is the same as the sign of `B − A`. (Input)

G — User-supplied `FUNCTION` to compute the lower limit of integration for the middle dimension. The form is `G(X [, …])`, where

Function Return Value

G — The function value. (Output)

Required Arguments

X — Independent variable. (Input)

Optional Arguments

FCN_DATA — A derived type, `s_fcn_data`, which may be used to pass additional information to/from the user-supplied function. For a detailed description of this argument see `FCN_DATA` below.

`G` must be declared `EXTERNAL` in the calling program.

H **—** User-supplied `FUNCTION` to compute the upper limit of integration for the middle dimension. The form is `H(X [, …])`, where

Function Return Value

H — The function value. (Output)

Required Arguments

X — Independent variable. (Input)

Optional Arguments

FCN_DATA — A derived type, `s_fcn_data`, which may be used to pass additional information to/from the user-supplied function. For a detailed description of this argument see `FCN_DATA` below.

`H` must be declared `EXTERNAL` in the calling program

P **—** User-supplied `FUNCTION` to compute the lower limit of integration for the inner dimension. The form is `P(X, Y [, …])`, where

Function Return Value

P — The function value. (Output)

Required Arguments

X — Independent variable. (Input)

Y — Independent variable. (Input)

Optional Arguments

FCN_DATA — A derived type, `s_fcn_data`, which may be used to pass additional information to/from the user-supplied function. For a detailed description of this argument see `FCN_DATA` below.

`P` must be declared `EXTERNAL` in the calling program.

Q **—** User-supplied `FUNCTION` to compute the upper limit of integration for the inner dimension. The form is `Q(X, Y [, …])`, where

Function Return Value

Q — The function value. (Output)

Required Arguments

X — Independent variable. (Input)

Y — Independent variable. (Input)

Optional Arguments

FCN_DATA — A derived type, `s_fcn_data`, which may be used to pass additional information to/from the user-supplied function. For a detailed description of this argument see `FCN_DATA` below.

`Q` must be declared `EXTERNAL` in the calling program

RESULT — Estimate of the integral from A to B of the integral from G(X) to H(X) of the integral from P(X,Y) to Q(X,Y) of F(X,Y,Z). (Output)

Optional Arguments

ERRABS — Absolute error tolerance. See *Comment 1* for a discussion of the error tolerances. (Input)
Default: ERRABS = 0.0.

ERRFRAC — A fraction expressing the (number of correct digits of accuracy desired)/(number of digits of achievable precision). See *Comment 1* for a discussion of the error tolerances. (Input)
Default: ERRFRAC = 0.75.

ERRREL — The error tolerance relative to the value of the integral. See *Comment 1* for a discussion of the error tolerances. (Input)
Default: ERRREL = 0.0.

ERRPOST — An a posteriori estimate of the absolute value of the error committed while evaluating the integrand. This value may be computed during the evaluation of the integrand. When this optional argument is used, FCN_DATA must also be used as FCN_DATA%RDATA(1) will be used to pass the newly calculated value of ERRPOST back from the evaluator, F. In this case, the user should not use FCN_DATA%RDATA(1) for passing other data. (Input)
Default: ERRPOST = 0.0.

ERRPRIOR— An a priori estimate of the absolute value of the relative error expected to be committed while evaluating the integrand. Changes to this value are not detected during evaluation of the integral. (Input)
Default: ERRPRIOR = 1.19e-7 for single precision and 2.22d-16 for double precision.

MAXFCN — The maximum number of function values to use to compute the integral. (Input)
Default: The number of function values is not bounded.

SINGULARITY — The real part of the abscissa of a singularity or discontinuity in the innermost integrand. If this option is used, SINGULARITY_TYPE must also be used. (Input)
Default: It is assumed that there is no singularity in the innermost integrand so SINGULARITY is not set. It is an error to set SINGULARITY without also setting SINGULARITY_TYPE.

SINGULARITY_TYPE— A signed integer specifying the type of singularity which occurs in the innermost integrand. If the singularity has a leading term of the form x^{α} where α is not an integer, if α is "large" or has the form $\alpha = (2n-1)/2$ where n is a nonnegative integer, or the singularity is well outside the interval, set SINGULARITY_TYPE to a positive integer. Otherwise, set SINGULARITY_TYPE to a negative integer. (Input)

Default: It is assumed that there is no singularity in the innermost integrand so SINGULARITY_TYPE is not set. It is an error to set SINGULARITY_TYPE without also setting SINGULARITY.

FCN_DATA — A derived type, s_fcn_data, which may be used to pass additional information to/from the user-supplied function. The derived type, s_fcn_data, is defined as:

```
type s_fcn_data
   real(kind(1e0)), pointer, dimension(:) :: rdata
   integer, pointer, dimension(:) :: idata
end type
```

in module mp_types. The double precision counterpart to s_fcn_data is named d_fcn_data. The user must include a use mp_types statement in the calling program to define this derived type. (Input/Output)

NEVAL — Number of function evaluations used to calculate the integral. (Output)

ERREST — An estimate of the upper bound of the magnitude of the difference between RESULT and the true value of the integral. (Output)

ISTATUS — A status flag indicating the error criteria which was satisfied on exit.
ISTATUS = −1 indicates normal termination with either the absolute or relative error tolerance criteria satisfied.
ISTATUS = −2 indicates normal termination with neither the absolute nor the relative error tolerance criteria satisfied, but the error tolerance based on the locally achievable precision is satisfied.
ISTATUS = −3 indicates normal termination with none of the error tolerance criteria satisfied.
ISTATUS = any value other than the above indicates abnormal termination due to an error condition. (Output)

FORTRAN 90 Interface

Generic: CALL QDAG3D (F, A, B, G, H, P, Q, RESULT [, …])

Specific: The specific interface names are S_QDAG3D and D_QDAG3D.

Description

QDAG3D, based on the JPL Library routine SINTM, approximates an iterated three-dimensional integral of the form

$$\int_a^b \int_{g(x)}^{h(x)} \int_{p(x,y)}^{q(x,y)} f(x,y,z)\, dz dy dx$$

The integral over three dimensions is computed by repeated integration over one dimension. The integration over one dimension is estimated using quadrature formulae due to T. N. L. Patterson (1968). Patterson described a family of formulae in which the k^{th} formula used all the integrand values used in the $k-1^{st}$ formula, and added 2^{k-1} new integrand values in an optimal way. The first formula is the midpoint rule, the second is the three point Gauss formula, and the third is the seven point Kronrod formula. Formulae of this family of higher degree had not previously been described. This program uses formulae up to $k = 8$.

An error estimate is obtained by comparing the values of the integral estimated by two adjacent formulae, examining differences up to the fifteenth order, integrating round-off error, integrating error declared to have been committed during computation of the integrand, integrating a first order estimate of the effect round-off error in the abscissa has on integrand values, and including errors in the limits. The latter four methods are also used to derive a bound on the achievable precision.

If the integral over an interval cannot be estimated with sufficient accuracy, the interval is subdivided. The difference table is used to discover whether the integral is difficult to compute because the integrand is too complex or has singular behavior. In the former case, the estimated error, requested error tolerance, and difference table are used to choose a step size.

In the latter case, the difference table is used in a search algorithm to find the abscissa of the singular behavior. If the singular behavior is discovered on the end of an interval, a change of independent variable is applied to reduce the strength of the singularity.

The program also uses the difference table to detect nonintegrable singularities, jump discontinuities, and computational noise.

Comments

1. The user provides the absolute error tolerance through optional argument `ERRABS`. Optional argument `ERRFRAC` represents the ratio of the (number of correct digits of accuracy desired) to (number of digits of achievable precision). Optional argument `ERRREL` represents the error tolerance relative to the value of the integral. The internal value for `ERRFRAC` is bounded between .5 and 1. By default, `ERRABS and ERRREL` are set to 0.0 and `ERRFRAC` is set to .75. These default values usually provide all the accuracy that can be obtained efficiently.

   The error tolerance relative to the value of the integral is applied globally (over the entire region of integration) rather than locally (one step at a time). This policy provides true control of error relative to the value of the integral when the integrand is not sign definite, as well as when the integrand is sign definite. To apply the criterion of error tolerance relative to the value of the integral, the value of the integral over the entire region, estimated without refinement of the region, is used to derive an absolute error tolerance that may be applied locally. If the preliminary estimate of the value of the integral is significantly in error, and the least restrictive error tolerance is relative to the value of the integral, the cost of computing the integral will be larger than the cost of computing the integral to the same degree of accuracy using appropriate values of either of the other tolerance criteria. The preliminary estimate of the integral may be significantly in error if the integrand is not sign definite or has large variation.

2. Optional arguments `SINGULARITY` and `SINGULARITY_TYPE` provide the user with a means to give the routine information about the location and type of any known singularity of the innermost integrand. When an integrand appears to have singular behavior at the end of the interval, a transformation of the variable of integration is applied to reduce the strength of the singularity. When an integrand appears to have singular behavior inside the interval, the abscissa of the singularity is determined as precisely as necessary, depending on the error tolerance, and the interval is subdivided. The discovery of singular behavior and determination of the abscissa of singular behavior are expensive. If the user knows of the existence of a singularity, the efficiency of computation of the integral may be improved by requesting an immediate transformation of the independent variable or subdivision of the interval. It is recommended that the user select these optional arguments for all singularities, even those outside `[A, B]`. If the singularity has a leading term of the form x^{α} where α is not an integer, if α is "large" or has the form $\alpha = (2n-1)/2$ where n is a nonnegative integer, or the singularity is well outside the interval, set `SINGULARITY_TYPE` to a positive value. Otherwise, set `SINGULARITY_TYPE` to a negative value. The meaning of "large" depends on the rest of the integrand and the length of the interval. For the typical case, a value of about 2 is considered "large". For a singularity of the form $x^{\alpha} \log x$ use the above rule, even if α is an integer. For other types of singularities make a reasonable guess based on the above. If several similar integrals are to be computed, some experimentation may be useful.

   When `SINGULARITY_TYPE` is positive, a transformation of the form $T = TA + (X - TA)^2 / (TB - TA)$ is applied, where *TA* is the abscissa of the singularity and *TB* is the end of the interval. If *TA* is outside the interval, *TB* will be the end of the interval farthest from *TA*. If *TA* is inside the interval, the interval will immediately be subdivided at *TA*, and both parts will be separately integrated with *TB* equal to each end of the original interval, respectively. When `SINGULARITY_TYPE` is negative, a transformation of the form $T = TA + (X - TA)^4 / (TB - TA)^3$ is applied, with *TA* and *TB* as above.

   If the integrand has singularities at more than one abscissa within the region, or more than one pole near the real axis such that the real parts are within the region of integration, then the interval should be subdivided at the abscissa of the singularities or the real parts of the poles, and the integrals should be computed as separate problems, with the results summed.

Example

The value of

$$\int_0^1 \int_0^{1-x} \int_0^{1-x-y} \left(1.0 + x + y + 2z\right) dz dy dx$$

is estimated.

```
      USE QDAG3D_INT
      USE UMACH_INT

      IMPLICIT NONE
!                                  Declare variables
      INTEGER    NOUT

      REAL    A, B, ERREST, F, G, H, P, Q, RESULT

      EXTERNAL      F, G, H, P, Q
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Set limits of integration
      A = 0.0
      B = 1.0
!                              Set singularity value and type
      CALL QDAG3D ( F, A, B, G, H, P, Q, RESULT, &
      ERREST=ERREST)
!                              Print the results
      WRITE(NOUT,*) 'Result = ', RESULT
      WRITE(NOUT,9999) ERREST
 9999 FORMAT('Error Estimate = ', 1PE9.1)
      END

      REAL FUNCTION F (X, Y, Z)
      REAL        X, Y, Z
      F = 1.0 + X + Y + 2.0*Z
      RETURN
      END

      REAL FUNCTION G (X)
      REAL        X
      G = 0.0
      RETURN
      END

      REAL FUNCTION H (X)
      REAL        X
      H = 1.0 - X
      RETURN
      END

      REAL FUNCTION P (X, Y)
      REAL        X, Y
      P = 0.0
      RETURN
      END

      REAL FUNCTION Q (X, Y)
      REAL        X, Y
      Q = 1.0 - X - Y
      RETURN
      END
```

Output

```
RESULT = 0.333333
```

```
 Error Estimate = 1.9E-07
```

QAND

Integrates a function on a hyper-rectangle.

Required Arguments

F — User-supplied FUNCTION to be integrated. The form is
F(N, X), where

N – The dimension of the hyper-rectangle. (Input)

X – The independent variable of dimension N. (Input)

F – The value of the integrand at X. (Output)

F must be declared EXTERNAL in the calling program.

N — The dimension of the hyper-rectangle. (Input)
N must be less than or equal to 20.

A — Vector of length N. (Input)
Lower limits of integration.

B — Vector of length N. (Input)
Upper limits of integration.

RESULT — Estimate of the integral from A to B of F. (Output)
The integral of F is approximated over the N-dimensional hyper-rectangle A.LE.X.LE.B.

Optional Arguments

ERRABS — Absolute accuracy desired. (Input)
Default: ERRABS = 1.e-3 for single precision and 1.d-8 for double precision.

ERRREL — Relative accuracy desired. (Input)
Default: ERRREL = 1.e-3 for single precision and 1.d-8 for double precision.

MAXFCN — Approximate maximum number of function evaluations to be permitted. (Input)
MAXFCN cannot be greater than 256^{N} or IMACH(5) if N is greater than 3.
Default: MAXFCN = 32**N.

ERREST — Estimate of the absolute value of the error. (Output)

FORTRAN 90 Interface

Generic: CALL QAND (F, N, A, B, RESULT [, …])

Specific: The specific interface names are S_QAND and D_QAND.

FORTRAN 77 Interface

Single: CALL QAND (F, N, A, B, ERRABS, ERRREL, MAXFCN, RESULT, ERREST)

Double: The double precision name is DQAND.

Description

The routine QAND approximates the *n*-dimensional iterated integral

$$\int_{a_1}^{b_1} \dots \int_{a_n}^{b_n} f\left(x_1, \dots, x_n\right) dx_n \dots dx_1$$

with the approximation returned in RESULT. An estimate of the error is returned in ERREST. The approximation is achieved by iterated applications of product Gauss formulas. The integral is first estimated by a two-point tensor product formula in each direction. Then for $i = 1, \dots, n$ the routine calculates a new estimate by doubling the number of points in the i-th direction, but halving the number immediately afterwards if the new estimate does not change appreciably. This process is repeated until either one complete sweep results in no increase in the number of sample points in any dimension, or the number of Gauss points in one direction exceeds 256, or the number of function evaluations needed to complete a sweep would exceed MAXFCN.

Comments

1. Informational errors

Type	Code	Description
3	1	MAXFCN was set greater than 256^N.
4	2	The maximum number of function evaluations has been reached, and convergence has not been attained.

2. If EXACT is the exact value, QAND attempts to find RESULT such that ABS(EXACT - RESULT).LE.MAX(ERRABS, ERRREL * ABS(EXACT)). To specify only a relative error, set ERRABS to zero. Similarly, to specify only an absolute error, set ERRREL to zero.

Example

In this example, we approximate the integral of

$$e^{-\left(x_1^2+x_2^2+x_3^2\right)}$$

on an expanding cube. The values of the error estimates are machine dependent. The exact integral over

$$R^3 \text{ is } \pi^{3/2}$$

```
      USE QAND_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    I, J, MAXFCN, N, NOUT
      REAL       A(3), B(3), CNST, ERRABS, ERREST, ERRREL, F, RESULT
      EXTERNAL   F
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!
      N      = 3
      MAXFCN = 100000
!                                  Set error tolerances
      ERRABS = 0.0001
      ERRREL = 0.001
!
      DO 20  I=1, 6
         CNST = I/2.0
!                                  Set limits of integration
!                                  As CNST approaches infinity, the
!                                  answer approaches PI**1.5
         DO 10  J=1, 3
            A(J) = -CNST
            B(J) = CNST
   10  CONTINUE
         CALL QAND (F, N, A, B, RESULT, ERRABS, ERRREL, MAXFCN, ERREST)
         WRITE (NOUT,99999) CNST, RESULT, ERREST
   20 CONTINUE
99999 FORMAT (1X, 'For CNST = ', F4.1, ', result = ', F7.3, ' with ', &
              'error estimate ', 1PE10.3)
      END
!
      REAL FUNCTION F (N, X)
      INTEGER    N
      REAL       X(N)
      REAL       EXP
      INTRINSIC  EXP
      F = EXP(-(X(1)*X(1)+X(2)*X(2)+X(3)*X(3)))
      RETURN
      END
```

Output

```
For CNST =  0.5, result =   0.785 with error estimate  3.934E-06
For CNST =  1.0, result =   3.332 with error estimate  2.100E-03
For CNST =  1.5, result =   5.021 with error estimate  1.192E-05
For CNST =  2.0, result =   5.491 with error estimate  2.413E-04
For CNST =  2.5, result =   5.561 with error estimate  4.232E-03
```

```
 For CNST =  3.0, result =   5.568 with error estimate  2.580E-04
```

QMC

Integrates a function over a hyper-rectangle using a quasi-Monte Carlo method.

Required Arguments

FCN — User-supplied `FUNCTION` to be integrated. The form is `FCN(X)`, where

`X` – The independent variable. (Input)

`FCN` – The value of the integrand at `X`. (Output)

`FCN` must be declared `EXTERNAL` in the calling program.

A — Vector containing lower limits of integration. (Input)

B — Vector containing upper limits of integration. (Input)

RESULT — The value of

$$\int_{a_1}^{b_1} \dots \int_{a_n}^{b_n} f\left(x_1, \dots, x_n\right) dx_n \dots dx_1$$

is returned, where *n* is the dimension of `X`. If no value can be computed, then NaN is returned. (Output)

Optional Arguments

ERRABS — Absolute accuracy desired. (Input)
Default: 1.0e-2.

ERRREL — Relative accuracy desired. (Input)
Default: 1.0e-2.

ERREST — Estimate of the absolute value of the error. (Output)

MAXEVALS — Number of evaluations allowed. (Input)
Default: No limit.

BASE — The base of the Faure sequence. (Input)
Default: The smallest prime number greater than or equal to the number of dimensions (length of *a* and *b*).

SKIP — The number of points to be skipped at the beginning of the Faure sequence. (Input)
Default: $\lfloor \mathtt{base}^{m/2-1} \rfloor$, where $m = \lfloor \log B / \log \mathtt{base} \rfloor$ and B is the largest representable integer.

FORTRAN 90 Interface

Generic: CALL QMC (FCN, A, B, RESULT [, …])

Specific: The specific interface names are S_QMC and D_QMC.

Description

Integration of functions over hyper rectangle by direct methods, such as QAND, is practical only for fairly low dimensional hypercubes. This is because the amount of work required increases exponentially as the dimension increases.

An alternative to direct methods is QMC, in which the integral is evaluated as the value of the function averaged over a sequence of randomly chosen points. Under mild assumptions on the function, this method will converge like

$$1/\sqrt{k}$$

where k is the number of points at which the function is evaluated.

It is possible to improve on the performance of QMC by carefully choosing the points at which the function is to be evaluated. Randomly distributed points tend to be non-uniformly distributed. The alternative to a sequence of random points is a *low-discrepancy* sequence. A low-discrepancy sequence is one that is highly uniform.

This function is based on the low-discrepancy Faure sequence as computed by FAURE_NEXT, see the Fortran Stat Library, Chapter 18, *"Random Number Generation"*.

Example

This example evaluates the n-dimensional integral

$$\int_0^1 \dots \int_0^1 \sum_{i=1}^{n} \prod_{j=1}^{i} (-1)^i x_j dx_1 \dots dx_n = -\tfrac{1}{3}\left[1-\left(-\tfrac{1}{2}\right)^n\right]$$

with n=10.

```
      use qmc_int
      implicit none
      integer, parameter    :: ndim=10
      real(kind(1d0))       :: a(ndim)
      real(kind(1d0))       :: b(ndim)
```

```
         real(kind(1d0))      :: result
         integer              :: I
         external fcn

         a = 0.d0
         b = 1.d0

         call qmc(fcn, a, b, result)
         write (*,*) 'result = ', result
        end

          real(kind(1d0)) function fcn(x)
              implicit none
              real(kind(1d0)), dimension(:)  :: x
              integer  :: i, j
              real(kind(1d0)) :: prod, sum, sign

              sign = -1.d0
              sum = 0.d0
              do i=1, size(x)
                  prod = 1.d0
                  prod = product(x(1:i))
                  sum = sum + (sign * prod)
                  sign = -sign
              end do
              fcn = sum
          end function fcn
```

Output

```
           result = -0.3334789
```

GQRUL

Computes a Gauss, Gauss-Radau, or Gauss-Lobatto quadrature rule with various classical weight functions.

Required Arguments

N — Number of quadrature points. (Input)

QX — Array of length `N` containing quadrature points. (Output)

QW — Array of length `N` containing quadrature weights. (Output)

Optional Arguments

IWEIGH — Index of the weight function. (Input)
Default: `IWEIGH` = 1.

IWEIGH	wt(x)	Interval	Name
1	1	(−1,1)	Legendre
2	$1/\sqrt{1-x^2}$	(−1,1)	Chebyshev 1st kind
3	$\sqrt{1-x^2}$	(−1,1)	Chebyshev 2nd kind
4	e^{-x^2}	(−∞,∞)	Hermite
5	$(1-x)^{\alpha}(1+x)^{\beta}$	(−1,1)	Jacobi
6	$e^{-x}x^{\alpha}$	(0,∞)	Generalized Laguerre
7	$1/\cosh(x)$	(−∞,∞)	Hyperbolic Cosine

ALPHA — Parameter used in the weight function with some values of `IWEIGH`, otherwise it is ignored. (Input)
Default: `ALPHA` = 2.0.

BETAW — Parameter used in the weight function with some values of IWEIGH, otherwise it is ignored. (Input)
Default: BETAW = 2.0.

NFIX — Number of fixed quadrature points. (Input)
NFIX = 0, 1 or 2. For the usual Gauss quadrature rules, NFIX = 0.
Default: NFIX = 0.

QXFIX — Array of length NFIX (ignored if NFIX = 0) containing the preset quadrature point(s). (Input)

FORTRAN 90 Interface

Generic: CALL GQRUL (N, QX, QW [, …])

Specific: The specific interface names are S_GQRUL and D_GQRUL.

FORTRAN 77 Interface

Single: CALL GQRUL (N, IWEIGH, ALPHA, BETAW, NFIX, QXFIX, QX, QW)

Double: The double precision name is DGQRUL.

Description

The routine GQRUL produces the points and weights for the Gauss, Gauss-Radau, or Gauss-Lobatto quadrature formulas for some of the most popular weights. In fact, it is slightly more general than this suggests because the extra one or two points that may be specified do not have to lie at the endpoints of the interval. This routine is a modification of the subroutine GAUSSQUADRULE (Golub and Welsch 1969).

In the simple case when NFIX = 0, the routine returns points in x = QX and weights in w = QW so that

$$\int_a^b f(x)w(x)\,dx = \sum_{i=1}^{N} f(x_i)w_i$$

for all functions f that are polynomials of degree less than $2N$.

If NFIX = 1, then one of the above x_i equals the first component of QXFIX. Similarly, if NFIX = 2, then two of the components of x will equal the first two components of QXFIX. In general, the accuracy of the above quadrature formula degrades when NFIX increases. The quadrature rule will integrate all functions f that are polynomials of degree less than $2N$ − NFIX.

Comments

1. Workspace may be explicitly provided, if desired, by use of G2RUL/DG2RUL. The reference is

   CALL G2RUL (N, IWEIGH, ALPHA, BETAW, NFIX, QXFIX, QX, QW, WK)

   The additional argument is

   WK — Work array of length N.

2. If IWEIGH specifies the weight WT(X) and the interval (*a*, *b*), then approximately

$$\int_a^b F(X) * WT(X) dX = \sum_{I=1}^{N} F(QX(I)) * QW(I)$$

3. Gaussian quadrature is always the method of choice when the function F(X) behaves like a polynomial. Gaussian quadrature is also useful on infinite intervals (with appropriate weight functions), because other techniques often fail.

4. The weight function 1/cosh(*X*) behaves like a polynomial near zero and like $e^{|X|}$ far from zero.

Examples

Example 1

In this example, we obtain the classical Gauss-Legendre quadrature formula, which is accurate for polynomials of degree less than 2*N*, and apply this when *N* = 6 to the function x^8 on the interval [−1, 1]. This quadrature rule is accurate for polynomials of degree less than 12.

```
      USE GQRUL_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    N
      PARAMETER (N=6)
      INTEGER    I, NOUT
      REAL       ANSWER, QW(N), QX(N), SUM
!                                 Get output unit number
      CALL UMACH (2, NOUT)
!
!                                 Get points and weights from GQRUL
      CALL GQRUL (N, QX, QW)
!                                 Write results from GQRUL
      WRITE (NOUT,99998) (I,QX(I),I,QW(I),I=1,N)
99998 FORMAT (6(6X,'QX(',I1,') = ',F8.4,7X,'QW(',I1,') = ',F8.5,/))
!                                 Evaluate the integral from these
!                                 points and weights
      SUM = 0.0
      DO 10  I=1, N
         SUM = SUM + QX(I)**8*QW(I)
   10 CONTINUE
      ANSWER = SUM
```

```
      WRITE (NOUT,99999) ANSWER
99999 FORMAT (/, ' The quadrature result making use of these ', &
             'points and weights is ', 1PE10.4, '.')
      END
```

Output

```
QX(1) =  -0.9325       QW(1) =  0.17132
QX(2) =  -0.6612       QW(2) =  0.36076
QX(3) =  -0.2386       QW(3) =  0.46791
QX(4) =   0.2386       QW(4) =  0.46791
QX(5) =   0.6612       QW(5) =  0.36076
QX(6) =   0.9325       QW(6) =  0.17132

The quadrature result making use of these points and weights is 2.2222E-01.
```

Example 2

We modify Example 1 by requiring that both endpoints be included in the quadrature formulas and again apply the new formulas to the function x^8 on the interval $[-1, 1]$. This quadrature rule is accurate for polynomials of degree less than 10.

```
      USE GQRUL_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    N
      PARAMETER (N=6)
      INTEGER    I, IWEIGH, NFIX, NOUT
      REAL       ALPHA, ANSWER, BETAW, QW(N), QX(N), QXFIX(2), SUM
!                                 Get output unit number
      CALL UMACH (2, NOUT)
!
      IWEIGH   = 1
      ALPHA    = 0.0
      BETAW     = 0.0
      NFIX     = 2
      QXFIX(1) = -1.0
      QXFIX(2) = 1.0
!                                 Get points and weights from GQRUL
      CALL GQRUL (N, QX, QW, ALPHA=ALPHA, BETAW=BETAW, NFIX=NFIX,   &
                 QXFIX=QXFIX)
!                                 Write results from GQRUL
      WRITE (NOUT,99998) (I,QX(I),I,QW(I),I=1,N)
99998 FORMAT (6(6X,'QX(',I1,') = ',F8.4,7X,'QW(',I1,') = ',F8.5,/))
!                                 Evaluate the integral from these
!                                 points and weights
      SUM = 0.0
      DO 10  I=1, N
         SUM = SUM + QX(I)**8*QW(I)
   10 CONTINUE
      ANSWER = SUM
      WRITE (NOUT,99999) ANSWER
99999 FORMAT (/, ' The quadrature result making use of these ', &
            'points and weights is ', 1PE10.4, '.')
      END
```

Output

```
QX(1) =  -1.0000       QW(1) =  0.06667
QX(2) =  -0.7651       QW(2) =  0.37847
```

```
QX(3) =  -0.2852       QW(3) =  0.55486
QX(4) =   0.2852       QW(4) =  0.55486
QX(5) =   0.7651       QW(5) =  0.37847
QX(6) =   1.0000       QW(6) =  0.06667

The quadrature result making use of these points and weights is 2.2222E-01.
```

GQRCF

Computes a Gauss, Gauss-Radau or Gauss-Lobatto quadrature rule given the recurrence coefficients for the monic polynomials orthogonal with respect to the weight function.

Required Arguments

N — Number of quadrature points. (Input)

B — Array of length `N` containing the recurrence coefficients. (Input)
See Comments for definitions.

C — Array of length `N` containing the recurrence coefficients. (Input)
See Comments for definitions.

QX — Array of length `N` containing quadrature points. (Output)

QW — Array of length `N` containing quadrature weights. (Output)

Optional Arguments

NFIX — Number of fixed quadrature points. (Input)
`NFIX` = 0, 1 or 2. For the usual Gauss quadrature rules `NFIX` = 0.
Default: `NFIX` = 0.

QXFIX — Array of length `NFIX` (ignored if `NFIX` = 0) containing the preset quadrature point(s). (Input)

FORTRAN 90 Interface

Generic: `CALL GQRCF (N, B, C, QX, QW [, …])`

Specific: The specific interface names are `S_GQRCF` and `D_GQRCF`.

FORTRAN 77 Interface

Single: `CALL GQRCF (N, B, C, NFIX, QXFIX, QX, QW)`

Double: The double precision name is `DGQRCF`.

Description

The routine GQRCF produces the points and weights for the Gauss, Gauss-Radau, or Gauss-Lobatto quadrature formulas given the three-term recurrence relation for the orthogonal polynomials. In particular, it is assumed that the orthogonal polynomials are monic, and hence, the three-term recursion may be written as

$$p_i(x) = (x - b_i)p_{i-1}(x) - c_i p_{i-2}(x) \text{ for } i = 1, \ldots, N$$

where $p_0 = 1$ and $p_{-1} = 0$. It is obvious from this representation that the degree of p_i is i and that p_i is monic. In order for the recurrence to give rise to a sequence of orthogonal polynomials (with respect to a nonnegative measure), it is necessary and sufficient that $c_i > 0$. This routine is a modification of the subroutine GAUSSQUADRULE (Golub and Welsch 1969). In the simple case when NFIX = 0, the routine returns points in x = QX and weights in w = QW so that

$$\int_a^b f(x)w(x)dx = \sum_{i=1}^{N} f(x_i)w_i$$

for all functions f that are polynomials of degree less than $2N$. Here, w is any weight function for which the above recurrence produces the orthogonal polynomials p_i on the interval $[a, b]$ and w is normalized by

$$\int_a^b w(x)dx = c_1$$

If NFIX = 1, then one of the above x_i equals the first component of QXFIX. Similarly, if NFIX = 2, then two of the components of x will equal the first two components of QXFIX. In general, the accuracy of the above quadrature formula degrades when NFIX increases. The quadrature rule will integrate all functions f that are polynomials of degree less than $2N$ − NFIX.

Comments

1. Workspace may be explicitly provided, if desired, by use of G2RCF/DG2RCF. The reference is:

   CALL G2RCF (N, B, C, NFIX, QXFIX, QX, QW, WK)

   The additional argument is:

   WK — Work array of length N.

2. Informational error

Type	Code	Description
4	1	No convergence in 100 iterations.

3. The recurrence coefficients B(I) and C(I) define the monic polynomials via the relation P(I) = (X − B(I + 1)) * P(I − 1) − C(I + 1) * P(I − 2). C(1) contains the zero-th moment

$$\int WT(X)\,dX$$

of the weight function. Each element of C must be greater than zero.

4. If *WT*(*X*) is the weight specified by the coefficients and the interval is (*a*, *b*), then approximately

$$\int_a^b F(X) * WT(X)\,dX = \sum_{I=1}^{N} F(QX(I)) * QW(I)$$

5. Gaussian quadrature is always the method of choice when the function F(X) behaves like a polynomial. Gaussian quadrature is also useful on infinite intervals (with appropriate weight functions) because other techniques often fail.

Example

We compute the Gauss quadrature rule (with $N = 6$) for the Chebyshev weight, $(1 + x^2)^{(-1/2)}$, from the recurrence coefficients. These coefficients are obtained by a call to the IMSL routine RECCF.

```
      USE GQRCF_INT
      USE UMACH_INT
      USE RECCF_INT

      IMPLICIT   NONE
      INTEGER    N
      PARAMETER (N=6)
      INTEGER    I, NFIX, NOUT
      REAL       B(N), C(N), QW(N), QX(N), QXFIX(2)
!                                 Get output unit number
      CALL UMACH (2, NOUT)
!                                 Recursion coefficients will come from
!                                 routine RECCF.
!                                 The call to RECCF finds recurrence
!                                 coefficients for Chebyshev
!                                 polynomials of the 1st kind.
      CALL RECCF (N, B, C)
!
!                                  The call to GQRCF will compute the
!                                 quadrature rule from the recurrence
!                                 coefficients determined above.
      CALL GQRCF (N, B, C, QX, QW)
      WRITE (NOUT,99999) (I,QX(I),I,QW(I),I=1,N)
99999 FORMAT (6(6X,'QX(',I1,') = ',F8.4,7X,'QW(',I1,') = ',F8.5,/))
!
      END
```

Output

```
QX(1) =  -0.9325        QW(1) =  0.17132
QX(2) =  -0.6612        QW(2) =  0.36076
QX(3) =  -0.2386        QW(3) =  0.46791
QX(4) =   0.2386        QW(4) =  0.46791
QX(5) =   0.6612        QW(5) =  0.36076
QX(6) =   0.9325        QW(6) =  0.17132
```

RECCF

Computes recurrence coefficients for various monic polynomials.

Required Arguments

N — Number of recurrence coefficients. (Input)

B — Array of length `N` containing recurrence coefficients. (Output)

C — Array of length `N` containing recurrence coefficients. (Output)

Optional Arguments

IWEIGH — Index of the weight function. (Input)
Default: `IWEIGH` = 1.

IWEIGH	wt(x)	Interval	Name
1	1	(−1,1)	Legendre
2	$1/\sqrt{1-x^2}$	(−1,1)	Chebyshev 1st kind
3	$\sqrt{1-x^2}$	(−1,1)	Chebyshev 2nd kind
4	e^{-x^2}	(−∞,∞)	Hermite
5	$(1-x)^{\alpha}(1+x)^{\beta}$	(−1,1)	Jacobi
6	$e^{-x}x^{\alpha}$	(0,∞)	Generalized Laguerre
7	$1/\cosh(x)$	(−∞,∞)	Hyperbolic Cosine

ALPHA — Parameter used in the weight function with some values of `IWEIGH`, otherwise it is ignored. (Input)
Default: `ALPHA`=1.0.

BETAW — Parameter used in the weight function with some values of `IWEIGH`, otherwise it is ignored. (Input)
Default: `BETAW`=1.0.

FORTRAN 90 Interface

Generic: `CALL RECCF (N, B, C [, …])`

Specific: The specific interface names are `S_RECCF` and `D_RECCF`.

FORTRAN 77 Interface

Single: `CALL RECCF (N, IWEIGH, ALPHA, BETAW, B, C)`

Double: The double precision name is `DRECCF`.

Description

The routine `RECCF` produces the recurrence coefficients for the orthogonal polynomials for some of the most important weights. It is assumed that the orthogonal polynomials are monic; hence, the three-term recursion may be written as

$$p_i(x) = \left(x - b_i\right) p_{i-1}(x) - c_i p_{i-2}(x) \text{ for } i = 1, \ldots, N$$

where $p_0 = 1$ and $p_{-1} = 0$. It is obvious from this representation that the degree of p_i is i and that p_i is monic. In order for the recurrence to give rise to a sequence of orthogonal polynomials (with respect to a nonnegative measure), it is necessary and sufficient that $c_i > 0$.

Comment

The recurrence coefficients `B(I)` and `C(I)` define the monic polynomials via the relation `P(I) = (X − B(I + 1)) * P(I − 1) − C(I + 1) * P(I − 2)`. The zero-th moment

$$\left(\int WT(X)dX\right)$$

of the weight function is returned in `C(1)`.

Example

Here, we obtain the well-known recurrence relations for the first six *monic* Legendre polynomials, Chebyshev polynomials of the first kind, and Laguerre polynomials.

```
      USE RECCF_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    N
      PARAMETER (N=6)
      INTEGER    I, IWEIGH, NOUT
      REAL       ALPHA, B(N), C(N), BETAW
!                                 Get output unit number
      CALL UMACH (2, NOUT)
!
      CALL RECCF (N, B, C)
      WRITE (NOUT,99996)
      WRITE (NOUT,99999) (I,B(I),I,C(I),I=1,N)
!
      IWEIGH = 2
      CALL RECCF (N, B, C, IWEIGH=IWEIGH)
      WRITE (NOUT,99997)
      WRITE (NOUT,99999) (I,B(I),I,C(I),I=1,N)
!
      IWEIGH = 6
      ALPHA = 0.0
      BETAW  = 0.0
      CALL RECCF (N, B, C, IWEIGH=IWEIGH, ALPHA=ALPHA)
      WRITE (NOUT,99998)
      WRITE (NOUT,99999) (I,B(I),I,C(I),I=1,N)
!
99996 FORMAT (1X, 'Legendre')
99997 FORMAT (/, 1X, 'Chebyshev, first kind')
99998 FORMAT (/, 1X, 'Laguerre')
99999 FORMAT (6(6X,'B(',I1,') = ',F8.4,7X,'C(',I1,') = ',F8.5,/))
      END
```

Output

```
Legendre
B(1) =   0.0000       C(1) =  2.00000
B(2) =   0.0000       C(2) =  0.33333
B(3) =   0.0000       C(3) =  0.26667
B(4) =   0.0000       C(4) =  0.25714
B(5) =   0.0000       C(5) =  0.25397
B(6) =   0.0000       C(6) =  0.25253

Chebyshev, first kind
B(1) =   0.0000       C(1) =  3.14159
B(2) =   0.0000       C(2) =  0.50000
B(3) =   0.0000       C(3) =  0.25000
B(4) =   0.0000       C(4) =  0.25000
B(5) =   0.0000       C(5) =  0.25000
B(6) =   0.0000       C(6) =  0.25000

Laguerre
B(1) =   1.0000       C(1) =  1.00000
B(2) =   3.0000       C(2) =  1.00000
B(3) =   5.0000       C(3) =  4.00000
B(4) =   7.0000       C(4) =  9.00000
B(5) =   9.0000       C(5) = 16.00000
```

```
  B(6) =  11.0000        C(6) = 25.00000
```

RECQR

Computes recurrence coefficients for monic polynomials given a quadrature rule.

Required Arguments

QX — Array of length `N` containing the quadrature points. (Input)

QW — Array of length `N` containing the quadrature weights. (Input)

B — Array of length `NTERM` containing recurrence coefficients. (Output)

C — Array of length `NTERM` containing recurrence coefficients. (Output)

Optional Arguments

N — Number of quadrature points. (Input)
Default: `N` = size (`QX`,1).

NTERM — Number of recurrence coefficients. (Input)
`NTERM` must be less than or equal to `N`.
Default: `NTERM` = size (`B`,1).

FORTRAN 90 Interface

Generic: `CALL RECQR (QX, QW, B, C [, …])`

Specific: The specific interface names are `S_RECQR` and `D_RECQR`.

FORTRAN 77 Interface

Single: `CALL RECQR (N, QX, QW, NTERM, B, C)`

Double: The double precision name is `DRECQR`.

Description

The routine `RECQR` produces the recurrence coefficients for the orthogonal polynomials given the points and weights for the Gauss quadrature formula. It is assumed that the orthogonal polynomials are monic; hence the three-term recursion may be written

$$p_i(x) = (x - b_i)p_{i-1}(x) - c_i p_{i-2}(x) \text{ for } i = 1, \dots, N$$

where $p_0 = 1$ and $p_{-1} = 0$. It is obvious from this representation that the degree of p_i is i and that p_i is monic. In order for the recurrence to give rise to a sequence of orthogonal polynomials (with respect to a nonnegative measure), it is necessary and sufficient that $c_i > 0$.

This routine is an inverse routine to `GQRCF`. Given the recurrence coefficients, the routine `GQRCF` produces the corresponding Gauss quadrature formula, whereas the routine `RECQR` produces the recurrence coefficients given the quadrature formula.

Comments

1. Workspace may be explicitly provided, if desired, by use of `R2CQR/DR2CQR`. The reference is:

   `CALL R2CQR (N, QX, QW, NTERM, B, C, WK)`

   The additional argument is:

   WK — Work array of length 2 * N.

2. The recurrence coefficients `B(I)` and `C(I)` define the monic polynomials via the relation `P(I)` = (`X` − `B(I` + 1)) * `P(I` − 1) − `C(I` + 1) * `P(I` − 2). The zero-th moment

$$\left(\int WT(X)\,dX\right)$$

   of the weight function is returned in C(1).

Example

To illustrate the use of `RECQR`, we will input a simple choice of recurrence coefficients, call `GQRCF` for the quadrature formula, put this information into `RECQR`, and recover the recurrence coefficients.

```
      USE RECQR_INT
      USE UMACH_INT
      USE GQRCF_INT

      IMPLICIT   NONE
      INTEGER    N
      PARAMETER (N=5)
      INTEGER    I, J, NFIX, NOUT, NTERM
      REAL       B(N), C(N), FLOAT, QW(N), QX(N), QXFIX(2)
      INTRINSIC  FLOAT
!                                 Get output unit number
      CALL UMACH (2, NOUT)
      NFIX = 0
!                                 Set arrays B and C of recurrence
!                                 coefficients
      DO 10  J=1, N
```

```
         B(J) = FLOAT(J)
         C(J) = FLOAT(J)/2.0
   10 CONTINUE
      WRITE (NOUT,99995)
99995 FORMAT (1X, 'Original recurrence coefficients')
      WRITE (NOUT,99996) (I,B(I),I,C(I),I=1,N)
99996 FORMAT (5(6X,'B(',I1,') = ',F8.4,7X,'C(',I1,') = ',F8.5,/))
!
!                                 The call to GQRCF will compute the
!                                 quadrature rule from the recurrence
!                                 coefficients given above.
!
      CALL GQRCF (N, B, C, QX, QW)
      WRITE (NOUT,99997)
99997 FORMAT (/, 1X, 'Quadrature rule from the recurrence coefficients' &
            )
      WRITE (NOUT,99998) (I,QX(I),I,QW(I),I=1,N)
99998 FORMAT (5(6X,'QX(',I1,') = ',F8.4,7X,'QW(',I1,') = ',F8.5,/))
!
!                                 Call RECQR to recover the original
!                                 recurrence coefficients
      NTERM = N
      CALL RECQR (QX, QW, B, C)
      WRITE (NOUT,99999)
99999 FORMAT (/, 1X, 'Recurrence coefficients determined by RECQR')
      WRITE (NOUT,99996) (I,B(I),I,C(I),I=1,N)
!
      END
```

Output

```
Original recurrence coefficients
B(1) =   1.0000      C(1) =  0.50000
B(2) =   2.0000      C(2) =  1.00000
B(3) =   3.0000      C(3) =  1.50000
B(4) =   4.0000      C(4) =  2.00000
B(5) =   5.0000      C(5) =  2.50000

Quadrature rule from the recurrence coefficients
QX(1) =   0.1525       QW(1) =  0.25328
QX(2) =   1.4237       QW(2) =  0.17172
QX(3) =   2.7211       QW(3) =  0.06698
QX(4) =   4.2856       QW(4) =  0.00790
QX(5) =   6.4171       QW(5) =  0.00012

Recurrence coefficients determined by RECQR
B(1) =   1.0000      C(1) =  0.50000
B(2) =   2.0000      C(2) =  1.00000
B(3) =   3.0000      C(3) =  1.50000
B(4) =   4.0000      C(4) =  2.00000
B(5) =   5.0000      C(5) =  2.50000
```

FQRUL

Computes a Fejér quadrature rule with various classical weight functions.

Required Arguments

N — Number of quadrature points. (Input)

A — Lower limit of integration. (Input)

B — Upper limit of integration. (Input)
B must be greater than A.

QX — Array of length N containing quadrature points. (Output)

QW — Array of length N containing quadrature weights. (Output)

Optional Arguments

IWEIGH — Index of the weight function. (Input)
Default: IWEIGH = 1.

IWEIGH	WT(X)
1	1
2	1/(X − ALPHA)
3	$(B - X)^{\alpha} (X - A)^{\beta}$
4	$(B - X)^{\alpha} (X - A)^{\beta} \log(X - A)$
5	$(B - X)^{\alpha} (X - A)^{\beta} \log(B - X)$

ALPHA — Parameter used in the weight function (except if IWEIGH = 1, it is ignored). (Input)
If IWEIGH = 2, then it must satisfy A.LT.ALPHA.LT.B. If IWEIGH = 3, 4, or 5, then ALPHA must be greater than −1.
Default: ALPHA= 0.0.

BETAW — Parameter used in the weight function (ignored if IWEIGH = 1 or 2). (Input)
BETAW must be greater than −1.0.
Default: BETAW= 0.0.

FORTRAN 90 Interface

Generic: `CALL FQRUL (N, A, B, QX, QW [, …])`

Specific: The specific interface names are `S_FQRUL` and `D_FQRUL`.

FORTRAN 77 Interface

Single: `CALL FQRUL (N, A, B, IWEIGH, ALPHA, BETAW, QX, QW)`

Double: The double precision name is `DFQRUL`.

Description

The routine `FQRUL` produces the weights and points for the Fejér quadrature rule. Since this computation is based on a quarter-wave cosine transform, the computations are most efficient when *N*, the number of points, is a product of small primes. These quadrature formulas may be an intermediate step in a more complicated situation, see for instance Gautschi and Milovanofic (1985).

The Fejér quadrature rules are based on polynomial interpolation. First, choose classical abscissas (in our case, the Gauss points for the Chebyshev weight function $(1 - x^2)^{-1/2}$), then derive the quadrature rule for a different weight. In order to keep the presentation simple, we will describe the case where the interval of integration is $[-1, 1]$ even though `FQRUL` allows rescaling to an arbitrary interval $[a, b]$.

We are looking for quadrature rules of the form

$$Q(f) := \sum_{j=1}^{N} w_j f(x_j)$$

where the

$$\{x_j\}_{j=1}^{N}$$

are the zeros of the *N*-th Chebyshev polynomial (of the first kind) $T_N(x) = \cos(N \arccos x)$. The weights in the quadrature rule *Q* are chosen so that, for all polynomials *p* of degree less than *N*,

$$Q(p) = \sum_{j=1}^{N} w_j p(x_j) = \int_{-1}^{1} p(x) w(x) dx$$

for some weight function *w*. In `FQRUL`, the user has the option of choosing *w* from five families of functions with various algebraic and logarithmic endpoint singularities.

These Fejér rules are important because they can be computed using specialized FFT quarter-wave transform routines. This means that rules with a large number of abscissas may be computed efficiently. If we insert T_l for *p* in the above formula, we obtain

$$Q(T_l) = \sum_{j=1}^{N} w_j T_l(x_j) = \int_{-1}^{1} T_l(x) w(x) dx$$

for l = 0, …, N − 1. This is a system of linear equations for the unknown weights w_j that can be simplified by noting that

$$x_j = \cos\frac{(2j-1)\pi}{2N} \qquad j = 1, \ldots, N$$

and hence,

$$\begin{aligned}\int_{-1}^{1} T_l(x) w(x) dx &= \sum_{j=1}^{N} w_j T_l(x_j) \\ &= \sum_{j=1}^{N} w_j \cos\frac{l(2j-1)\pi}{2N}\end{aligned}$$

The last expression is the cosine quarter-wave forward transform for the sequence

$$\{w_j\}_{j=1}^{N}$$

that is implemented in *Chapter 6, "Transforms"* under the name QCOSF. More importantly, QCOSF has an inverse QCOSB. It follows that if the integrals on the left in the last expression can be computed, then the Fejér rule can be derived efficiently for highly composite integers *N* utilizing QCOSB. For more information on this topic, consult Davis and Rabinowitz (1984, pages 84−86) and Gautschi (1968, page 259).

Comments

1. Workspace may be explicitly provided, if desired, by use of F2RUL/DF2RUL. The reference is:

   CALL F2RUL (N, A, B, IWEIGH, ALPHA, BETAW, QX, QW, WK)

   The additional argument is:

   WK — Work array of length 3 * N + 15.

2. If IWEIGH specifies the weight WT(X) and the interval (A, B), then approximately

$$\int_A^B F(X) * WT(X)dX = \sum_{I=1}^{N} F(QX(I)) * QW(I)$$

3. The routine `FQRUL` uses an *fft*, so it is most efficient when `N` is the product of small primes.

Example

Here, we obtain the Fejér quadrature rules using 10, 100, and 200 points. With these rules, we get successively better approximations to the integral

$$\int_0^1 x\sin\left(41\pi x^2\right)dx = \frac{1}{41\pi}$$

```
      USE FQRUL_INT
      USE UMACH_INT
      USE CONST_INT

      IMPLICIT   NONE
      INTEGER    NMAX
      PARAMETER (NMAX=200)
      INTEGER    I, K, N, NOUT
      REAL       A, ANSWER, B, F, QW(NMAX), &
                QX(NMAX), SIN, SUM, X, PI, ERROR
      INTRINSIC  SIN, ABS
!
      F(X) = X*SIN(41.0*PI*X**2)
!                                 Get output unit number
      CALL UMACH (2, NOUT)
!
      PI = CONST('PI')
      DO 20  K=1, 3
         IF (K .EQ. 1) N = 10
         IF (K .EQ. 2) N = 100
         IF (K .EQ. 3) N = 200
         A      = 0.0
         B      = 1.0

!                                 Get points and weights from FQRUL
         CALL FQRUL (N, A, B, QX, QW)
!                                 Evaluate the integral from these
!                                 points and weights
         SUM = 0.0
         DO 10  I=1, N
            SUM = SUM + F(QX(I))*QW(I)
   10  CONTINUE
         ANSWER = SUM
         ERROR = ABS(ANSWER - 1.0/(41.0*PI))
         WRITE (NOUT,99999) N, ANSWER, ERROR
   20 CONTINUE
!
99999 FORMAT (/, 1X, 'When N = ', I3, ', the quadrature result making ' &
            , 'use of these points ', /, ' and weights is ', 1PE11.4, &
            ', with error ', 1PE9.2, '.')
      END
```

Output

```
When N =  10, the quadrature result making use of these points and weights is -1.6523E-01,
with error  1.73E-01.

When N = 100, the quadrature result making use of these points and weights is  7.7637E-03,
with error  2.79E-08.

When N = 200, the quadrature result making use of these points and weights is  7.7636E-03,
with error  1.40E-08.
```

DERIV

This function computes the first, second or third derivative of a user-supplied function.

Function Return Value

DERIV — Estimate of the first (KORDER = 1), second (KORDER = 2) or third (KORDER = 3) derivative of FCN at X. (Output)

Required Arguments

FCN — User-supplied FUNCTION whose derivative at X will be computed. The form is FCN(X), where

X – Independent variable. (Input)

FCN – The function value. (Output)

FCN must be declared EXTERNAL in the calling program.

X — Point at which the derivative is to be evaluated. (Input)

Optional Arguments

KORDER — Order of the derivative desired (1, 2 or 3). (Input)
Default: KORDER = 1.

BGSTEP — Beginning value used to compute the size of the interval used in computing the derivative. (Input)
The interval used is the closed interval (X − 4 * BGSTEP, X + 4 * BGSTEP). BGSTEP must be positive.
Default: BGSTEP = .01.

TOL — Relative error desired in the derivative estimate. (Input)
Default: TOL = 1.e-2 for single precision and 1.d-4 for double precision.

FORTRAN 90 Interface

Generic: DERIV (FCN, X [, …])

Specific: The specific interface names are S_DERIV and D_DERIV.

FORTRAN 77 Interface

Single: `DERIV (FCN, KORDER, X, BGSTEP, TOL)`

Double: The double precision function name is `DDERIV`.

Description

`DERIV` produces an estimate to the first, second, or third derivative of a function. The estimate originates from first computing a spline interpolant to the input function using values within the interval (`X` – 4.0 * `BGSTEP`, `X` + 4.0 * `BGSTEP`), then differentiating the spline at `X`.

Comments

Informational errors

Type	Code	Description
3	2	Roundoff error became dominant before estimates converged. Increase precision and/or increase `BGSTEP`.
4	1	Unable to achieve desired tolerance in derivative estimation. Increase precision, increase `TOL` and/or change `BGSTEP`. If this error continues, the function may not have a derivative at `X`.

2. Convergence is assumed when

$$\frac{2}{3}|D2 - D1| < TOL$$

for two successive derivative estimates `D1` and `D2`.

3. The initial step size, `BGSTEP`, must be chosen small enough that `FCN` is defined and reasonably smooth in the interval (`X` – 4 * `BGSTEP`, `X` + 4 * `BGSTEP`), yet large enough to avoid roundoff problems.

Examples

Example 1

In this example, we obtain the approximate first derivative of the function

$$f(x) = -2\sin(3x/2)$$

at the point $x = 2$.

```
      USE DERIV_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    KORDER, NCOUNT, NOUT
      REAL       BGSTEP, DERV, TOL, X
      EXTERNAL   FCN
!                                 Get output unit number
      CALL UMACH (2, NOUT)
!
      X      = 2.0
      BGSTEP = 0.2
      NCOUNT = 1
      DERV   = DERIV(FCN,X, BGSTEP=BGSTEP)
      WRITE (NOUT,99999) DERV
99999 FORMAT (/, 1X, 'First derivative of FCN is ', 1PE10.3)
      END
!
      REAL FUNCTION FCN (X)
      REAL       X
      REAL       SIN
      INTRINSIC  SIN
      FCN = -2.0*SIN(1.5*X)
      RETURN
      END
```

Output

```
 First derivative of FCN is  2.970E+00
```

Example 2

In this example, we attempt to approximate in single precision the third derivative of the function

$$f(x) = 2x^4 + 3x$$

at the point $x = 0.75$. Although the function is well-behaved near $x = 0.75$, finding derivatives is often computationally difficult on 32-bit machines. The difficulty is overcome in double precision.

```
      USE IMSL_LIBRARIES

      IMPLICIT   NONE
      INTEGER    KORDER, NOUT
      REAL       BGSTEP, DERV, X, TOL
      DOUBLE PRECISION DBGSTE, DDERV, DFCN, DTOL, DX
      EXTERNAL   DFCN, FCN
!                                 Get output unit number
      CALL UMACH (2, NOUT)
!                                 Turn off stopping due to error
!                                 condition
      CALL ERSET (0, -1, 0)
!
      X      = 0.75
      BGSTEP = 0.1
      KORDER = 3
!                                 In single precision, on a 32-bit
!                                 machine, the following attempt
!                                 produces an error message
      DERV = DERIV(FCN, X, KORDER, BGSTEP,TOL)
!                                 In double precision, we get good
!                                 results
```

```
      DX     = 0.75D0
      DBGSTE = 0.1D0
      DTOL   = 0.01D0
      KORDER = 3
      DDERV  = DERIV(DFCN, DX,KORDER, DBGSTE, DTOL)
      WRITE (NOUT,99999) DDERV
99999 FORMAT (/, 1X, 'The third derivative of DFCN is ', 1PD10.4)
      END
!
      REAL FUNCTION FCN (X)
      REAL       X
      FCN = 2.0*X**4 + 3.0*X
      RETURN
      END
!
      DOUBLE PRECISION FUNCTION DFCN (X)
      DOUBLE PRECISION X
      DFCN = 2.0D0*X**4 + 3.0D0*X
      RETURN
      END
```

Output

```
*** FATAL    ERROR 1 from DERIV.  Unable to achieve desired tolerance.
***          Increase precision, increase TOL = 1.000000E-02 and/or change
***          BGSTEP = 1.000000E-01.  If this error continues the function
***          may not have a derivative at X = 7.500000E-01

The third derivative of DFCN is 3.6000D+01
```

Differential Equations

Routines

Usage Notes

A *differential equation* is an equation involving one or more dependent variables (called y_i or u_i), their derivatives, and one or more independent variables (called t, x, and y). Users will typically need to relabel their own model variables so that they correspond to the variables used in the solvers described here. A differential equation with one independent variable is called an *ordinary differential equation* (ODE). A system of equations involving derivatives in one independent variable and other dependent variables is called a *differential-algebraic system*. A differential equation with more than one independent variable is called a *partial differential equation* (PDE).

The *order* of a differential equation is the highest order of any of the derivatives in the equation. Some of the routines in this chapter require the user to reduce higher-order problems to systems of first-order differential equations.

Ordinary Differential Equations

It is convenient to use the vector notation below. We denote the number of equations as the value N. The problem statement is abbreviated by writing it as a *system* of first-order ODEs

$$y(t) = \left[y_1(t), \ldots ,y_N(t) \right]^T, \quad f(t,y) = \left[f_1(t,y), \ldots ,f_N(t,y) \right]^T$$

The problem becomes

$$y' = \frac{dy(t)}{dt} = f(t,y)$$

with initial values $y(t_0)$. Values of $y(t)$ for $t > t_0$ or $t < t_0$ are required. The routines IVPRK, IVMRK, and IVPAG, solve the IVP for systems of ODEs of the form $y' = f(t, y)$ with $y(t = t_0)$ specified. Here, f is a user supplied function that must be evaluated at any set of values $(t, y_1, \ldots, y_N)$; $i = 1, \ldots, N$. The routines IVPAG, and DAESL, will also solve implicit systems of the form $Ay' = f(t, y)$ where A is a user supplied matrix. For IVPAG, the matrix A must be nonsingular.

The system $y' = f(t, y)$ is said to be *stiff* if some of the eigenvalues of the Jacobian matrix $\{\partial f_i/\partial y_j\}$ have large, negative real parts. This is often the case for differential equations representing the behavior of physical systems such as chemical reactions proceeding to equilibrium where subspecies effectively complete their reaction in different epochs. An alternate model concerns discharging capacitors such that different parts of the system have widely varying decay rates (or *time constants*). This definition of stiffness, based on the eigenvalues of the Jacobian matrix, is not satisfactory. Users typically identify stiff systems by the fact that numerical differential equation solvers such as IVPRK, are inefficient, or else they fail. The most common inefficiency is that a large number of evaluations of the functions f_i are required. In such cases, use routine IVPAG, or DAESL. For more about stiff systems, see Gear (1971, Chapter 11) or Shampine and Gear (1979).

In the *boundary value problem* (BVP) for ODEs, constraints on the dependent variables are given at the endpoints of the interval of interest, [*a*, *b*]. The routines BVPFD and BVPMS solve the BVP for systems of the form $y'(t) = f(t, y)$, subject to the conditions

$$h_i(y_1(a), \ldots, y_N(a), y_1(b), \ldots, y_N(b)) = 0 \quad i = 1, \ldots, N$$

Here, f and $h = [h_1, \ldots, h_N]^T$ are user-supplied functions.

IVOAM solves systems of ordinary differential equations of order one, order two, or mixed order one and two.

Differential-Algebraic Equations

Frequently, it is not possible or not convenient to express the model of a dynamical system as a set of ODEs. Rather, an implicit equation is available in the form

$$g_i(t, y, \ldots, y_N, y'_1, \ldots, y'_N) = 0 \quad i = 1, \ldots, N$$

The g_i are user-supplied functions. The system is abbreviated as

$$g(t, y, y') = \left[g_1(t, y, y'), \ldots, g_N(t, y, y') \right]^T = 0$$

With initial value $y(t_0)$. Any system of ODEs can be trivially written as a differential-algebraic system by defining

$$g(t, y, y') = f(t, y) - y'$$

The routine DAESL solves differential-algebraic systems of index 1 or index 0. For a definition of *index* of a differential-algebraic system, see (Brenan et al. 1989). Also, see Gear and Petzold (1984) for an outline of the computing methods used.

Partial Differential Equations

The routine MMOLCH solves the IVP problem for systems of the form

$$\frac{\delta u_i}{\delta t} = f_i\left(x, t, u_1, \ldots, u_N, \frac{\delta u_1}{\delta x}, \ldots, \frac{\delta u_N}{\delta x}, \frac{\delta^2 u_1}{\delta x^2}, \ldots, \frac{\delta^2 u_N}{\delta x^2}\right)$$

subject to the boundary conditions

$$\begin{aligned} \alpha_1^{(i)} u_i(a) + \beta_1^{(i)} \frac{\partial u_i}{\partial x}(a) &= \gamma_1^{(i)}(t) \\ \alpha_2^{(i)} u_i(b) + \beta_2^{(i)} \frac{\partial u_i}{\partial x}(b) &= \gamma_2^{(i)}(t) \end{aligned}$$

and subject to the initial conditions

$$u_{\boldsymbol{i}}(x, t = t_0) = g_{\boldsymbol{i}}(x)$$

for $i = 1, \ldots, N$. Here, $f_{\boldsymbol{i}}$, $g_{\boldsymbol{i}}$, $\alpha_j^{(i)}$, $\beta_j^{(i)}$ and $\gamma_j^{(i)}(t)$ are user-supplied, $j = 1, 2$.

The routines FPS2H and FPS3H solve Laplace's, Poisson's, or Helmholtz's equation in two or three dimensions. FPS2H uses a fast Poisson method to solve a PDE of the form

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + cu = f(x,y)$$

over a rectangle, subject to boundary conditions on each of the four sides. The scalar constant *c* and the function *f* are user specified. FPS3H solves the three-dimensional analogue of this problem.

Summary

The following table summarizes the types of problems handled by the routines in this chapter. With the exception of FPS2H and FPS3H, the routines can handle more than one differential equation.

Problem	Consideration	Routine
$Ay' = f(t, y)$ $y(t_0) = y_0$	*A* is a general, symmetric positive definite, band or symmetric positive definite band matrix.	IVPAG
	Stiff or expensive to evaluate $f(t, y)$, banded Jacobian or finely spaced output needed.	IVPAG
$y' = f(t, y)$, $y(t_0) = y_0$	High accuracy needed and not stiff. (Uses Adams methods)	IVPAG
	Moderate accuracy needed and not stiff.	IVPRK
$y' = f(t, y)$ $h(y(a), y(b)) = 0$	BVP solver using finite differences	BVPFD
	BVP solver using multiple shooting	BVPMS
$g(t, y, y') = 0$ $y(t_0), y'(t_0)$ given	Stiff, differential-algebraic solver for systems of index 1 or 0. **Note:** DAESL uses the user-supplied $y'(t_0)$ only as an initial guess to help it find the correct initial $y'(t_0)$ to get started.	DAESL

$u_t = f(x, t, u, u_x, u_{xx})$ $\alpha_1 u(a) + \beta_1 u_x(a) = \gamma_1(t)$ $\alpha_2 u(b) + \beta_2 u_x(b) = \gamma_2(t)$	Method of lines using cubic Hermites and ODEs.	`MMOLCH`
$u_{xx} + u_{yy} + cu = f(x, y)$ on a rectangle, given u or u_n on each edge.	Fast Poisson solver	`FPS2H`
$u_{xx} + u_{yy} + u_{zz} + cu = f(x, y, z)$ on a box, given u or u_n on each face.	Fast Poisson solver	`FPS3H`
$-(pu')' + qu = \lambda ru,$ $\alpha_1 u(a) - \alpha_2(pu'(a))$ $= \lambda(\alpha'_1 u(a) - \alpha'_2(pu'(a)))$ $\beta_1 u(b) + \beta_2(pu'(b)) = 0$	Sturm-Liouville problems	`SLEIG`

IVPRK

Solves an initial-value problem for ordinary differential equations using the Runge-Kutta-Verner fifth-order and sixth-order method.

Required Arguments

IDO — Flag indicating the state of the computation. (Input/Output)

IDO	State
1	Initial entry
2	Normal re-entry
3	Final call to release workspace
4	Return because of interrupt 1
5	Return because of interrupt 2 with step accepted
6	Return because of interrupt 2 with step rejected

Normally, the initial call is made with IDO = 1. The routine then sets IDO = 2, and this value is used for all but the last call that is made with IDO = 3. This final call is used to release workspace, which was automatically allocated by the initial call with IDO = 1. No integration is performed on this final call. See Comment 3 for a description of the other interrupts.

FCN — User-supplied subroutine to evaluate functions. The usage is CALL FCN (N, T, Y, YPRIME), where

N – Number of equations. (Input)

T – Independent variable, *t*. (Input)

Y – Array of size N containing the dependent variable values, *y*. (Input)

YPRIME – Array of size N containing the values of the vector *y*′ evaluated at (*t*, y). (Output)

FCN must be declared EXTERNAL in the calling program.

T — Independent variable. (Input/Output)
On input, T contains the initial value. On output, T is replaced by TEND unless error conditions have occurred. See IDO for details.

TEND — Value of *t* where the solution is required. (Input)
The value TEND may be less than the initial value of *t*.

Y — Array of size NEQ of dependent variables. (Input/Output)
On input, Y contains the initial values. On output, Y contains the approximate solution.

Optional Arguments

NEQ — Number of differential equations. (Input)
Default: NEQ = size (Y,1).

TOL — Tolerance for error control. (Input)
An attempt is made to control the norm of the local error such that the global error is proportional to TOL.
Default: TOL = machine precision.

PARAM — A *floating-point* array of size 50 containing optional parameters. (Input/ Output)
If a parameter is zero, then a default value is used. These default values are given below. Parameters that concern values of step size are applied in the direction of integration. The following parameters may be set by the user:

	PARAM	**Meaning**
1	HINIT	Initial value of the step size. Default: 10.0 * MAX (AMACH (1), AMACH(4) * MAX(ABS(TEND), ABS(T)))
2	HMIN	Minimum value of the step size. Default: 0.0
3	HMAX	Maximum value of the step size. Default: 2.0
4	MXSTEP	Maximum number of steps allowed. Default: 500
5	MXFCN	Maximum number of function evaluations allowed. Default: No enforced limit.
6		Not used.
7	INTRP1	If nonzero, then return with IDO = 4 before each step. See Comment 3. Default: 0.
8	INTRP2	If nonzero, then return with IDO = 5 after every successful step and with IDO = 6 after every unsuccessful step. See Comment 3. Default: 0.
9	SCALE	A measure of the scale of the problem, such as an approximation to the average value of a norm of the Jacobian matrix along the solution. Default: 1.0

	PARAM	Meaning
10	INORM	Switch determining error norm. In the following, e_i is the absolute value of an estimate of the error in $y_i(t)$. Default: 0.0 — min(absolute error, relative error) = max(e_i/w_i); i = 1, …, NEQ, where w_i = max($\lvert y_i(t)\rvert$, 1.0). 1 — absolute error = max(e_i), i = 1, …, NEQ. 2— max(e_i/w_i), i = 1, …, NEQ where w_i = max($\lvert y_i(t)\rvert$, FLOOR), and FLOOR is PARAM(11). 3 — Scaled Euclidean norm defined as $YMAX = \sqrt{\sum_{i=1}^{NEQ} e_i^2 / w_i^2}$ where w_i = max($\lvert y_i(t)\rvert$, 1.0). Other definitions of YMAX can be specified by the user, as explained in Comment 1.
11	FLOOR	Used in the norm computation associated with parameter INORM. Default: 1.0.
12-30		Not used.

The following entries in PARAM are set by the program.

	PARAM	Meaning
31	HTRIAL	Current trial step size.
32	HMINC	Computed minimum step size allowed.
33	HMAXC	Computed maximum step size allowed.
34	NSTEP	Number of steps taken.
35	NFCN	Number of function evaluations used.
36-50		Not used.

FORTRAN 90 Interface

Generic: CALL IVPRK (IDO, FCN, T, TEND, Y [, …])

Specific: The specific interface names are S_IVPRK and D_IVPRK.

FORTRAN 77 Interface

Single: CALL IVPRK (IDO, NEQ, FCN, T, TEND, TOL, PARAM, Y)

Double: The double precision name is DIVPRK.

Description

Routine IVPRK finds an approximation to the solution of a system of first-order differential equations of the form $y_0 = f(t, y)$ with given initial data. The routine attempts to keep the global error proportional to a user-specified tolerance. This routine is efficient for nonstiff systems where the derivative evaluations are not expensive.

The routine IVPRK is based on a code designed by Hull, Enright and Jackson (1976, 1977). It uses Runge-Kutta formulas of order five and six developed by J. H. Verner.

Comments

1. Workspace may be explicitly provided, if desired, by use of I2PRK/DI2PRK. The reference is:

   CALL I2PRK (IDO, NEQ, FCN, T, TEND, TOL, PARAM, Y, VNORM, WK)

   The additional arguments are as follows:

   VNORM — A Fortran subroutine to compute the norm of the error. (Input)
   The routine may be provided by the user, or the IMSL routine I3PRK/DI3PRK may be used. In either case, the name must be declared in a Fortran EXTERNAL statement. If usage of the IMSL routine is intended, then the name I3PRK/DI3PRK should be used. The usage of the error norm routine is
   CALL VNORM (N, V, Y, YMAX, ENORM), where

Arg	**Definition**
N	Number of equations. (Input).
V	Array of size N containing the vector whose norm is to be computed. (Input)
Y	Array of size N containing the values of the dependent variable. (Input)
YMAX	Array of size N containing the maximum values of $\|y(t)\|$. (Input).
ENORM	Norm of the vector V. (Output).

   VNORM must be declared EXTERNAL in the calling program.

   WK — Work array of size 10N using the working precision. The contents of WK must not be changed from the first call with IDO = 1 until after the final call with IDO = 3.

2. Informational errors

Type	Code	Description
4	1	Cannot satisfy error condition. The value of TOL may be too small.
4	2	Too many function evaluations needed.
4	3	Too many steps needed. The problem may be stiff.

3. If PARAM(7) is nonzero, the subroutine returns with IDO = 4 and will resume calculation at the point of interruption if re-entered with IDO = 4. If PARAM(8) is nonzero, the subroutine will interrupt the calculations immediately after it decides whether or not to accept the result of the most recent trial step. The values used are IDO = 5 if the routine plans to accept, or IDO = 6 if it plans to reject the step. The values of IDO may be changed by the user (by changing IDO from 6 to 5) in order to force acceptance of a step that would otherwise be rejected. Some parameters the user might want to examine after return from an interrupt are IDO, HTRIAL, NSTEP, NFCN, T, and Y. The array Y contains the newly computed trial value for $y(t)$, accepted or not.

Examples

Example 1

Consider a predator-prey problem with rabbits and foxes. Let r be the density of rabbits and let f be the density of foxes. In the absence of any predator-prey interaction, the rabbits would increase at a rate proportional to their number, and the foxes would die of starvation at a rate proportional to their number. Mathematically,

$$r' = 2r$$
$$f' = -f$$

The rate at which the rabbits are eaten by the foxes is $2rf$, and the rate at which the foxes increase, because they are eating the rabbits, is rf. So, the model to be solved is

$$r' = 2r - 2rf$$
$$f' = -f + rf$$

The initial conditions are $r(0) = 1$ and $f(0) = 3$ over the interval $0 \le t \le 10$.

In the program Y(1) = r and Y(2) = f. Note that the parameter vector PARAM is first set to zero with IMSL routine SSET (*Chapter 9, "Basic Matrix/Vector Operations"*). Then, absolute error control is selected by setting PARAM(10) = 1.0.

The last call to IVPRK with IDO = 3 deallocates IMSL workspace allocated on the first call to IVPRK. It is not necessary to release the workspace in this example because the program ends after solving a single problem. The call to release workspace is made as a model of what would be needed if the program included further calls to IMSL routines.

```
      USE IVPRK_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    MXPARM, N
      PARAMETER  (MXPARM=50, N=2)
!                                 SPECIFICATIONS FOR LOCAL VARIABLES
      INTEGER    IDO, ISTEP, NOUT
      REAL       PARAM(MXPARM), T, TEND, TOL, Y(N)
!                                 SPECIFICATIONS FOR SUBROUTINES
      EXTERNAL   FCN
!
      CALL UMACH (2, NOUT)
!                                 Set initial conditions
      T = 0.0
      Y(1) = 1.0
      Y(2) = 3.0
!                                 Set error tolerance
      TOL = 0.0005
!                                 Set PARAM to default
      PARAM = 0.E0
!                                 Select absolute error control
      PARAM(10) = 1.0
!                                 Print header
      WRITE (NOUT,99999)
      IDO = 1
      ISTEP = 0
   10 CONTINUE
      ISTEP = ISTEP + 1
      TEND = ISTEP
      CALL IVPRK (IDO, FCN, T, TEND, Y, TOL=TOL, PARAM=PARAM)
      IF (ISTEP .LE. 10) THEN
         WRITE (NOUT,'(I6,3F12.3)') ISTEP, T, Y
!                                 Final call to release workspace
         IF (ISTEP .EQ. 10) IDO = 3
         GO TO 10
      END IF
99999 FORMAT (4X, 'ISTEP', 5X, 'Time', 9X, 'Y1', 11X, 'Y2')
      END
      SUBROUTINE FCN (N, T, Y, YPRIME)
!                                 SPECIFICATIONS FOR ARGUMENTS
      INTEGER    N
      REAL       T, Y(N), YPRIME(N)
!
      YPRIME(1) = 2.0*Y(1) - 2.0*Y(1)*Y(2)
      YPRIME(2) = -Y(2) + Y(1)*Y(2)
      RETURN
      END
```

Output

```
ISTEP     Time         Y1          Y2
  1       1.000       0.078       1.465
  2       2.000       0.085       0.578
  3       3.000       0.292       0.250
  4       4.000       1.449       0.187
  5       5.000       4.046       1.444
  6       6.000       0.176       2.256
  7       7.000       0.066       0.908
  8       8.000       0.148       0.367
  9       9.000       0.655       0.188
 10      10.000       3.157       0.352
```

Example 2

This is a mildly stiff problem (F2) from the test set of Enright and Pryce (1987). It is included here because it illustrates the inefficiency of requiring more function evaluations with a nonstiff solver, for a requested accuracy, than would be required using a stiff solver. Also, see `IVPAG` Example 2, where the problem is solved using a BDF method. The number of function evaluations may vary, depending on the accuracy and other arithmetic characteristics of the computer. The test problem has n = 2 equations:

$$\begin{aligned}
y'_1 &= -y_1 - y_1 y_2 + k_1 y_2 \\
y'_2 &= -k_2 y_2 + k_3 \left(1 - y_2\right) y_1 \\
y_1\left(0\right) &= 1 \\
y_2\left(0\right) &= 0 \\
k_1 &= 294 \\
k_2 &= 3 \\
k_3 &= 0.01020408 \\
tend &= 240
\end{aligned}$$

```
      USE IVPRK_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    MXPARM, N
      PARAMETER  (MXPARM=50, N=2)
!                                 SPECIFICATIONS FOR LOCAL VARIABLES
      INTEGER    IDO, ISTEP, NOUT
      REAL       PARAM(MXPARM), T, TEND, TOL, Y(N)
!                                 SPECIFICATIONS FOR SUBROUTINES
!                                 SPECIFICATIONS FOR FUNCTIONS
      EXTERNAL   FCN
!
      CALL UMACH (2, NOUT)
!                                 Set initial conditions
      T = 0.0
      Y(1) = 1.0
      Y(2) = 0.0
!                                 Set error tolerance
      TOL = 0.001
!                                 Set PARAM to default
      PARAM = 0.0E0
!                                 Select absolute error control
      PARAM(10) = 1.0
!                                 Print header
      WRITE (NOUT,99998)
      IDO = 1
      ISTEP = 0
   10 CONTINUE
      ISTEP = ISTEP + 24
      TEND = ISTEP
      CALL IVPRK (IDO, FCN, T, TEND, Y, TOL=TOL, PARAM=PARAM)
      IF (ISTEP .LE. 240) THEN
         WRITE (NOUT,'(I6,3F12.3)') ISTEP/24, T, Y
!                                 Final call to release workspace
         IF (ISTEP .EQ. 240) IDO = 3
```

```
         GO TO 10
      END IF
!                                  Show number of function calls.
      WRITE (NOUT,99999) PARAM(35)
99998 FORMAT (4X, 'ISTEP', 5X, 'Time', 9X, 'Y1', 11X, 'Y2')
99999 FORMAT (4X, 'Number of fcn calls with IVPRK =', F6.0)
      END
      SUBROUTINE FCN (N, T, Y, YPRIME)
!                                  SPECIFICATIONS FOR ARGUMENTS
      INTEGER    N
      REAL       T, Y(N), YPRIME(N)
!                                  SPECIFICATIONS FOR DATA VARIABLES
      REAL       AK1, AK2, AK3
!
      DATA AK1, AK2, AK3/294.0E0, 3.0E0, 0.01020408E0/
!
      YPRIME(1) = -Y(1) - Y(1)*Y(2) + AK1*Y(2)
      YPRIME(2) = -AK2*Y(2) + AK3*(1.0E0-Y(2))*Y(1)
      RETURN
      END
```

Output

```
ISTEP     Time         Y1           Y2
 1      24.000       0.688        0.002
 2      48.000       0.634        0.002
 3      72.000       0.589        0.002
 4      96.000       0.549        0.002
 5     120.000       0.514        0.002
 6     144.000       0.484        0.002
 7     168.000       0.457        0.002
 8     192.000       0.433        0.001
 9     216.000       0.411        0.001
10     240.000       0.391        0.001
Number of fcn calls with IVPRK = 2153.
```

IVMRK

Solves an initial-value problem $y' = f(t, y)$ for ordinary differential equations using Runge-Kutta pairs of various orders.

Required Arguments

IDO — Flag indicating the state of the computation. (Input/Output)

IDO	State
1	Initial entry
2	Normal re-entry
3	Final call to release workspace
4	Return after a step
5	Return for function evaluation (reverse communication)

Normally, the initial call is made with IDO = 1. The routine then sets IDO = 2, and this value is used for all but the last call that is made with IDO = 3. This final call is used to release workspace, which was automatically allocated by the initial call with IDO = 1.

FCN — User-supplied subroutine to evaluate functions. The usage is CALL FCN (N, T, Y, YPRIME), where

N — Number of equations. (Input)

T — Independent variable. (Input)

Y — Array of size N containing the dependent variable values, y. (Input)

YPRIME — Array of size N containing the values of the vector y' evaluated at (t, y). (Output)

FCN must be declared EXTERNAL in the calling program.

T — Independent variable. (Input/Output)
On input, T contains the initial value. On output, T is replaced by TEND unless error conditions have occurred.

TEND — Value of t where the solution is required. (Input)
The value of TEND may be less than the initial value of t.

Y — Array of size N of dependent variables. (Input/Output)
On input, Y contains the initial values. On output, Y contains the approximate solution.

YPRIME — Array of size `N` containing the values of the vector y' evaluated at (t, y). (Output)

Optional Arguments

N — Number of differential equations. (Input)
Default: `N`= size (`Y`,1).

FORTRAN 90 Interface

Generic: `CALL IVMRK (IDO, FCN, T, TEND, Y, YPRIME [, …])`

Specific: The specific interface names are `S_IVMRK` and `D_IVMRK`.

FORTRAN 77 Interface

Single: `CALL IVMRK (IDO, N, FCN, T, TEND, Y, YPRIME)`

Double: The double precision name is `DIVMRK`.

Description

Routine `IVMRK` finds an approximation to the solution of a system of first-order differential equations of the form $y' = f(t, y)$ with given initial data. Relative local error is controlled according to a user-supplied tolerance. For added efficiency, three Runge-Kutta formula pairs, of orders 3, 5, and 8, are available.

Optionally, the values of the vector y' can be passed to `IVMRK` by reverse communication, avoiding the user-supplied subroutine `FCN`. Reverse communication is especially useful in applications that have complicated algorithmic requirement for the evaluations of $f(t, y)$. Another option allows assessment of the global error in the integration.

The routine `IVMRK` is based on the codes contained in `RKSUITE`, developed by R. W. Brankin, I. Gladwell, and L. F. Shampine (1991).

Comments

1. Workspace may be explicitly provided, if desired, by use of `I2MRK/DI2MRK`. The reference is:

   `CALL I2MRK (IDO, N, FCN, T, TEND, Y, YPRIME, TOL, THRES, PARAM, YMAX, RMSERR, WORK, IWORK)`

   The additional arguments are as follows:

   TOL — Tolerance for error control. (Input)

THRES — Array of size `N`. (Input)
`THRES(I)` is a threshold for solution component `Y(I)`. It is chosen so that the value of `Y(L)` is not important when `Y(L)` is smaller in magnitude than `THRES(L)`. `THRES(L)` must be greater than or equal to `sqrt(amach(4))`.

PARAM — A floating-point array of size 50 containing optional parameters. (Input/Output)
If a parameter is zero, then a default value is used. These default values are given below. The following parameters must be set by the user:

	PARAM	Definition
1	HINIT	Initial value of the step size. Must be chosen such that 0.01 ≥ HINIT ≥ 10.0 amach(4). Default: automatic selection of stepsize
2	METHOD	1 – use the (2, 3) pair 2 – use the (4, 5) pair 3 – use the (7, 8) pair. Default: METHOD = 1 if 1.e-2 ≥ tol > 1.e-4 METHOD = 2 if 1.e-4 ≥ tol > 1.e-6 METHOD = 3 if 1.e-6 ≥ tol
3	ERREST	ERREST = 1 attempts to assess the true error, the difference between the numerical solution and the true solution. The cost of this is roughly twice the cost of the integration itself with METHOD = 2 or METHOD = 3, and three times with METHOD = 1. Default: ERREST = 0.
4	INTRP	If nonzero, then return the IDO = 4 before each step. See Comment 3. Default: 0.
5	RCSTAT	If nonzero, then reverse communication is used to get derivative information. See Comment 4. Default: 0.
6 – 30		Not used.
	The following entries are set by the program:	
31	HTRIAL	Current trial step size.
32	NSTEP	Number of steps taken.
33	NFCN	Number of function evaluations.
34	ERRMAX	The maximum approximate weighted true error taken over all solution components and all steps from T
35	TERRMX	First value of the independent variable where an approximate true error attains the maximum value ERRMAX.

YMAX — *Array of size* N, where YMAX(L) is the largest value of ABS(Y(L)) computed at any step in the integration so far.

RMSERR — Array of size N where RMSERR(L) approximates the RMS average of the true error of the numerical solution for the L-th solution component, L = 1, …, *N*. The average is taken over all steps from T through the current integration point. RMSERR is accessed and set only if PARAM(3) = 1.

WORK — Floating point work array of size 39N using the working precision. The contents of WORK must not be changed from the first call with IDO = 1 until after the final call with IDO = 3.

IWORK — Length of array work. (Input)

2. Informational errors

Type	Code	Description
4	1	It does not appear possible to achieve the accuracy specified by TOL and THRES(*) using the current precision and METHOD. A larger value for METHOD, if possible, will permit greater accuracy with this precision. The integration must be restarted.
4	2	The global error assessment may not be reliable beyond the current integration point T. This may occur because either too little or too much accuracy has been requested or because *f*(*t*, *y*) is not smooth enough for values of *t* just past TEND and current values of the solution *y*. This return does not mean that you cannot integrate past TEND, rather that you cannot do it with PARAM(3) = 1.

3 If PARAM(4) is nonzero, the subroutine returns with IDO = 4 and will resume calculation at the point of interruption if re-entered with IDO = 4. Some parameters the user might want to examine are IDO, HTRIAL, NSTEP, NFCN, T, and Y. The array Y contains the newly computed trial value for *y*(*t*), accepted or not.

4 If PARAM(5) is nonzero, the subroutine will return with IDO = 5. At this time, evaluate the derivatives at T, place the result in YPRIME, and call IVMRK again. The dummy function I40RK/DI40RK may be used in place of FCN.

Examples

Example 1

This example integrates the small system (A.2.B2) from the test set of Enright and Pryce (1987):

$$
\begin{aligned}
y_1{}' &= y_1 + y_2 \\
y_2{}' &= y_1 - 2y_2 + y_3 \\
y_3{}' &= y_2 - y_3 \\
y_1(0) &= 2 \\
y_2(0) &= 0 \\
y_3(0) &= 1
\end{aligned}
$$

```
      USE IVMRK_INT
      USE WRRRN_INT

      IMPLICIT   NONE
      INTEGER    N

      PARAMETER  (N=3)
!                                  Specifications for local variables
      INTEGER    IDO
      REAL       T, TEND, Y(N), YPRIME(N)
      EXTERNAL FCN
!                                  Set initial conditions
      T = 0.0
      TEND = 20.0
      Y(1) = 2.0
      Y(2) = 0.0
      Y(3) = 1.0
      IDO = 1
      CALL IVMRK (IDO, FCN, T, TEND, Y, YPRIME)
!
!                                  Final call to release workspace
      IDO = 3
      CALL IVMRK (IDO, FCN, T, TEND, Y, YPRIME)
!
      CALL WRRRN ('Y', Y)
      END
!
      SUBROUTINE FCN (N, T, Y, YPRIME)
!                                  Specifications for arguments
      INTEGER    N
      REAL       T, Y(*), YPRIME(*)
!
      YPRIME(1) = -Y(1) + Y(2)
      YPRIME(2) = Y(1) - 2.0*Y(2) + Y(3)
      YPRIME(3) = Y(2) - Y(3)
      RETURN
      END
```

Output

```
         Y
1    1.000
2    1.000
3    1.000
```

Example 2

This problem is the same mildly stiff problem (A.1.F2) from the test set of Enright and Pryce as Example 2 for IVPRK.

$$
\begin{aligned}
y_1' &= y_1 - y_1 y_2 + k_1 y_2 \\
y_2' &= -k_2 y_2 + k_3 (1 - y_2) y_1 \\
y_1(0) &= 1 \\
y_2(0) &= 0 \\
k_1 &= 294 \\
k_2 &= 3 \\
k_3 &= 0.01020408 \\
tend &= 240
\end{aligned}
$$

Although not a stiff solver, one notes the greater efficiency of IVMRK over IVPRK, in terms of derivative evaluations. Reverse communication is also used in this example. Users will find this feature particularly helpful if their derivative evaluation scheme is difficult to isolate in a separate subroutine.

```
      USE I2MRK_INT
      USE UMACH_INT
      USE AMACH_INT

      IMPLICIT   NONE
      INTEGER    N

      PARAMETER  (N=2)
!                                  Specifications for local variables
      INTEGER    IDO, ISTEP, LWORK, NOUT
      REAL       PARAM(50), PREC, RMSERR(N), T, TEND, THRES(N), TOL, &
                  WORK(1000), Y(N), YMAX(N), YPRIME(N)
      REAL       AK1, AK2, AK3
      SAVE       AK1, AK2, AK3
!                                  Specifications for intrinsics
      INTRINSIC  SQRT
      REAL       SQRT
!                                  Specifications for subroutines
      EXTERNAL   I40RK
!                                  Specifications for functions
!
      DATA AK1, AK2, AK3/294.0, 3.0, 0.01020408/
!
      CALL UMACH (2, NOUT)
!                                  Set initial conditions
      T    = 0.0
      Y(1) = 1.0
      Y(2) = 0.0
!                                  Set tolerance for error control,
!                                  threshold vector and parameter
!                                  vector
      TOL = .001
      PREC = AMACH(4)
      THRES = SQRT (PREC)
      PARAM = 0.0E0
      LWORK = 1000
```

```
!                                   Turn on derivative evaluation by
!                                   reverse communication
      PARAM(5) = 1
      IDO      = 1
      ISTEP    = 24
!                                   Print header
      WRITE (NOUT,99998)
   10 CONTINUE
      TEND = ISTEP
      CALL I2MRK (IDO, N, I40RK, T, TEND, Y, YPRIME, TOL, THRES, PARAM,&
                 YMAX, RMSERR, WORK, LWORK)
      IF (IDO .EQ. 5) THEN
!                                   Evaluate derivatives
!
         YPRIME(1) = -Y(1) - Y(1)*Y(2) + AK1*Y(2)
         YPRIME(2) = -AK2*Y(2) + AK3*(1.0-Y(2))*Y(1)
         GO TO 10
      ELSE IF (ISTEP .LE. 240) THEN
!
!                                   Integrate to 10 equally spaced points
!
         WRITE (NOUT,'(I6,3F12.3)') ISTEP/24, T, Y
         IF (ISTEP .EQ. 240) IDO = 3
         ISTEP = ISTEP + 24
         GO TO 10
      END IF
!                                   Show number of derivative evaluations
!
      WRITE (NOUT,99999) PARAM(33)
99998 FORMAT (3X, 'ISTEP', 5X, 'TIME', 9X, 'Y1', 10X, 'Y2')
99999 FORMAT (/, 4X, 'NUMBER OF DERIVATIVE EVALUATIONS WITH IVMRK =', &
            F6.0)
      END

!     DUMMY FUNCTION TO TAKE THE PLACE OF DERIVATIVE EVALUATOR
      SUBROUTINE I40RK (N, T, Y, YPRIME)
      INTEGER N
      REAL     T, y(*), YPRIME(*)
      RETURN
      END
```

Output

```
ISTEP     TIME         Y1          Y2
1       24.000       0.688       0.002
2       48.000       0.634       0.002
3       72.000       0.589       0.002
4       96.000       0.549       0.002
5      120.000       0.514       0.002
6      144.000       0.484       0.002
7      168.000       0.457       0.002
8      192.000       0.433       0.001
9      216.000       0.411       0.001
10     240.000       0.391       0.001
NUMBER OF DERIVATIVE EVALUATIONS WITH IVMRK = 1375.
```

Example 3

This example demonstrates how exceptions may be handled. The problem is from Enright and Pryce (A.2.F1), and has discontinuities. We choose this problem to force a failure in the global error estimation scheme, which requires some smoothness in *y*. We also request an initial relative error tolerance which happens to be unsuitably small in this precision.

If the integration fails because of problems in global error assessment, the assessment option is turned off, and the integration is restarted. If the integration fails because the requested accuracy is not achievable, the tolerance is increased, and global error assessment is requested. The reason error assessment is turned on is that prior assessment failures may have been due more in part to an overly stringent tolerance than lack of smoothness in the derivatives.

When the integration is successful, the example prints the final relative error tolerance, and indicates whether or not global error estimation was possible.

$$
\begin{aligned}
y'_1 &= y_2 \\
y'_2 &= \begin{cases} 2ay_2 - \left(\pi^2 + a^2\right)y_1 + 1, \lfloor x \rfloor \text{ even} \\ 2ay_2 - \left(\pi^2 + a^2\right)y_1 - 1, \lfloor x \rfloor \text{ odd} \end{cases} \\
y_1(0) &= 0 \\
y_2(0) &= 0 \\
a &= 0.1 \\
\lfloor x \rfloor &= \text{largest integer} \le x
\end{aligned}
$$

```
      USE IMSL_LIBRARIES

      IMPLICIT   NONE
      INTEGER    N
      PARAMETER  (N=2)
!                                  Specifications for local variables
      INTEGER    IDO, LWORK, NOUT
      REAL       PARAM(50), PREC, RMSERR(N), T, TEND, THRES(N), TOL,&
                WORK(100), Y(N), YMAX(N), YPRIME(N)
!
!                                  Specifications for intrinsics
      INTRINSIC  SQRT
      REAL       SQRT
!                                  Specifications for subroutines
!
!
!                                  Specifications for functions
      EXTERNAL   FCN
!
!
      CALL UMACH (2, NOUT)
!                                  Turn off stopping for FATAL errors
      CALL ERSET (4, -1, 0)
!                                  Initialize input, turn on global
!                                  error assessment
      LWORK = 100
      PREC = AMACH(4)
      TOL   = SQRT(PREC)
      PARAM = 0.0E01
      THRES = TOL
      TEND     = 20.0E0
      PARAM(3) = 1
!
   10 CONTINUE
!                                  Set initial values
```

```
      T    = 0.0E0
      Y(1) = 0.0E0
      Y(2) = 0.0E0
      IDO  = 1
      CALL I2MRK (IDO, N, FCN, T, TEND, Y, YPRIME, TOL, THRES, PARAM,&
                  YMAX, RMSERR, WORK, LWORK)
      IF (IERCD() .EQ. 32) THEN
!                                  Unable to achieve requested
!                                  accuracy, so increase tolerance.
!                                  Activate global error assessment
         TOL      = 10.0*TOL
         PARAM(3) = 1
         WRITE (NOUT,99995) TOL
         GO TO 10
      ELSE IF (IERCD() .EQ. 34) THEN
!                                  Global error assessment has failed,
!                                  cannot continue from this point,
!                                  so restart integration
         WRITE (NOUT,99996)
         PARAM(3) = 0
         GO TO 10
      END IF
!
!                                  Final call to release workspace
      IDO = 3
      CALL I2MRK (IDO, N, FCN, T, TEND, Y, YPRIME, TOL, THRES, PARAM,&
                  YMAX, RMSERR, WORK, LWORK)
!
!                                  Summarize status
      WRITE (NOUT,99997) TOL
      IF (PARAM(3) .EQ. 1) THEN
         WRITE (NOUT,99998)
      ELSE
         WRITE (NOUT,99999)
      END IF
      CALL WRRRN ('Y', Y)
!
99995 FORMAT (/, 'CHANGING TOLERANCE TO ', E9.3, ' AND RESTARTING ...'&
            , /, 'ALSO (RE)ENABLING GLOBAL ERROR ASSESSMENT', /)
99996 FORMAT (/, 'DISABLING GLOBAL ERROR ASSESSMENT AND RESTARTING ...'&
            , /)
99997 FORMAT (/, 72('-'), //, 'SOLUTION OBTAINED WITH TOLERANCE = ',&
            E9.3)
99998 FORMAT ('GLOBAL ERROR ASSESSMENT IS AVAILABLE')
99999 FORMAT ('GLOBAL ERROR ASSESSMENT IS NOT AVAILABLE')
!
      END
!
      SUBROUTINE FCN (N, T, Y, YPRIME)
      USE CONST_INT
!                                  Specifications for arguments
      INTEGER    N
      REAL       T, Y(*), YPRIME(*)
!                                  Specifications for local variables
      REAL       A
      REAL       PI
      LOGICAL    FIRST
      SAVE       FIRST, PI
!                                  Specifications for intrinsics
      INTRINSIC  INT, MOD
      INTEGER    INT, MOD
!                                  Specifications for functions
!
      DATA FIRST/.TRUE./
!
      IF (FIRST) THEN
```

```
            PI    = CONST('PI')
            FIRST = .FALSE.
         END IF
!
         A          = 0.1E0
         YPRIME(1) = Y(2)
         IF (MOD(INT(T),2) .EQ. 0) THEN
            YPRIME(2) = 2.0E0*A*Y(2) - (PI*PI+A*A)*Y(1) + 1.0E0
         ELSE
            YPRIME(2) = 2.0E0*A*Y(2) - (PI*PI+A*A)*Y(1) - 1.0E0
         END IF
         RETURN
         END
```

Output

```
 *** FATAL    ERROR 34 from i2mrk.  The global error assessment may not
 ***          be reliable for T past 9.994749E-01.  The integration is
 ***          being terminated.


DISABLING GLOBAL ERROR ASSESSMENT AND RESTARTING ...


 *** FATAL    ERROR 32 from i2mrk.  In order to satisfy the error
 ***          requirement I6MRK would have to use a step size of
 ***          3.647129E- 06 at TNOW = 9.999932E-01.  This is too small
 ***          for the current precision.


CHANGING TOLERANCE TO 0.345E-02 AND RESTARTING ...
ALSO (RE)ENABLING GLOBAL ERROR ASSESSMENT


 *** FATAL    ERROR 34 from i2mrk.  The global error assessment may
 ***          not be reliable for T past 9.986024E-01.  The integration
 ***          is being terminated.

DISABLING GLOBAL ERROR ASSESSMENT AND RESTARTING ...

------------------------------------------------------------------------

SOLUTION OBTAINED WITH TOLERANCE = 0.345E-02
GLOBAL ERROR ASSESSMENT IS NOT AVAILABLE

      Y
 1  -12.30
 2    0.95
```

IVPAG

more...

Solves an initial-value problem for ordinary differential equations using either Adams-Moulton's or Gear's BDF method.

Required Arguments

IDO — Flag indicating the state of the computation. (Input/Output)

IDO	State
1	Initial entry
2	Normal re-entry
3	Final call to release workspace
4	Return because of interrupt 1
5	Return because of interrupt 2 with step accepted
6	Return because of interrupt 2 with step rejected
7	Return for new value of matrix A.

Normally, the initial call is made with IDO = 1. The routine then sets IDO = 2, and this value is then used for all but the last call that is made with IDO = 3. This final call is only used to release workspace, which was automatically allocated by the initial call with IDO = 1. See Comment 5 for a description of the interrupts.

When IDO = 7, the matrix *A* at *t* must be recomputed and IVPAG/DIVPAG called again. No other argument (including IDO) should be changed. This value of IDO is returned only if PARAM(19) = 2.

FCN — User-supplied subroutine to evaluate functions. The usage is CALL FCN (N, T, Y, YPRIME), where

N – Number of equations. (Input)

T – Independent variable, *t*. (Input)

Y – Array of size N containing the dependent variable values, *y*. (Input)

YPRIME – Array of size N containing the values of the vector y' evaluated at (t, y). (Output)
See Comment 3.

FCN must be declared EXTERNAL in the calling program.

FCNJ — User-supplied subroutine to compute the Jacobian. The usage is
CALL FCNJ (N, T, Y, DYPDY) where

N – Number of equations. (Input)

T – Independent variable, *t*. (Input)

Y – Array of size N containing the dependent variable values, $y(t)$. (Input)

DYPDY – An array, with data structure and type determined by PARAM(14) = MTYPE, containing the required partial derivatives $\partial f_i / \partial y_j$. (Output)

These derivatives are to be evaluated at the current values of (t, y). When the Jacobian is dense, MTYPE = 0 or MTYPE = 2, the leading dimension of DYPDY has the value N. When the Jacobian matrix is banded, MTYPE = 1, and the leading dimension of DYPDY has the value 2 * NLC + NUC + 1. If the matrix is banded positive definite symmetric, MTYPE = 3, and the leading dimension of DYPDY has the value NUC + 1.

FCNJ must be declared EXTERNAL in the calling program. If PARAM(19) = IATYPE is nonzero, then FCNJ should compute the Jacobian of the righthand side of the equation $Ay' = f(t, y)$. The subroutine FCNJ is used only if PARAM(13) = MITER = 1.

T — Independent variable, *t*. (Input/Output)
On input, T contains the initial independent variable value. On output, T is replaced by TEND unless error or other normal conditions arise. See IDO for details.

TEND — Value of $t = tend$ where the solution is required. (Input)
The value *tend* may be less than the initial value of *t*.

Y — Array of size NEQ of dependent variables, $y(t)$. (Input/Output)
On input, Y contains the initial values, $y(t_0)$. On output, Y contains the approximate solution, $y(t)$.

Optional Arguments

NEQ— Number of differential equations. (Input)
Default: NEQ = size (Y,1)

A — Matrix structure used when the system is implicit. (Input)
The matrix *A* is referenced only if PARAM(19) = IATYPE is nonzero. Its data structure is determined by PARAM(14) = MTYPE. The matrix A must be nonsingular and MITER must be 1 or 2. See Comment 3.

TOL — Tolerance for error control. (Input)
An attempt is made to control the norm of the local error such that the global error is proportional to `TOL`.
Default: `TOL` = .001

PARAM — A *floating-point* array of size 50 containing optional parameters. (Input/Output)
If a parameter is zero, then the default value is used. These default values are given below. Parameters that concern values of the step size are applied in the direction of integration. The following parameters may be set by the user:

	PARAM	Meaning
1	HINIT	Initial value of the step size `H`. Always nonnegative. Default: $0.001\,\lvert tend - t_0 \rvert$.
2	HMIN	Minimum value of the step size `H`. Default: 0.0.
3	HMAX	Maximum value of the step size `H`. Default: No limit, beyond the machine scale, is imposed on the step size.
4	MXSTEP	Maximum number of steps allowed. Default: 500.
5	MXFCN	Maximum number of function evaluations allowed. Default: No enforced limit.
6	MAXORD	Maximum order of the method. Default: If Adams-Moulton method is used, then 12. If Gear's or BDF method is used, then 5. The defaults are the maximum values allowed.
7	INTRP1	If this value is set nonzero, the subroutine will return before every step with `IDO` = 4. See Comment 5. Default: 0.
8	INTRP2	If this value is nonzero, the subroutine will return after every successful step with `IDO` = 5 and return with `IDO` = 6 after every unsuccessful step. See Comment 5. Default: 0
9	SCALE	A measure of the scale of the problem, such as an approximation to the average value of a norm of the Jacobian along the solution. Default: 1.0

	PARAM	Meaning
10	INORM	Switch determining error norm. In the following, e_i is the absolute value of an estimate of the error in $y_i(t)$. Default: 0. 0 — min(absolute error, relative error) = max($e_i w_i$); i = 1, …, N, where w_i = max(|$y_i(t)$|, 1.0). 1 — absolute error = max(e_i), i = 1, …, NEQ. 2 — max(e_i / w_i), i = 1, …, N where w_i = max(|$y_i(t)$|, FLOOR), and FLOOR is the value PARAM(11). 3 — Scaled Euclidean norm defined as $YMAX = \sqrt{\sum_{i=1}^{NEQ} e_i^2 / w_i^2}$ where w_i = max(|$y_i(t)$|, 1.0). Other definitions of YMAX can be specified by the user, as explained in Comment 1.
11	FLOOR	Used in the norm computation associated the parameter INORM. Default: 1.0.
12	METH	Integration method indicator. 1 = METH selects the Adams-Moulton method. 2 = METH selects Gear's BDF method. Default: 1.
13	MITER	Nonlinear solver method indicator. Note: If the problem is stiff and a chord or modified Newton method is most efficient, use MITER = 1 or = 2. 0 = MITER selects functional iteration. The value IATYPE must be set to zero with this option. 1 = MITER selects a chord method with a user-provided Jacobian. 2 = MITER selects a chord method with a divided-difference Jacobian. 3 = MITER selects a chord method with the Jacobian replaced by a diagonal matrix based on a directional derivative. The value IATYPE must be set to zero with this option. Default: 0.
14	MTYPE	Matrix type for A (if used) and the Jacobian (if MITER = 1 or MITER = 2). When both are used, A and the Jacobian must be of the same type. 0 = MTYPE selects full matrices. 1 = MTYPE selects banded matrices. 2 = MTYPE selects symmetric positive definite matrices. 3 = MTYPE selects banded symmetric positive definite matrices. Default: 0.
15	NLC	Number of lower codiagonals, used if MTYPE = 1. Default: 0.
16	NUC	Number of upper codiagonals, used if MTYPE = 1 or MTYPE = 3. Default: 0.

	PARAM	Meaning
17		Not used.
18	EPSJ	Relative tolerance used in computing divided difference Jacobians. Default: SQRT(AMACH(4)) .
19	IATYPE	Type of the matrix *A*. 0 = IATYPE implies *A* is not used (the system is explicit). 1 = IATYPE if *A* is a constant matrix. 2 = IATYPE if *A* depends on *t*. Default: 0.
20	LDA	Leading dimension of array *A* exactly as specified in the dimension statement in the calling program. Used if IATYPE is not zero. Default: N if MTYPE = 0 or = 2 NUC + NLC + 1 if MTYPE = 1 NUC + 1 if MTYPE = 3
21–30		Not used.

The following entries in the array PARAM are set by the program:

	PARAM	Meaning
31	HTRIAL	Current trial step size.
32	HMINC	Computed minimum step size.
33	HMAXC	Computed maximum step size.
34	NSTEP	Number of steps taken.
35	NFCN	Number of function evaluations used.
36	NJE	Number of Jacobian evaluations.
37–50		Not used.

FORTRAN 90 Interface

Generic: CALL IVPAG (IDO, FCN, FCNJ, T, TEND, Y [, …])

Specific: The specific interface names are S_IVPAG and D_IVPAG.

FORTRAN 77 Interface

Single: CALL IVPAG (IDO, NEQ, FCN, FCNJ, A, T, TEND, TOL, PARAM, Y)

Double: The double precision name is DIVPAG.

Description

The routine IVPAG solves a system of first-order ordinary differential equations of the form $y' = f(t, y)$ or $Ay' = f(t, y)$ with initial conditions where A is a square nonsingular matrix of order N. Two classes of implicit linear multistep methods are available. The first is the implicit Adams-Moulton method (up to order twelve); the second uses the backward differentiation formulas BDF (up to order five). The BDF method is often called Gear's stiff method. In both cases, because basic formulas are implicit, a system of nonlinear equations must be solved at each step. The deriviative matrix in this system has the form $L = A + \eta J$ where η is a small number computed by IVPAG and J is the Jacobian. When it is used, this matrix is computed in the user-supplied routine FCNJ or else it is approximated by divided differences as a default. Using defaults, A is the identity matrix. The data structure for the matrix L may be identified to be real general, real banded, symmetric positive definite, or banded symmetric positive definite. The default structure for L is real general.

Comments

1. Workspace and a user-supplied error norm subroutine may be explicitly provided, if desired, by use of I2PAG/DI2PAG. The reference is:

```
CALL I2PAG(IDO, NEQ, FCN, FCNJ, A, T, TEND, TOL, PARAM, Y, YTEMP, YMAX,
    ERROR, SAVE1, SAVE2, PW, IPVT, VNORM)
```

None of the additional array arguments should be changed from the first call with IDO = 1 until after the final call with IDO = 3. The additional arguments are as follows:

YTEMP — Array of size NMETH. (Workspace)

YMAX — Array of size NEQ containing the maximum Y-values computed so far. (Output)

ERROR — Array of size NEQ containing error estimates for each component of Y. (Output)

SAVE1 — Array of size NEQ. (Workspace)

SAVE2 — Array of size NEQ. (Workspace)

PW — Array of size NPW. (Workspace)

IPVT — Array of size NEQ. (Workspace)

VNORM — A Fortran subroutine to compute the norm of the error. (Input)
The routine may be provided by the user, or the IMSL routine I3PRK/DI3PRK may be used. In either case, the name must be declared in a Fortran EXTERNAL statement. If usage of the IMSL routine is intended, then the name I3PRK/DI3PRK should be specified. The usage of the error norm routine is CALL VNORM (NEQ, V, Y, YMAX, ENORM) where

Arg	Definition
NEQ	Number of equations. (Input).
V	Array of size N containing the vector whose norm is to be computed. (Input)

Arg	Definition
Y	Array of size N containing the values of the dependent variable. (Input)
YMAX	Array of size N containing the maximum values of $\|y(t)\|$. (Input).
ENORM	Norm of the vector V. (Output).

VNORM must be declared EXTERNAL in the calling program.

2. Informational errors

Type	Code	Description
4	1	After some initial success, the integration was halted by repeated error-test failures.
4	2	The maximum number of function evaluations have been used.
4	3	The maximum number of steps allowed have been used. The problem may be stiff.
4	4	On the next step T + H will equal T. Either TOL is too small, or the problem is stiff. Note: If the Adams-Moulton method is the one used in the integration, then users can switch to the BDF methods. If the BDF methods are being used, then these comments are gratuitous and indicate that the problem is too stiff for this combination of method and value of TOL.
4	5	After some initial success, the integration was halted by a test on TOL.
4	6	Integration was halted after failing to pass the error test even after dividing the initial step size by a factor of 1.0E + 10. The value TOL may be too small.
4	7	Integration was halted after failing to achieve corrector convergence even after dividing the initial step size by a factor of 1.0E + 10. The value TOL may be too small.
4	8	IATYPE is nonzero and the input matrix *A* multiplying y′ is singular.

3. Both explicit systems, of the form $y' = f(t, y)$, and implicit systems, $Ay' = f(t, y)$, can be solved. If the system is explicit, then PARAM(19) = 0; and the matrix *A* is not referenced. If the system is implicit, then PARAM(14) determines the data structure of the array A. If PARAM(19) = 1, then A is assumed to be a constant matrix. The value of A used on the first call (with IDO = 1) is saved until after a call with IDO = 3. The value of A must not be changed between these calls. If PARAM(19) = 2, then the matrix is assumed to be a function of *t*.

4. If MTYPE is greater than zero, then MITER must equal 1 or 2.

5. If PARAM(7) is nonzero, the subroutine returns with IDO= 4 and will resume calculation at the point of interruption if re-entered with IDO = 4. If PARAM(8) is nonzero, the subroutine will interrupt immediately after decides to accept the result of the most recent trial step. The value IDO = 5 is returned if

the routine plans to accept, or IDO = 6 if it plans to reject. The value IDO may be changed by the user (by changing IDO from 6 to 5) to force acceptance of a step that would otherwise be rejected. Relevant parameters to observe after return from an interrupt are IDO, HTRIAL, NSTEP, NFCN, NJE, T and Y. The array Y contains the newly computed trial value $y(t)$.

Examples

Example 1

Euler's equation for the motion of a rigid body not subject to external forces is

$$\begin{aligned} y'_1 &= y_2 y_3 & y_1(0) &= 0 \\ y'_2 &= -y_1 y_3 & y_2(0) &= 1 \\ y'_3 &= -0.51 y_1 y_2 & y_3(0) &= 1 \end{aligned}$$

Its solution is, in terms of Jacobi elliptic functions, $y(t) = \mathrm{sn}(t; k)$, $y_2(t) = \mathrm{cn}(t; k)$, $y_3(t) = \mathrm{dn}(t; k)$ where $k^2 = 0.51$. The Adams-Moulton method of IVPAG is used to solve this system, since this is the default. All parameters are set to defaults.

The last call to IVPAG with IDO = 3 releases IMSL workspace that was reserved on the first call to IVPAG. It is not necessary to release the workspace in this example because the program ends after solving a single problem. The call to release workspace is made as a model of what would be needed if the program included further calls to IMSL routines.

Because PARAM(13) = MITER = 0, functional iteration is used and so subroutine FCNJ is never called. It is included only because the calling sequence for IVPAG requires it.

```
      USE IVPAG_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    N, NPARAM
      PARAMETER  (N=3, NPARAM=50)
!                                 SPECIFICATIONS FOR LOCAL VARIABLES
      INTEGER    IDO, IEND, NOUT
      REAL       A(1,1), T, TEND, TOL, Y(N)
!                                 SPECIFICATIONS FOR SUBROUTINES
!                                 SPECIFICATIONS FOR FUNCTIONS
      EXTERNAL   FCN, FCNJ
!                                 Initialize
!
      IDO  = 1
      T    = 0.0
      Y(1) = 0.0
      Y(2) = 1.0
      Y(3) = 1.0
      TOL  = 1.0E-6
!                                 Write title
```

```
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99998)
!                                   Integrate ODE
      IEND = 0
   10 CONTINUE
      IEND = IEND + 1
      TEND = IEND
!                                   The array a(*,*) is not used.
      CALL IVPAG (IDO, FCN, FCNJ, T, TEND, Y, TOL=TOL)
      IF (IEND .LE. 10) THEN
         WRITE (NOUT,99999) T, Y
!                                   Finish up
         IF (IEND .EQ. 10) IDO = 3
         GO TO 10
      END IF
99998 FORMAT (11X, 'T', 14X, 'Y(1)', 11X, 'Y(2)', 11X, 'Y(3)')
99999 FORMAT (4F15.5)
      END
!
      SUBROUTINE FCN (N, X, Y, YPRIME)
!                                   SPECIFICATIONS FOR ARGUMENTS
      INTEGER    N
      REAL       X, Y(N), YPRIME(N)
!
      YPRIME(1) = Y(2)*Y(3)
      YPRIME(2) = -Y(1)*Y(3)
      YPRIME(3) = -0.51*Y(1)*Y(2)
      RETURN
      END
!
      SUBROUTINE FCNJ (N, X, Y, DYPDY)
!                                   SPECIFICATIONS FOR ARGUMENTS
      INTEGER    N
      REAL       X, Y(N), DYPDY(N,*)
!                                   This subroutine is never called
      RETURN
      END
```

Output

```
      T              Y(1)           Y(2)           Y(3)
 1.00000        0.80220        0.59705        0.81963
 2.00000        0.99537       -0.09615        0.70336
 3.00000        0.64141       -0.76720        0.88892
 4.00000       -0.26961       -0.96296        0.98129
 5.00000       -0.91173       -0.41079        0.75899
 6.00000       -0.95751        0.28841        0.72967
 7.00000       -0.42877        0.90342        0.95197
 8.00000        0.51092        0.85963        0.93106
 9.00000        0.97567        0.21926        0.71730
10.00000        0.87790       -0.47884        0.77906
```

Example 2

The BDF method of `IVPAG` is used to solve Example 2 of `IVPRK`. We set `PARAM`(12) = 2 to designate the BDF method. A chord or modified Newton method, with the Jacobian computed by divided differences, is used to solve the nonlinear equations. Thus, we set `PARAM`(13) = 2. The number of evaluations of y' is printed after the last output point, showing the efficiency gained when using a stiff solver compared to using `IVPRK` on this problem. The number of evaluations may vary, depending on the accuracy and other arithmetic characteristics of the computer.

```
      USE IVPAG_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    MXPARM, N
      PARAMETER  (MXPARM=50, N=2)
!                                 SPECIFICATIONS FOR PARAMETERS
      INTEGER    MABSE, MBDF, MSOLVE
      PARAMETER  (MABSE=1, MBDF=2, MSOLVE=2)
!                                 SPECIFICATIONS FOR LOCAL VARIABLES
      INTEGER    IDO, ISTEP, NOUT
      REAL       A(1,1), PARAM(MXPARM), T, TEND, TOL, Y(N)
!                                 SPECIFICATIONS FOR SUBROUTINES
!                                 SPECIFICATIONS FOR FUNCTIONS
      EXTERNAL   FCN, FCNJ
!
      CALL UMACH (2, NOUT)
!                                 Set initial conditions
      T = 0.0
      Y(1) = 1.0
      Y(2) = 0.0
!                                 Set error tolerance
      TOL = 0.001
!                                 Set PARAM to defaults
      PARAM = 0.0E0
!
      PARAM(10) = MABSE
!                                 Select BDF method
      PARAM(12) = MBDF
!                                 Select chord method and
!                                 a divided difference Jacobian.
      PARAM(13) = MSOLVE
!                                 Print header
      WRITE (NOUT,99998)
      IDO = 1
      ISTEP = 0
   10 CONTINUE
      ISTEP = ISTEP + 24
      TEND = ISTEP
!                                 The array a(*,*) is not used.
      CALL IVPAG (IDO, FCN, FCNJ, T, TEND, Y, TOL=TOL, &
                 PARAM=PARAM)
      IF (ISTEP .LE. 240) THEN
         WRITE (NOUT,'(I6,3F12.3)') ISTEP/24, T, Y
!                                 Final call to release workspace
         IF (ISTEP .EQ. 240) IDO = 3
         GO TO 10
      END IF
!                                 Show number of function calls.
      WRITE (NOUT,99999) PARAM(35)
99998 FORMAT (4X, 'ISTEP', 5X, 'Time', 9X, 'Y1', 11X, 'Y2')
99999 FORMAT (4X, 'Number of fcn calls with IVPAG =', F6.0)
      END
      SUBROUTINE FCN (N, T, Y, YPRIME)
!                                 SPECIFICATIONS FOR ARGUMENTS
      INTEGER    N
      REAL       T, Y(N), YPRIME(N)
!                                 SPECIFICATIONS FOR SAVE VARIABLES
      REAL       AK1, AK2, AK3
      SAVE       AK1, AK2, AK3
!
      DATA AK1, AK2, AK3/294.0E0, 3.0E0, 0.01020408E0/
!
      YPRIME(1) = -Y(1) - Y(1)*Y(2) + AK1*Y(2)
      YPRIME(2) = -AK2*Y(2) + AK3*(1.0E0-Y(2))*Y(1)
```

```
      RETURN
      END
      SUBROUTINE FCNJ (N, T, Y, DYPDY)
!                                  SPECIFICATIONS FOR ARGUMENTS
      INTEGER    N
      REAL       T, Y(N), DYPDY(N,*)
!
      RETURN
      END
```

Output

```
ISTEP     Time          Y1          Y2
 1      24.000        0.689       0.002
 2      48.000        0.636       0.002
 3      72.000        0.590       0.002
 4      96.000        0.550       0.002
 5     120.000        0.515       0.002
 6     144.000        0.485       0.002
 7     168.000        0.458       0.002
 8     192.000        0.434       0.001
 9     216.000        0.412       0.001
10     240.000        0.392       0.001
Number of fcn calls with IVPAG =   73.
```

Example 3

The BDF method of `IVPAG` is used to solve the so-called Robertson problem:

$$\begin{aligned}
&y_1{}' = -c_1 y_1 + c_2 y_2 y_3 && y_1(0) = 1 \\
&y_2{}' = -y_1{}' - y_3{}' && y_2(0) = 0 \\
&y_3{}' = c_3 y_2{}^2 && y_3(0) = 0 \\
&c_1 = 0.04,\ c_2 = 10^4,\ c_3 = 3 \times 10^7 && 0 \le t \le 10
\end{aligned}$$

Output is obtained after each unit of the independent variable. A user-provided subroutine for the Jacobian matrix is used. An absolute error tolerance of 10^{-5} is required.

```
      USE IVPAG_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    MXPARM, N
      PARAMETER  (MXPARM=50, N=3)
!                                  SPECIFICATIONS FOR PARAMETERS
      INTEGER    MABSE, MBDF, MSOLVE
      PARAMETER  (MABSE=1, MBDF=2, MSOLVE=1)
!                                  SPECIFICATIONS FOR LOCAL VARIABLES
      INTEGER    IDO, ISTEP, NOUT
      REAL       A(1,1), PARAM(MXPARM), T, TEND, TOL, Y(N)
!                                  SPECIFICATIONS FOR SUBROUTINES
!                                  SPECIFICATIONS FOR FUNCTIONS
      EXTERNAL   FCN, FCNJ
!
      CALL UMACH (2, NOUT)
!                                  Set initial conditions
```

```
      T = 0.0
      Y(1) = 1.0
      Y(2) = 0.0
      Y(3) = 0.0
!                                  Set error tolerance
      TOL = 1.0E-5
!                                  Set PARAM to defaults
      PARAM = 0.0E0

!                                  Select absolute error control
      PARAM(10) = MABSE
!                                  Select BDF method
      PARAM(12) = MBDF
!                                  Select chord method and
!                                  a user-provided Jacobian.
      PARAM(13) = MSOLVE
!                                  Print header
      WRITE (NOUT,99998)
      IDO = 1
      ISTEP = 0
   10 CONTINUE
      ISTEP = ISTEP + 1
      TEND = ISTEP
!                                  The array a(*,*) is not used.
      CALL IVPAG (IDO, FCN, FCNJ, T, TEND, Y, TOL=TOL, PARAM=PARAM)
      IF (ISTEP .LE. 10) THEN
         WRITE (NOUT,'(I6,F12.2,3F13.5)') ISTEP, T, Y
!                                  Final call to release workspace
         IF (ISTEP .EQ. 10) IDO = 3
         GO TO 10
      END IF
99998 FORMAT (4X, 'ISTEP', 5X, 'Time', 9X, 'Y1', 11X, 'Y2', 11X, &
            'Y3')
      END
      SUBROUTINE FCN (N, T, Y, YPRIME)
!                                  SPECIFICATIONS FOR ARGUMENTS
      INTEGER    N
      REAL       T, Y(N), YPRIME(N)
!                                  SPECIFICATIONS FOR SAVE VARIABLES
      REAL       C1, C2, C3
      SAVE       C1, C2, C3
!
      DATA C1, C2, C3/0.04E0, 1.0E4, 3.0E7/
!
      YPRIME(1) = -C1*Y(1) + C2*Y(2)*Y(3)
      YPRIME(3) = C3*Y(2)**2
      YPRIME(2) = -YPRIME(1) - YPRIME(3)
      RETURN
      END
      SUBROUTINE FCNJ (N, T, Y, DYPDY)
!                                  SPECIFICATIONS FOR ARGUMENTS
      INTEGER    N
      REAL       T, Y(N), DYPDY(N,*)
!                                  SPECIFICATIONS FOR SAVE VARIABLES
      REAL       C1, C2, C3
      SAVE       C1, C2, C3
!                                  SPECIFICATIONS FOR SUBROUTINES
      EXTERNAL   SSET
!
      DATA C1, C2, C3/0.04E0, 1.0E4, 3.0E7/
!                                  Clear array to zero
      CALL SSET (N**2, 0.0, DYPDY, 1)
!                                  Compute partials
      DYPDY(1,1) = -C1
      DYPDY(1,2) = C2*Y(3)
      DYPDY(1,3) = C2*Y(2)
```

```
      DYPDY(3,2) = 2.0*C3*Y(2)
      DYPDY(2,1) = -DYPDY(1,1)
      DYPDY(2,2) = -DYPDY(1,2) - DYPDY(3,2)
      DYPDY(2,3) = -DYPDY(1,3)
      RETURN
      END
```

Output

```
 ISTEP     Time         Y1           Y2           Y3
 1         1.00       0.96647      0.00003      0.03350
 2         2.00       0.94164      0.00003      0.05834
 3         3.00       0.92191      0.00002      0.07806
 4         4.00       0.90555      0.00002      0.09443
 5         5.00       0.89153      0.00002      0.10845
 6         6.00       0.87928      0.00002      0.12070
 7         7.00       0.86838      0.00002      0.13160
 8         8.00       0.85855      0.00002      0.14143
 9         9.00       0.84959      0.00002      0.15039
10        10.00       0.84136      0.00002      0.15862
```

Example 4

Solve the partial differential equation

$$e^{-t}\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}$$

with the initial condition

$$u(t = 0, x) = \sin x$$

and the boundary conditions

$$u(t, x = 0) = u(t, x = \pi) = 0$$

on the square $[0, 1] \times [0, \pi]$, using the method of lines with a piecewise-linear Galerkin discretization. The exact solution is $u(t, x) = \exp(1 - e^t) \sin x$. The interval $[0, \pi]$ is divided into equal intervals by choosing breakpoints $x_k = k\pi/(N + 1)$ for $k = 0, \ldots, N + 1$. The unknown function $u(t, x)$ is approximated by

$$\sum_{k=1}^{N} c_k(t)\phi_k(x)$$

where $\phi_k(x)$ is the piecewise linear function that equals 1 at x_k and is zero at all of the other breakpoints. We approximate the partial differential equation by a system of N ordinary differential equations, $A\, dc/dt = Rc$ where A and R are matrices of order N. The matrix A is given by

$$A_{ij} = \begin{cases} e^{-t}2h/3 \quad \text{if } i = j \\ e^{-t}\int_0^{\pi}\phi_i(x)\phi_j(x)\,dx = e^{-t}h/6 \quad \text{if } i = j \pm 1 \\ 0 \quad \text{otherwise} \end{cases}$$

where $h = 1/(N + 1)$ is the mesh spacing. The matrix R is given by

$$R_{ij} = \begin{cases} & -2/h \quad \text{if } i = j \\ \int_0^\pi \phi_i''(x)\phi_j(x)\,dx = & -\int_0^\pi \phi_i'(x)\phi_j'(x)\,dx = 1/h \quad \text{if } i = j \pm 1 \\ & 0 \text{ otherwise} \end{cases}$$

The integrals involving

$$\phi''_i$$

are assigned the values of the integrals on the right-hand side, by using the boundary values and integration by parts. Because this system may be stiff, Gear's BDF method is used.

In the following program, the array `Y`(1:`N`) corresponds to the vector of coefficients, c. Note that `Y` contains `N` + 2 elements; `Y`(0) and `Y`(`N` + 1) are used to store the boundary values. The matrix A depends on t so we set `PARAM`(19) = 2 and evaluate A when `IVPAG` returns with `IDO` = 7. The subroutine `FCN` computes the vector Rc, and the subroutine `FCNJ` computes R. The matrices A and R are stored as band-symmetric positive-definite structures having one upper co-diagonal.

```
      USE IVPAG_INT
      USE CONST_INT
      USE WRRRN_INT
      USE SSET_INT

      IMPLICIT   NONE
      INTEGER    LDA, N, NPARAM, NUC
      PARAMETER  (N=9, NPARAM=50, NUC=1, LDA=NUC+1)
!                                 SPECIFICATIONS FOR PARAMETERS
      INTEGER    NSTEP
      PARAMETER  (NSTEP=4)
!                                 SPECIFICATIONS FOR LOCAL VARIABLES
      INTEGER    I, IATYPE, IDO, IMETH, INORM, ISTEP, MITER, MTYPE
      REAL       A(LDA,N), C, HINIT, PARAM(NPARAM), PI, T, TEND, TMAX, &
                TOL, XPOINT(0:N+1), Y(0:N+1)
      CHARACTER  TITLE*10
!                                 SPECIFICATIONS FOR COMMON /COMHX/
      COMMON     /COMHX/ HX
      REAL       HX
!                                 SPECIFICATIONS FOR INTRINSICS
      INTRINSIC  EXP, REAL, SIN
      REAL       EXP, REAL, SIN
!                                 SPECIFICATIONS FOR SUBROUTINES
!                                 SPECIFICATIONS FOR FUNCTIONS
      EXTERNAL   FCN, FCNJ
!                                 Initialize PARAM
      HINIT  = 1.0E-3
      INORM  = 1
      IMETH  = 2
      MITER  = 1
      MTYPE  = 3
      IATYPE = 2
      PARAM = 0.0E0
      PARAM(1)  = HINIT
      PARAM(10) = INORM
```

```
      PARAM(12) = IMETH
      PARAM(13) = MITER
      PARAM(14) = MTYPE
      PARAM(16) = NUC
      PARAM(19) = IATYPE
!                                   Initialize other arguments
      PI = CONST('PI')
      HX = PI/REAL(N+1)
      CALL SSET (N-1, HX/6., A(1:,2), LDA)
      CALL SSET (N, 2.*HX/3., A(2:,1), LDA)
      DO 10  I=0, N + 1
         XPOINT(I) = I*HX
         Y(I)      = SIN(XPOINT(I))
   10 CONTINUE
      TOL  = 1.0E-6
      T    = 0.0
      TMAX = 1.0
!                                   Integrate ODE
      IDO   = 1
      ISTEP = 0
   20 CONTINUE
      ISTEP = ISTEP + 1
      TEND  = TMAX*REAL(ISTEP)/REAL(NSTEP)
   30 CALL IVPAG (IDO, FCN, FCNJ, T, TEND, Y(1:), NEQ=N, A=A, &
                 TOL=TOL, PARAM=PARAM)
!                                   Set matrix A
      IF (IDO .EQ. 7) THEN
         C = EXP(-T)
         CALL SSET (N-1, C*HX/6., A(1:,2), LDA)
         CALL SSET (N, 2.*C*HX/3., A(2:,1), LDA)
         GO TO 30
      END IF
      IF (ISTEP .LE. NSTEP) THEN
!                                   Print solution
         WRITE (TITLE,'(A,F5.3,A)') 'U(T=', T, ')'
         CALL WRRRN (TITLE, Y, 1, N+2, 1)
!                                   Final call to release workspace
         IF (ISTEP .EQ. NSTEP) IDO = 3
         GO TO 20
       END IF
       END
!
      SUBROUTINE FCN (N, T, Y, YPRIME)
!                                   SPECIFICATIONS FOR ARGUMENTS
      INTEGER    N
      REAL       T, Y(*), YPRIME(N)
!                                   SPECIFICATIONS FOR LOCAL VARIABLES
      INTEGER    I
!                                   SPECIFICATIONS FOR COMMON /COMHX/
      COMMON     /COMHX/ HX
      REAL       HX
!                                   SPECIFICATIONS FOR SUBROUTINES
      EXTERNAL   SSCAL
!
      YPRIME(1) = -2.0*Y(1) + Y(2)
      DO 10  I=2, N - 1
         YPRIME(I) = -2.0*Y(I) + Y(I-1) + Y(I+1)
   10 CONTINUE
      YPRIME(N) = -2.0*Y(N) + Y(N-1)
      CALL SSCAL (N, 1.0/HX, YPRIME, 1)
      RETURN
      END
!
      SUBROUTINE FCNJ (N, T, Y, DYPDY)
!                                   SPECIFICATIONS FOR ARGUMENTS
```

```
      INTEGER    N
      REAL       T, Y(*), DYPDY(2,*)
!                                  SPECIFICATIONS FOR COMMON /COMHX/
      COMMON     /COMHX/ HX
      REAL       HX
!                                  SPECIFICATIONS FOR SUBROUTINES
      EXTERNAL   SSET
!
      CALL SSET (N-1, 1.0/HX, DYPDY(1,2), 2)
      CALL SSET (N, -2.0/HX, DYPDY(2,1), 2)
      RETURN
      END
```

Output

```
                               U(T=0.250)
     1         2         3         4         5         6         7         8
0.0000    0.2321    0.4414    0.6076    0.7142    0.7510    0.7142    0.6076
     9        10        11
0.4414    0.2321    0.0000
                               U(T=0.500)
     1         2         3         4         5         6         7         8
0.0000    0.1607    0.3056    0.4206    0.4945    0.5199    0.4945    0.4206
     9        10        11
0.3056    0.1607    0.0000
                               U(T=0.750)
     1         2         3         4         5         6         7         8
0.0000    0.1002    0.1906    0.2623    0.3084    0.3243    0.3084    0.2623
     9        10        11
0.1906    0.1002    0.0000
                               U(T=1.000)
     1         2         3         4         5         6         7         8
0.0000    0.0546    0.1039    0.1431    0.1682    0.1768    0.1682    0.1431
     9        10        11
0.1039    0.0546    0.0000
```

BVPFD

Solves a (parameterized) system of differential equations with boundary conditions at two points, using a variable order, variable step size finite difference method with deferred corrections.

Required Arguments

FCNEQN — User-supplied `subroutine` to evaluate derivatives. The usage is
`CALL FCNEQN (N, T, Y, P, DYDT)`, where

`N` – Number of differential equations. (Input)

`T` – Independent variable, t. (Input)

`Y` – Array of size `N` containing the dependent variable values, y(t). (Input)

`P` – Continuation parameter, p. (Input)
See Comment 3.

`DYDT` – Array of size `N` containing the derivatives $y'(t)$. (Output)

The name `FCNEQN` must be declared `EXTERNAL` in the calling program.

FCNJAC — User-supplied `subroutine` to evaluate the Jacobian. The usage is
`CALL FCNJAC (N, T, Y, P, DYPDY)`, where

`N` – Number of differential equations. (Input)

`T` – Independent variable, t. (Input)

`Y` – Array of size `N` containing the dependent variable values. (Input)

`P` – Continuation parameter, p. (Input)
See Comments 3.

`DYPDY` – `N` by `N` array containing the partial derivatives $a_{i,j} = \partial f_i / \partial y_j$ evaluated at (t, y). The values $a_{i,j}$ are returned in `DYPDY(i, j)`. (Output)

The name `FCNJAC` must be declared `EXTERNAL` in the calling program.

FCNBC — User-supplied `subroutine` to evaluate the boundary conditions. The usage is
`CALL FCNBC (N, YLEFT, YRIGHT, P, H)`, where

`N` – Number of differential equations. (Input)

`YLEFT` – Array of size `N` containing the values of the dependent variable at the left endpoint. (Input)

`YRIGHT` – Array of size `N` containing the values of the dependent variable at the right endpoint. (Input)

`P` – Continuation parameter, p. (Input)
See Comment 3.

H – Array of size N containing the boundary condition residuals. (Output)
The boundary conditions are defined by $h_i = 0$; for $i = 1, \ldots, N$. The left endpoint conditions must be defined first, then, the conditions involving both endpoints, and finally the right endpoint conditions.

The name FCNBC must be declared EXTERNAL in the calling program.

FCNPEQ — User-supplied subroutine to evaluate the derivative of y' with respect to the parameter p. The usage is CALL FCNPEQ (N, T, Y, P, DYPDP), where

N – Number of differential equations. (Input)

T – Dependent variable, t. (Input)

Y – Array of size N containing the dependent variable values. (Input)

P – Continuation parameter, p. (Input)
See Comment 3.

DYPDP – Array of size N containing the derivative of y' evaluated at (t, y). (Output)

The name FCNPEQ must be declared EXTERNAL in the calling program.

FCNPBC — User-supplied subroutine to evaluate the derivative of the boundary conditions with respect to the parameter p. The usage is
CALL FCNPBC (N, YLEFT, YRIGHT, P, H), where

N – Number of differential equations. (Input)

YLEFT – Array of size N containing the values of the dependent variable at the left endpoint. (Input)

YRIGHT – Array of size N containing the values of the dependent variable at the right endpoint. (Input)

P – Continuation parameter, p. (Input)
See Comment 3.

H – Array of size N containing the derivative of f_i with respect to p. (Output)

The name FCNPBC must be declared EXTERNAL in the calling program.

NLEFT — Number of initial conditions. (Input)
The value NLEFT must be greater than or equal to zero and less than N.

NCUPBC — Number of coupled boundary conditions. (Input)
The value NLEFT + NCUPBC must be greater than zero and less than or equal to N.

TLEFT — The left endpoint. (Input)

TRIGHT — The right endpoint. (Input)

PISTEP — Initial increment size for p. (Input)
If this value is zero, continuation will not be used in this problem. The routines FCNPEQ and FCNPBC will not be called.

TOL — Relative error control parameter. (Input)
The computations stop when ABS(ERROR(J, I))/MAX(ABS(Y(J, I)), 1.0).LT.TOL for all J = 1, …, N and I = 1, …, NGRID. Here, ERROR(J, I) is the estimated error in Y(J, I).

TINIT — Array of size NINIT containing the initial grid points. (Input)

YINIT — Array of size N by NINIT containing an initial guess for the values of Y at the points in TINIT. (Input)

LINEAR — Logical .TRUE. if the differential equations and the boundary conditions are linear. (Input)

MXGRID — Maximum number of grid points allowed. (Input)

NFINAL — Number of final grid points, including the endpoints. (Output)

TFINAL — Array of size MXGRID containing the final grid points. (Output)
Only the first NFINAL points are significant.

YFINAL — Array of size N by MXGRID containing the values of Y at the points in TFINAL. (Output)

ERREST — Array of size N. (Output)
ERREST(J) is the estimated error in Y(J).

Optional Arguments

N — Number of differential equations. (Input)
Default: N = size (YINIT,1).

NINIT — Number of initial grid points, including the endpoints. (Input)
It must be at least 4.
Default: NINIT = size (TINIT,1).

LDYINI — Leading dimension of YINIT exactly as specified in the dimension statement of the calling program. (Input)
Default: LDYINI = size (YINIT,1).

PRINT — Logical .TRUE. if intermediate output is to be printed. (Input)
Default: PRINT = .FALSE.

LDYFIN — Leading dimension of YFINAL exactly as specified in the dimension statement of the calling program. (Input)
Default: LDYFIN = size (YFINAL,1).

FORTRAN 90 Interface

Generic: CALL BVPFD (FCNEQN, FCNJAC, FCNBC, FCNPEQ, FCNPBC, NLEFT, NCUPBC, TLEFT, TRIGHT, PISTEP, TOL, TINIT, YINIT, LINEAR, MXGRID, NFINAL, TFINAL, YFINAL, ERREST [, …])

Specific: The specific interface names are S_BVPFD and D_BVPFD.

FORTRAN 77 Interface

Single: CALL BVPFD (FCNEQN, FCNJAC, FCNBC, FCNPEQ, FCNPBC, N, NLEFT, NCUPBC, TLEFT, TRIGHT, PISTEP, TOL, NINIT, TINIT, YINIT, LDYINI, LINEAR, PRINT, MXGRID, NFINAL, TFINAL, YFINAL, LDYFIN, ERREST)

Double: The double precision name is DBVPFD.

Description

The routine BVPFD is based on the subprogram PASVA3 by M. Lentini and V. Pereyra (see Pereyra 1978). The basic discretization is the trapezoidal rule over a nonuniform mesh. This mesh is chosen adaptively, to make the local error approximately the same size everywhere. Higher-order discretizations are obtained by deferred corrections. Global error estimates are produced to control the computation. The resulting nonlinear algebraic system is solved by Newton's method with step control. The linearized system of equations is solved by a special form of Gauss elimination that preserves the sparseness.

Comments

1. Workspace may be explicitly provided, if desired, by use of B2PFD/DB2PFD. The reference is:

   CALL B2PFD (FCNEQN, FCNJAC, FCNBC, FCNPEQ, FCNPBC, N, NLEFT, NCUPBC, TLEFT, TRIGHT, PISTEP, TOL, NINIT, TINIT, YINIT, LDYINI, LINEAR, PRINT, MXGRID, NFINAL, TFINAL, YFINAL, LDYFIN, ERREST, RWORK, IWORK)

   The additional arguments are as follows:

   RWORK — Floating-point work array of size N(3N * MXGRID + 4N + 1) + MXGRID * (7N + 2).

   IWORK — Integer work array of size 2N * MXGRID + N + MXGRID.

2. Informational errors

Type	Code	Description
4	1	More than MXGRID grid points are needed to solve the problem.
4	2	Newton's method diverged.
3	3	Newton's method reached roundoff error level.

3. If the value of PISTEP is greater than zero, then the routine BVPFD assumes that the user has embedded the problem into a one-parameter family of problems:

$$y' = y'(t, y, p)$$
$$h(y_{tleft}, y_{tright}, p) = 0$$

such that for $p = 0$ the problem is simple. For $p = 1$, the original problem is recovered. The routine BVPFD automatically attempts to increment from $p = 0$ to $p = 1$. The value PISTEP is the beginning increment used in this continuation. The increment will usually be changed by routine BVPFD, but an arbitrary minimum of 0.01 is imposed.

4. The vectors TINIT and TFINAL may be the same.

5. The arrays YINIT and YFINAL may be the same.

Examples

Example 1

This example solves the third-order linear equation

$$y''' - 2y'' + y' - y = \sin t$$

subject to the boundary conditions $y(0) = y(2\pi)$ and $y'(0) = y'(2\pi) = 1$. (Its solution is $y = \sin t$.) To use BVPFD, the problem is reduced to a system of first-order equations by defining $y_1 = y, y_2 = y'$, and $y_3 = y''$. The resulting system is

$$\begin{aligned} y'_1 &= y_2 & y_2(0) - 1 &= 0 \\ y'_2 &= y_3 & y_1(0) - y_1(2\pi) &= 0 \\ y'_3 &= 2y_3 - y_2 + y_1 + \sin t & y_2(2\pi) - 1 &= 0 \end{aligned}$$

Note that there is one boundary condition at the left endpoint $t = 0$ and one boundary condition coupling the left and right endpoints. The final boundary condition is at the right endpoint. The total number of boundary conditions must be the same as the number of equations (in this case 3).

Note that since the parameter p is not used in the call to BVPFD, the routines FCNPEQ and FCNPBC are not needed. Therefore, in the call to BVPFD, FCNEQN and FCNBC were used in place of FCNPEQ and FCNPBC.

```
      USE BVPFD_INT
      USE UMACH_INT
      USE CONST_INT

      IMPLICIT   NONE
!                                  SPECIFICATIONS FOR PARAMETERS
      INTEGER    LDYFIN, LDYINI, MXGRID, NEQNS, NINIT
      PARAMETER  (MXGRID=45, NEQNS=3, NINIT=10, LDYFIN=NEQNS, &
```

```
                  LDYINI=NEQNS)
!                                   SPECIFICATIONS FOR LOCAL VARIABLES
      INTEGER    I, J, NCUPBC, NFINAL, NLEFT, NOUT
      REAL       ERREST(NEQNS), PISTEP, TFINAL(MXGRID), TINIT(NINIT), &
                 TLEFT, TOL, TRIGHT, YFINAL(LDYFIN,MXGRID), &
                 YINIT(LDYINI,NINIT)
      LOGICAL    LINEAR, PRINT
!                                   SPECIFICATIONS FOR INTRINSICS
      INTRINSIC  FLOAT
      REAL       FLOAT
!                                   SPECIFICATIONS FOR SUBROUTINES
!                                   SPECIFICATIONS FOR FUNCTIONS
      EXTERNAL   FCNBC, FCNEQN, FCNJAC
!                                   Set parameters
      NLEFT  = 1
      NCUPBC = 1
      TOL    = .001
      TLEFT  = 0.0
      TRIGHT = CONST('PI')
      TRIGHT = 2.0*TRIGHT
      PISTEP = 0.0
      PRINT  = .FALSE.
      LINEAR = .TRUE.
!                                   Define TINIT
      DO 10  I=1, NINIT
      TINIT(I) = TLEFT + (I-1)*(TRIGHT-TLEFT)/FLOAT(NINIT-1)
   10 CONTINUE
!                                   Set YINIT to zero
      YINIT = 0.0E0
!                                   Solve problem
      CALL BVPFD (FCNEQN, FCNJAC, FCNBC, FCNEQN, FCNBC, NLEFT, &
                  NCUPBC, TLEFT, TRIGHT, PISTEP, TOL, TINIT, &
                  YINIT, LINEAR, MXGRID, NFINAL, &
                  TFINAL, YFINAL, ERREST)
!                                   Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99997)
      WRITE (NOUT,99998) (I,TFINAL(I),(YFINAL(J,I),J=1,NEQNS),I=1, &
                        NFINAL)
      WRITE (NOUT,99999) (ERREST(J),J=1,NEQNS)
99997 FORMAT (4X, 'I', 7X, 'T', 14X, 'Y1', 13X, 'Y2', 13X, 'Y3')
99998 FORMAT (I5, 1P4E15.6)
99999 FORMAT (' Error estimates', 4X, 1P3E15.6)
      END
      SUBROUTINE FCNEQN (NEQNS, T, Y, P, DYDX)
!                                   SPECIFICATIONS FOR ARGUMENTS
      INTEGER    NEQNS
      REAL       T, P, Y(NEQNS), DYDX(NEQNS)
!                                   SPECIFICATIONS FOR INTRINSICS
      INTRINSIC  SIN
      REAL       SIN
!                                   Define PDE
      DYDX(1) = Y(2)
      DYDX(2) = Y(3)
      DYDX(3) = 2.0*Y(3) - Y(2) + Y(1) + SIN(T)
      RETURN
      END
      SUBROUTINE FCNJAC (NEQNS, T, Y, P, DYPDY)
!                                   SPECIFICATIONS FOR ARGUMENTS
      INTEGER    NEQNS
      REAL       T, P, Y(NEQNS), DYPDY(NEQNS,NEQNS)
!                                   Define d(DYDX)/dY
      DYPDY(1,1) = 0.0
      DYPDY(1,2) = 1.0
      DYPDY(1,3) = 0.0
      DYPDY(2,1) = 0.0
```

```
      DYPDY(2,2) = 0.0
      DYPDY(2,3) = 1.0
      DYPDY(3,1) = 1.0
      DYPDY(3,2) = -1.0
      DYPDY(3,3) = 2.0
      RETURN
      END
      SUBROUTINE FCNBC (NEQNS, YLEFT, YRIGHT, P, F)
!                                 SPECIFICATIONS FOR ARGUMENTS
      INTEGER    NEQNS
      REAL       P, YLEFT(NEQNS), YRIGHT(NEQNS), F(NEQNS)
!                                 Define boundary conditions
      F(1) = YLEFT(2) - 1.0
      F(2) = YLEFT(1) - YRIGHT(1)
      F(3) = YRIGHT(2) - 1.0
      RETURN
      END
```

Output

```
 I       T              Y1             Y2             Y3
 1   0.000000E+00  -1.123191E-04   1.000000E+00   6.242319E-05
 2   3.490659E-01   3.419107E-01   9.397087E-01  -3.419580E-01
 3   6.981317E-01   6.426908E-01   7.660918E-01  -6.427230E-01
 4   1.396263E+00   9.847531E-01   1.737333E-01  -9.847453E-01
 5   2.094395E+00   8.660529E-01  -4.998747E-01  -8.660057E-01
 6   2.792527E+00   3.421830E-01  -9.395474E-01  -3.420648E-01
 7   3.490659E+00  -3.417234E-01  -9.396111E-01   3.418948E-01
 8   4.188790E+00  -8.656880E-01  -5.000588E-01   8.658733E-01
 9   4.886922E+00  -9.845794E-01   1.734571E-01   9.847518E-01
10   5.585054E+00  -6.427721E-01   7.658258E-01   6.429526E-01
11   5.934120E+00  -3.420819E-01   9.395434E-01   3.423986E-01
12   6.283185E+00  -1.123186E-04   1.000000E+00   6.743190E-04
Error estimates     2.840430E-04   1.792939E-04   5.588399E-04
```

Example 2

In this example, the following nonlinear problem is solved:

$$y'' - y^3 + (1 + \sin^2 t) \sin t = 0$$

with $y(0) = y(\pi) = 0$. Its solution is $y = \sin t$. As in Example 1, this equation is reduced to a system of first-order differential equations by defining $y_1 = y$ and $y_2 = y'$. The resulting system is

$$\begin{aligned} y'_1 &= y_2 & y_1(0) &= 0 \\ y'_2 &= y_1^3 - \left(1 + \sin^2 t\right)\sin t & y_1(\pi) &= 0 \end{aligned}$$

In this problem, there is one boundary condition at the left endpoint and one at the right endpoint; there are no coupled boundary conditions.

Note that since the parameter p is not used, in the call to BVPFD the routines FCNPEQ and FCNPBC are not needed. Therefore, in the call to BVPFD, FCNEQN and FCNBC were used in place of FCNPEQ and FCNPBC.

```
      USE BVPFD_INT
      USE UMACH_INT
      USE CONST_INT
```

```
      IMPLICIT   NONE

!                                 SPECIFICATIONS FOR PARAMETERS
      INTEGER    LDYFIN, LDYINI, MXGRID, NEQNS, NINIT
      PARAMETER  (MXGRID=45, NEQNS=2, NINIT=12, LDYFIN=NEQNS, &
                 LDYINI=NEQNS)
!                                 SPECIFICATIONS FOR LOCAL VARIABLES
      INTEGER    I, J, NCUPBC, NFINAL, NLEFT, NOUT
      REAL       ERREST(NEQNS), PISTEP, TFINAL(MXGRID), TINIT(NINIT), &
                 TLEFT, TOL, TRIGHT, YFINAL(LDYFIN,MXGRID), &
                 YINIT(LDYINI,NINIT)
      LOGICAL    LINEAR, PRINT
!                                 SPECIFICATIONS FOR INTRINSICS
      INTRINSIC  FLOAT
      REAL       FLOAT
!                                 SPECIFICATIONS FOR FUNCTIONS
      EXTERNAL   FCNBC, FCNEQN, FCNJAC
!                                 Set parameters
      NLEFT  = 1
      NCUPBC = 0
      TOL    = .001
      TLEFT  = 0.0
      TRIGHT = CONST('PI')
      PISTEP = 0.0
      PRINT  = .FALSE.
      LINEAR = .FALSE.
!                                 Define TINIT and YINIT
      DO 10  I=1, NINIT
         TINIT(I)   = TLEFT + (I-1)*(TRIGHT-TLEFT)/FLOAT(NINIT-1)
         YINIT(1,I) = 0.4*(TINIT(I)-TLEFT)*(TRIGHT-TINIT(I))
         YINIT(2,I) = 0.4*(TLEFT-TINIT(I)+TRIGHT-TINIT(I))
   10 CONTINUE
!                                 Solve problem
      CALL BVPFD (FCNEQN, FCNJAC, FCNBC, FCNEQN, FCNBC, NLEFT, &
                  NCUPBC, TLEFT, TRIGHT, PISTEP, TOL, TINIT, &
                  YINIT, LINEAR, MXGRID, NFINAL, &
                  TFINAL, YFINAL, ERREST)
!                                 Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99997)
      WRITE (NOUT,99998) (I,TFINAL(I),(YFINAL(J,I),J=1,NEQNS),I=1, &
                        NFINAL)
      WRITE (NOUT,99999) (ERREST(J),J=1,NEQNS)
99997 FORMAT (4X, 'I', 7X, 'T', 14X, 'Y1', 13X, 'Y2')
99998 FORMAT (I5, 1P3E15.6)
99999 FORMAT (' Error estimates', 4X, 1P2E15.6)
      END
      SUBROUTINE FCNEQN (NEQNS, T, Y, P, DYDT)
!                                 SPECIFICATIONS FOR ARGUMENTS
      INTEGER    NEQNS
      REAL       T, P, Y(NEQNS), DYDT(NEQNS)
!                                 SPECIFICATIONS FOR INTRINSICS
      INTRINSIC  SIN
      REAL       SIN
!                                 Define PDE
      DYDT(1) = Y(2)
      DYDT(2) = Y(1)**3 - SIN(T)*(1.0+SIN(T)**2)
      RETURN
      END
      SUBROUTINE FCNJAC (NEQNS, T, Y, P, DYPDY)
!                                 SPECIFICATIONS FOR ARGUMENTS
      INTEGER    NEQNS
      REAL       T, P, Y(NEQNS), DYPDY(NEQNS,NEQNS)
!                                 Define d(DYDT)/dY
      DYPDY(1,1) = 0.0
```

```
      DYPDY(1,2) = 1.0
      DYPDY(2,1) = 3.0*Y(1)**2
      DYPDY(2,2) = 0.0
      RETURN
      END
      SUBROUTINE FCNBC (NEQNS, YLEFT, YRIGHT, P, F)
!                                SPECIFICATIONS FOR ARGUMENTS
      INTEGER    NEQNS
      REAL       P, YLEFT(NEQNS), YRIGHT(NEQNS), F(NEQNS)
!                                Define boundary conditions
      F(1) = YLEFT(1)
      F(2) = YRIGHT(1)
      RETURN
      END
```

Output

```
  I       T              Y1              Y2
  1   0.000000E+00   0.000000E+00   9.999277E-01
  2   2.855994E-01   2.817682E-01   9.594315E-01
  3   5.711987E-01   5.406458E-01   8.412407E-01
  4   8.567980E-01   7.557380E-01   6.548904E-01
  5   1.142397E+00   9.096186E-01   4.154530E-01
  6   1.427997E+00   9.898143E-01   1.423307E-01
  7   1.713596E+00   9.898143E-01  -1.423307E-01
  8   1.999195E+00   9.096185E-01  -4.154530E-01
  9   2.284795E+00   7.557380E-01  -6.548903E-01
 10   2.570394E+00   5.406460E-01  -8.412405E-01
 11   2.855994E+00   2.817683E-01  -9.594313E-01
 12   3.141593E+00   0.000000E+00  -9.999274E-01
 Error estimates     3.906105E-05   7.124186E-05
```

Example 3

In this example, the following nonlinear problem is solved:

$$y'' - y^3 = \frac{40}{9}\left(t - \frac{1}{2}\right)^{2/3} - \left(t - \frac{1}{2}\right)^8$$

with $y(0) = y(1) = \pi/2$. As in the previous examples, this equation is reduced to a system of first-order differential equations by defining $y_1 = y$ and $y_2 = y'$. The resulting system is

$$\begin{aligned} y'_1 &= y_2 & y_1(0) &= \pi/2 \\ y'_2 &= y_1^3 - \tfrac{40}{9}\left(t - \tfrac{1}{2}\right)^{2/3} + \left(t - \tfrac{1}{2}\right)^8 & y_1(1) &= \pi/2 \end{aligned}$$

The problem is embedded in a family of problems by introducing the parameter p and by changing the second differential equation to

$$y'_2 = py_1^3 + \frac{40}{9}\left(t - \frac{1}{2}\right)^{2/3} - \left(t - \frac{1}{2}\right)^8$$

At $p = 0$, the problem is linear; and at $p = 1$, the original problem is recovered. The derivatives $\partial y'/\partial p$ must now be specified in the subroutine FCNPEQ. The derivatives $\partial f/\partial p$ are zero in FCNPBC.

```
      USE BVPFD_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                  SPECIFICATIONS FOR PARAMETERS
      INTEGER    LDYFIN, LDYINI, MXGRID, NEQNS, NINIT
      PARAMETER  (MXGRID=45, NEQNS=2, NINIT=5, LDYFIN=NEQNS, &
                 LDYINI=NEQNS)
!                                  SPECIFICATIONS FOR LOCAL VARIABLES
      INTEGER    NCUPBC, NFINAL, NLEFT, NOUT
      REAL       ERREST(NEQNS), PISTEP, TFINAL(MXGRID), TLEFT, TOL, &
                 XRIGHT, YFINAL(LDYFIN,MXGRID)
      LOGICAL    LINEAR, PRINT
!                                  SPECIFICATIONS FOR SAVE VARIABLES
      INTEGER    I, J
      REAL       TINIT(NINIT), YINIT(LDYINI,NINIT)
      SAVE       I, J, TINIT, YINIT
!                                  SPECIFICATIONS FOR FUNCTIONS
      EXTERNAL   FCNBC, FCNEQN, FCNJAC, FCNPBC, FCNPEQ
!
      DATA TINIT/0.0, 0.4, 0.5, 0.6, 1.0/
      DATA ((YINIT(I,J),J=1,NINIT),I=1,NEQNS)/0.15749, 0.00215, 0.0, &
          0.00215, 0.15749, -0.83995, -0.05745, 0.0, 0.05745, 0.83995/
!                                  Set parameters
      NLEFT  = 1
      NCUPBC = 0
      TOL    = .001
      TLEFT  = 0.0
      XRIGHT = 1.0
      PISTEP = 0.1
      PRINT  = .FALSE.
      LINEAR = .FALSE.
!
      CALL BVPFD (FCNEQN, FCNJAC, FCNBC, FCNPEQ, FCNPBC, NLEFT, &
                  NCUPBC, TLEFT, XRIGHT, PISTEP, TOL, TINIT, &
                  YINIT, LINEAR, MXGRID, NFINAL,TFINAL, YFINAL, ERREST)
!                                  Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99997)
      WRITE (NOUT,99998) (I,TFINAL(I),(YFINAL(J,I),J=1,NEQNS),I=1, &
                       NFINAL)
      WRITE (NOUT,99999) (ERREST(J),J=1,NEQNS)
99997 FORMAT (4X, 'I', 7X, 'T', 14X, 'Y1', 13X, 'Y2')
99998 FORMAT (I5, 1P3E15.6)
99999 FORMAT (' Error estimates', 4X, 1P2E15.6)
      END
      SUBROUTINE FCNEQN (NEQNS, T, Y, P, DYDT)
!                                   SPECIFICATIONS FOR ARGUMENTS
      INTEGER    NEQNS
      REAL       T, P, Y(NEQNS), DYDT(NEQNS)
!                                  Define PDE
      DYDT(1) = Y(2)
      DYDT(2) = P*Y(1)**3 + 40./9.*((T-0.5)**2)**(1./3.) - (T-0.5)**8
      RETURN
      END
      SUBROUTINE FCNJAC (NEQNS, T, Y, P, DYPDY)
!                                  SPECIFICATIONS FOR ARGUMENTS
      INTEGER    NEQNS
      REAL       T, P, Y(NEQNS), DYPDY(NEQNS,NEQNS)
!                                  Define d(DYDT)/dY
      DYPDY(1,1) = 0.0
      DYPDY(1,2) = 1.0
      DYPDY(2,1) = P*3.*Y(1)**2
      DYPDY(2,2) = 0.0
      RETURN
```

```
      END
      SUBROUTINE FCNBC (NEQNS, YLEFT, YRIGHT, P, F)
      USE CONST_INT
!                                 SPECIFICATIONS FOR ARGUMENTS
      INTEGER    NEQNS
      REAL       P, YLEFT(NEQNS), YRIGHT(NEQNS), F(NEQNS)
!                                 SPECIFICATIONS FOR LOCAL VARIABLES
      REAL       PI
!                                 Define boundary conditions
      PI   = CONST('PI')
      F(1) = YLEFT(1) - PI/2.0
      F(2) = YRIGHT(1) - PI/2.0
      RETURN
      END
      SUBROUTINE FCNPEQ (NEQNS, T, Y, P, DYPDP)
!                                 SPECIFICATIONS FOR ARGUMENTS
      INTEGER    NEQNS
      REAL       T, P, Y(NEQNS), DYPDP(NEQNS)
!                                 Define d(DYDT)/dP
      DYPDP(1) = 0.0
      DYPDP(2) = Y(1)**3
      RETURN
      END
      SUBROUTINE FCNPBC (NEQNS, YLEFT, YRIGHT, P, DFDP)
!                                 SPECIFICATIONS FOR ARGUMENTS
      INTEGER    NEQNS
      REAL       P, YLEFT(NEQNS), YRIGHT(NEQNS), DFDP(NEQNS)
!                                 SPECIFICATIONS FOR SUBROUTINES
      EXTERNAL   SSET
!                                 Define dF/dP
      CALL SSET (NEQNS, 0.0, DFDP, 1)
      RETURN
      END
```

Output

```
  I      T              Y1             Y2
  1   0.000000E+00   1.570796E+00  -1.949336E+00
  2   4.444445E-02   1.490495E+00  -1.669567E+00
  3   8.888889E-02   1.421951E+00  -1.419465E+00
  4   1.333333E-01   1.363953E+00  -1.194307E+00
  5   2.000000E-01   1.294526E+00  -8.958461E-01
  6   2.666667E-01   1.243628E+00  -6.373191E-01
  7   3.333334E-01   1.208785E+00  -4.135206E-01
  8   4.000000E-01   1.187783E+00  -2.219351E-01
  9   4.250000E-01   1.183038E+00  -1.584200E-01
 10   4.500000E-01   1.179822E+00  -9.973146E-02
 11   4.625000E-01   1.178748E+00  -7.233893E-02
 12   4.750000E-01   1.178007E+00  -4.638248E-02
 13   4.812500E-01   1.177756E+00  -3.399763E-02
 14   4.875000E-01   1.177582E+00  -2.205547E-02
 15   4.937500E-01   1.177480E+00  -1.061177E-02
 16   5.000000E-01   1.177447E+00  -1.479182E-07
 17   5.062500E-01   1.177480E+00   1.061153E-02
 18   5.125000E-01   1.177582E+00   2.205518E-02
 19   5.187500E-01   1.177756E+00   3.399727E-02
 20   5.250000E-01   1.178007E+00   4.638219E-02
 21   5.375000E-01   1.178748E+00   7.233876E-02
 22   5.500000E-01   1.179822E+00   9.973124E-02
 23   5.750000E-01   1.183038E+00   1.584199E-01
 24   6.000000E-01   1.187783E+00   2.219350E-01
 25   6.666667E-01   1.208786E+00   4.135205E-01
 26   7.333333E-01   1.243628E+00   6.373190E-01
 27   8.000000E-01   1.294526E+00   8.958461E-01
 28   8.666667E-01   1.363953E+00   1.194307E+00
```

```
 29   9.111111E-01   1.421951E+00   1.419465E+00
 30   9.555556E-01   1.490495E+00   1.669566E+00
 31   1.000000E+00   1.570796E+00   1.949336E+00
 Error estimates     3.448358E-06   5.549869E-05
```

BVPMS

more...

Solves a (parameterized) system of differential equations with boundary conditions at two points, using a multiple-shooting method.

Required Arguments

FCNEQN — User-supplied `subroutine` to evaluate derivatives. The usage is
`CALL FCNEQN (NEQNS, T, Y, P, DYDT)`, where

`NEQNS` – Number of equations. (Input)

`T` – Independent variable, *t*. (Input)

`Y` – Array of length `NEQNS` containing the dependent variable. (Input)

`P` – Continuation parameter used in solving highly nonlinear problems. (Input)
See Comment 4.

`DYDT` – Array of length `NEQNS` containing y' at `T`. (Output)

The name `FCNEQN` must be declared `EXTERNAL` in the calling program.

FCNJAC — User-supplied `subroutine` to evaluate the Jacobian. The usage is
`CALL FCNJAC (NEQNS, T, Y, P, DYPDY)`, where

`NEQNS` – Number of equations. (Input)

`T` – Independent variable. (Input)

`Y` – Array of length `NEQNS` containing the dependent variable. (Input)

`P` – Continuation parameter used in solving highly nonlinear problems. (Input)
See Comment 4.

`DYPDY` – Array of size `NEQNS` by `NEQNS` containing the Jacobian. (Output)
The entry `DYPDY`(*i*, *j*) contains the partial derivative $\partial f_i / \partial y_j$ evaluated at (*t*, *y*).

The name `FCNJAC` must be declared `EXTERNAL` in the calling program.

FCNBC — User-supplied `subroutine` to evaluate the boundary conditions. The usage is `CALL FCNBC (NEQNS, YLEFT, YRIGHT, P, H)`, where

`NEQNS` – Number of equations. (Input)

YLEFT – Array of length NEQNS containing the values of Y at TLEFT. (Input)

YRIGHT – Array of length NEQNS containing the values of Y at TRIGHT. (Input)

P – Continuation parameter used in solving highly nonlinear problems. (Input)
See Comment 4.

H – Array of length NEQNS containing the boundary function values. (Output)
The computed solution satisfies (within BTOL) the conditions $h_i = 0$, $i = 1, \ldots,$ NEQNS.

The name FCNBC must be declared EXTERNAL in the calling program.

TLEFT — The left endpoint. (Input)

TRIGHT — The right endpoint. (Input)

NMAX — Maximum number of shooting points to be allowed. (Input)
If NINIT is nonzero, then NMAX must equal NINIT. It must be at least 2.

NFINAL — Number of final shooting points, including the endpoints. (Output)

TFINAL — Vector of length NMAX containing the final shooting points. (Output)
Only the first NFINAL points are significant.

YFINAL — Array of size NEQNS by NMAX containing the values of Y at the points in TFINAL. (Output)

Optional Arguments

NEQNS — Number of differential equations. (Input)

DTOL — Differential equation error tolerance. (Input)
An attempt is made to control the local error in such a way that the global error is proportional to DTOL.
Default: DTOL = 1.0e-4.

BTOL — Boundary condition error tolerance. (Input)
The computed solution satisfies the boundary conditions, within BTOL tolerance.
Default: BTOL = 1.0e-4.

MAXIT — Maximum number of Newton iterations allowed. (Input)
Iteration stops if convergence is achieved sooner. Suggested values are MAXIT = 2 for linear problems and MAXIT = 9 for nonlinear problems.
Default: MAXIT = 9.

NINIT — Number of shooting points supplied by the user. (Input)
It may be 0. A suggested value for the number of shooting points is 10.
Default: NINIT = 0.

TINIT — Vector of length NINIT containing the shooting points supplied by the user. (Input)
If NINIT = 0, then TINIT is not referenced and the routine chooses all of the shooting points. This automatic selection of shooting points may be expensive and should only be used for linear problems. If NINIT is nonzero, then the points must be an increasing sequence with TINIT(1) = TLEFT and TINIT(NINIT) = TRIGHT. By default, TINIT is not used.

YINIT — Array of size NEQNS by NINIT containing an initial guess for the values of Y at the points in TINIT. (Input)
YINIT is not referenced if NINIT = 0. By default, YINIT is not used.

LDYINI — Leading dimension of YINIT exactly as specified in the dimension statement of the calling program. (Input)
Default: LDYINI = size (YINIT ,1).

LDYFIN — Leading dimension of YFINAL exactly as specified in the dimension statement of the calling program. (Input)
Default: LDYFIN = size (YFINAL,1).

FORTRAN 90 Interface

Generic: CALL BVPMS (FCNEQN, FCNJAC, FCNBC, TLEFT, TRIGHT, NMAX, NFINAL, TFINAL, YFINAL [, …])

Specific: The specific interface names are S_BVPMS and D_BVPMS.

FORTRAN 77 Interface

Single: CALL BVPMS (FCNEQN, FCNJAC, FCNBC, NEQNS, TLEFT, TRIGHT, DTOL, BTOL, MAXIT, NINIT, TINIT, YINIT, LDYINI, NMAX, NFINAL, TFINAL, YFINAL, LDYFIN)

Double: The double precision name is DBVPMS.

Description

Define N = NEQNS, M = NFINAL, t_a = TLEFT and t_b = TRIGHT. The routine BVPMS uses a multiple-shooting technique to solve the differential equation system $y' = f(t, y)$ with boundary conditions of the form

$$\mathrm{h}_k(y_1(t_a), \ldots, y_N(t_a), y_1(t_b), \ldots, y_N(t_b)) = 0 \quad \text{for } k = 1, \ldots, N$$

A modified version of IVPRK is used to compute the initial-value problem at each "shot." If there are M shooting points (including the endpoints t_a and t_b), then a system of NM simultaneous nonlinear equations must be solved. Newton's method is used to solve this system, which has a Jacobian matrix with a "periodic band" structure. Evaluation of the NM functions and the $NM \times NM$ (almost banded) Jacobian for one iteration of Newton's method is accomplished in one pass from t_a to t_b of the modified IVPRK, operating on a system of $N(N + 1)$ differential equations. For most problems, the total amount of work should not be highly dependent on M. Multiple shooting avoids many of the serious ill-conditioning problems that plague simple shooting methods. For more details on the algorithm, see Sewell (1982).

The boundary functions should be scaled so that all components h_k are of comparable magnitude since the absolute error in each is controlled.

Comments

1. Workspace may be explicitly provided, if desired, by use of B2PMS/DB2PMS. The reference is:

   CALL B2PMS (FCNEQN, FCNJAC, FCNBC, NEQNS, TLEFT, TRIGHT, DTOL, BTOL, MAXIT, NINIT, TINIT, YINIT, LDYINI, NMAX, NFINAL, TFINAL, YFINAL, LDYFIN, WORK, IWK)

   The additional arguments are as follows:

   WORK — Work array of length NEQNS * (NEQNS + 1) (NMAX + 12) + NEQNS + 30.

   IWK — Work array of length NEQNS.

2. Informational errors

Type	Code	Description
1	5	Convergence has been achieved; but to get acceptably accurate approximations to $y(t)$, it is often necessary to start an initial-value solver, for example IVPRK, at the nearest TFINAL(i) point to t with $t \geq$ TFINAL (i). The vectors YFINAL(j, i), $j = 1, \ldots,$ NEQNS are used as the initial values.
4	1	The initial-value integrator failed. Relax the tolerance DTOL or see Comment 3.
4	2	More than NMAX shooting points are needed for stability.
4	3	Newton's iteration did not converge in MAXIT iterations. If the problem is linear, do an extra iteration. If this error still occurs, check that the routine FCNJAC is giving the correct derivatives. If this does not fix the problem, see Comment 3.
4	4	Linear-equation solver failed. The problem may not have a unique solution, or the problem may be highly nonlinear. In the latter case, see Comment 3.

3. Many linear problems will be successfully solved using program-selected shooting points. Nonlinear problems may require user effort and input data. If the routine fails, then increase NMAX or parameterize the problem. With many shooting points the program essentially uses a finite-difference

method, which has less trouble with nonlinearities than shooting methods. After a certain point, however, increasing the number of points will no longer help convergence. To parameterize the problem, see Comment 4.

4. If the problem to be solved is highly nonlinear, then to obtain convergence it may be necessary to embed the problem into a one-parameter family of boundary value problems, $y' = f(t, y, p)$, $h(y(t_a, t_b, p)) = 0$ such that for $p = 0$, the problem is simple, e.g., linear; and for $p = 1$, the stated problem is solved. The routine `BVPMS/DBVPMS` automatically moves the parameter from $p = 0$ toward $p = 1$.

5. This routine is not recommended for stiff systems of differential equations.

Example

The differential equations that model an elastic beam are (see Washizu 1968, pages 142−143):

$$
\begin{aligned}
&M_{xx} - \frac{NM}{EI} + L(x) = 0 \\
&EIW_{xx} + M = 0 \\
&EA_0\left(U_x + W_x^2/2\right) - N = 0 \\
&N_x = 0
\end{aligned}
$$

where **U** is the axial displacement, **W** is the transverse displacement, **N** is the axial force, **M** is the bending moment, **E** is the elastic modulus, **I** is the moment of inertia, $\mathbf{A}_0$ is the cross-sectional area, and **L**(x) is the transverse load.

Assume we have a clamped cylindrical beam of radius 0.1in, a length of 10in, and an elastic modulus $\mathbf{E} = 10.6 \times 10^6$ lb/in^2. Then, $\mathbf{I} = 0.784 \times 10^{-4}$, and $\mathbf{A}_0 = \pi 10^{-2}$ in^2, and the boundary conditions are $\mathbf{U} = \mathbf{W} = \mathbf{W}_x = 0$ at each end. If we let $y_1 = \mathbf{U}$, $y_2 = \mathbf{N}/\mathbf{EA}_0$, $y_3 = \mathbf{W}$, $y_4 = \mathbf{W}_x$, $y_5 = \mathbf{M}/\mathbf{EI}$, and $y_6 = \mathbf{M}_x/\mathbf{EI}$, then the above nonlinear equations can be written as a system of six first-order equations.

$$y'_1 = y_2 - \frac{y_4^2}{2}$$
$$y'_2 = 0$$
$$y'_3 = y_4$$
$$y'_4 = -y_5$$
$$y'_5 = y_6$$
$$y'_6 = \frac{\mathbf{A}_0 y_2 y_5}{\mathbf{I}} - \frac{\mathbf{L}(x)}{\mathbf{EI}}$$

The boundary conditions are $y_1 = y_3 = y_4 = 0$ at $x = 0$ and at $x = 10$. The loading function is $\mathbf{L}(x) = -2$, if $3 \le x \le 7$, and is zero elsewhere.

The material parameters, $\mathbf{A}_0$ = `A0`, $\mathbf{I}$ = `AI`, and $\mathbf{E}$, are passed to the evaluation subprograms using the common block `PARAM`.

```
      USE BVPMS_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    LDY, NEQNS, NMAX
      PARAMETER  (NEQNS=6, NMAX=21, LDY=NEQNS)
!                                  SPECIFICATIONS FOR LOCAL VARIABLES
      INTEGER    I, MAXIT, NFINAL, NINIT, NOUT
      REAL       TOL, X(NMAX), XLEFT, XRIGHT, Y(LDY,NMAX)
!                                  SPECIFICATIONS FOR COMMON /PARAM/
      COMMON     /PARAM/ A0, A1, E
      REAL       A0, A1, E
!                                  SPECIFICATIONS FOR INTRINSICS
      INTRINSIC  REAL
      REAL       REAL
!                                  SPECIFICATIONS FOR SUBROUTINES
      EXTERNAL   FCNBC, FCNEQN, FCNJAC
!                                  Set material parameters
      A0 = 3.14E-2
      A1 = 0.784E-4
      E  = 10.6E6
!                                  Set parameters for BVPMS
      XLEFT  = 0.0
      XRIGHT = 10.0
      MAXIT  = 19
      NINIT  = NMAX
      Y = 0.0E0
!                                  Define the shooting points
      DO 10  I=1, NINIT
         X(I) = XLEFT + REAL(I-1)/REAL(NINIT-1)*(XRIGHT-XLEFT)
   10 CONTINUE
!                                  Solve problem
      CALL BVPMS (FCNEQN, FCNJAC, FCNBC, XLEFT, XRIGHT, NMAX, NFINAL, &
                  X, Y,  MAXIT=MAXIT, NINIT=NINIT, TINIT=X, YINIT=Y)

!                                  Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,'(26X,A/12X,A,10X,A,7X,A)') 'Displacement', &
                                      'X', 'Axial', 'Transvers'// &
                                      'e'
      WRITE (NOUT,'(F15.1,1P2E15.3)') (X(I),Y(1,I),Y(3,I),I=1,NFINAL)
      END
```

```
      SUBROUTINE FCNEQN (NEQNS, X, Y, P, DYDX)
!                                SPECIFICATIONS FOR ARGUMENTS
      INTEGER    NEQNS
      REAL       X, P, Y(NEQNS), DYDX(NEQNS)
!                                SPECIFICATIONS FOR LOCAL VARIABLES
      REAL       FORCE
!                                SPECIFICATIONS FOR COMMON /PARAM/
      COMMON     /PARAM/ A0, A1, E
      REAL       A0, A1, E
!                                Define derivatives
      FORCE = 0.0
      IF (X.GT.3.0 .AND. X.LT.7.0) FORCE = -2.0
      DYDX(1) = Y(2) - P*0.5*Y(4)**2
      DYDX(2) = 0.0
      DYDX(3) = Y(4)
      DYDX(4) = -Y(5)
      DYDX(5) = Y(6)
      DYDX(6) = P*A0*Y(2)*Y(5)/A1 - FORCE/E/A1
      RETURN
      END
      SUBROUTINE FCNBC (NEQNS, YLEFT, YRIGHT, P, F)
!                                SPECIFICATIONS FOR ARGUMENTS
      INTEGER    NEQNS
      REAL       P, YLEFT(NEQNS), YRIGHT(NEQNS), F(NEQNS)
!                                SPECIFICATIONS FOR COMMON /PARAM/
      COMMON     /PARAM/ A0, A1, E
      REAL       A0, A1, E
!                                Define boundary conditions
      F(1) = YLEFT(1)
      F(2) = YLEFT(3)
      F(3) = YLEFT(4)
      F(4) = YRIGHT(1)
      F(5) = YRIGHT(3)
      F(6) = YRIGHT(4)
      RETURN
      END
      SUBROUTINE FCNJAC (NEQNS, X, Y, P, DYPDY)
!                                SPECIFICATIONS FOR ARGUMENTS
      INTEGER    NEQNS
      REAL       X, P, Y(NEQNS), DYPDY(NEQNS,NEQNS)
!                                SPECIFICATIONS FOR COMMON /PARAM/
      COMMON     /PARAM/ A0, A1, E
      REAL       A0, A1, E
!                                SPECIFICATIONS FOR SUBROUTINES
!                                Define partials, d(DYDX)/dY
      DYPDY = 0.0E0
      DYPDY(1,2) = 1.0
      DYPDY(1,4) = -P*Y(4)
      DYPDY(3,4) = 1.0
      DYPDY(4,5) = -1.0
      DYPDY(5,6) = 1.0
      DYPDY(6,2) = P*Y(5)*A0/A1
      DYPDY(6,5) = P*Y(2)*A0/A1
      RETURN
      END
```

Output

```
                  Displacement
   X          Axial         Transverse
  0.0       1.631E-11      -8.677E-10
  5.0       1.914E-05      -1.273E-03
 10.0       2.839E-05      -4.697E-03
 15.0       2.461E-05      -9.688E-03
 20.0       1.008E-05      -1.567E-02
```

```
  25.0     -9.550E-06     -2.206E-02
  30.0     -2.721E-05     -2.830E-02
  35.0     -3.644E-05     -3.382E-02
  40.0     -3.379E-05     -3.811E-02
  45.0     -2.016E-05     -4.083E-02
  50.0     -4.414E-08     -4.176E-02
  55.0      2.006E-05     -4.082E-02
  60.0      3.366E-05     -3.810E-02
  65.0      3.627E-05     -3.380E-02
  70.0      2.702E-05     -2.828E-02
  75.0      9.378E-06     -2.205E-02
  80.0     -1.021E-05     -1.565E-02
  85.0     -2.468E-05     -9.679E-03
  90.0     -2.842E-05     -4.692E-03
  95.0     -1.914E-05     -1.271E-03
 100.0      0.000E+00      0.000E+00
```

DAESL

more...

Solves a first order differential-algebraic system of equations, $g(t, y, y') = 0$, with optional additional constraints and user-defined linear system solver.

> **Note:** `DAESL` replaces deprecated routine `DASPG`.

Required Arguments

T — Independent variable, t. (Input/Output)
Set `T` to the starting value t_0 at the first step. On output, `T` is set to the value to which the integration has advanced. Normally, this new value is `TEND`.

TEND — Final value of the independent variable. (Input)
Update this value when re-entering after output with `IDO` = 2.

IDO — Flag indicating the state of the computation. (Input/Output)

IDO	State
1	Initial entry
2	Normal re-entry after obtaining output
3	Release workspace, last call

The user sets `IDO` = 1 on the first call at `T` = t_0. The routine then sets `IDO` = 2, and this value is used for all but the last entry, which is made with `IDO` = 3.

Y — Array of size `NEQ` containing the dependent variable values, y. (Input/Output)
On input, `Y` must contain initial values. On output, `Y` contains the computed solution at `TEND`.

YPRIME — Array of size `NEQ` containing derivative values, y'. (Input/Output)
This array must contain initial values, but they need not be such that $g(t, y, y') = 0$ at $t = t_0$. See the description of parameter ***IYPR*** for more information.

GCN — User-supplied subroutine to evaluate $g(t, y, y')$, and any constraints. Also partial derivative evaluations and optionally linear solving steps occur here. The equations $g(t, y, y') = 0$ consist of NEQ differential-algebraic equations of the form.

$$F_{\boldsymbol{i}}(t, y_1, \ldots y_{\boldsymbol{NEQ}}, y_1', \ldots y'_{\boldsymbol{NEQ}}) \equiv F_{\boldsymbol{i}}(t, y, y') = 0, \quad i = 1, \ldots, NEQ$$

The routine ***GCN*** is also used to evaluate the NCON additional algebraic constraints

$$G_{\boldsymbol{i}}(t, y_1, \ldots, y_{\boldsymbol{NEQ}}) \equiv G_{\boldsymbol{i}}(t, y) = 0, \quad i = 1, \ldots, NCON \quad NCON \geq 0$$

The usage is CALL GCN (T, Y, YPRIME, DELTA, D, LDD, IRES [, …]) where

Required Arguments

T — Integration variable *t*. (Input)

Y — Array of NEQ dependent variables, *y*. (Input)

YPRIME — Array of NEQ derivative values, *y′*. (Input)

DELTA — Output array of length MAX(NEQ, NCON) containing residuals. See parameter IRES for definition. (Input/Output)

D — Output array dimensioned D(LDD,NEQ), containing partial derivatives. See parameter IRES for definition. (Input/Output)

LDD — Leading dimension of D. (Input)

IRES — Flag indicating what is to be calculated in the user routine, GCN. (Input/Output) Note: IRES is input only, except when IRES = 6. It is input/output when IRES = 6. For a detailed description see the table below.

The code calls GCN with IRES = 0, 1, 2, 3, 4, 5, 6, or 7, defined as follows:

IRES Value	Explanation
0	Do initializations, if any are required.
1	Compute DELTA(*i*) $= F_i\left(t, y, y'\right)$, the *i*-th residual, for *i* = 1, …, NEQ.
2	(Required only if IUJAC = 1 and MATSTR = 0 or 1.) Compute D(*i*, *j*) = $\frac{\partial F_i\left(t, y, y'\right)}{\partial y_j}$, the partial derivative matrix. These are derivatives of $F_{\boldsymbol{i}}$ with respect to $y_{\boldsymbol{j}}$, for *i* = 1, …, NEQ and *j* = 1, …, NEQ.
3	(Required only if IUJAC = 1 and MATSTR = 0 or 1.) Compute D(*i*, *j*) = $\frac{\partial F_i\left(t, y, y'\right)}{\partial y'_j}$, the partial derivative matrix. These are derivatives of $F_{\boldsymbol{i}}$ with respect to $y_{\boldsymbol{j}}'$, for *i* = 1, …, NEQ and *j* = 1, …, NEQ.
4	(Required only if IYPR=2.) Compute DELTA(i) = $\frac{\partial F_i\left(t, y, y'\right)}{\partial t}$, the partial derivative of $F_{\boldsymbol{i}}$ with respect to *t*, for i = 1, …, NEQ.

IRES Value	Explanation
5	(Required only if NCON > 0.) Compute DELTA(i) = $G_i(t, y)$, the *i-th* residual in the additional constraints, for i = 1, …, NCON, and D(i, j) = $\frac{\partial G_i(t,y)}{\partial y_j}$, the partial derivative of G_i with respect to y_j for i = 1, …, NCON and j = 1, …, NEQ.
6	(Required only if ISOLVE = 1.) If MATSTR = 2, the user must compute the matrix $A = \frac{\partial F}{\partial y} + cj\frac{\partial F}{\partial y'}$, where cj = DELTA (1), and save this matrix in any user-defined format. This is for later use when IRES = 7. The matrix may also be factored in this step, if desired. The array D is not referenced if MATSTR = 2. If MATSTR = 0 or 1, the A matrix will already be defined and passed to GCN in the array D, which will be in full matrix format if MATSTR = 0, and band matrix format, if MATSTR = 1. The user may factor D in this step, if desired. Note: For MATSTR = 0, 1, or 2, the user must set IRES = 0 to signal that A is nonsingular. If A is nearly singular, leave IRES = 6. This results in using a smaller step-size internally.
7	(Required only if ISOLVE = 1.) The user must solve $Ax = b$, where b is passed to GCN in the vector DELTA, and x is returned in DELTA. If MATSTR = 2, A is the matrix which was computed and saved at the call with IRES = 6; if MATSTR = 0 or 1, A is passed to GCN in the array D. In either case, the A matrix will remain factored if the user factored it when IRES = 6.

Optional Arguments

FCN_DATA — A derived type, s_fcn_data, which may be used to pass additional integer or floating point information to or from the user-supplied subroutine. For a description of this argument see FCN_DATA below. (Input/Output)

GCN must be declared EXTERNAL in the calling program.

Optional Arguments

NEQ — Number of dependent variables, and number of differential/algebraic equations, not counting any additional constraints. (Input)

Default: NEQ = size (Y).

NCON — Number of additional constraints. (Input)

Default: NCON = 0.

IUJAC — Jacobian calculation option. (Input)

Value	Description
0	Calculates using finite difference approximations.
1	User supplies the Jacobian matrices of partial derivatives of F_i, i = 1, …, *NEQ*, in the subroutine `GCN`, when `IRES` = 2 and 3.

Default: `IUJAC` = 0 for `MATSTR` = 0 or 1.
`IUJAC` = 1 for `MATSTR` = 2.

IYPR — Initial y' calculation method. (Input)

Value	Description
0	The initial input values of `YPRIME` are already consistent with the input values of `Y`. That is $g(t, y, y') = 0$ at $t = t_0$. Any constraints must be satisfied at $t = t_0$.
1	Consistent values of `YPRIME` are calculated by Petzold's original `DASSL` algorithm.
2	Consistent values of `YPRIME` are calculated using a new algorithm [Hanson and Krogh, 2008], which is generally more robust but requires that `IUJAC` = 1 and `ISOLVE` = 0, and additional derivatives corresponding to `IRES` = 4 are to be calculated in `GCN`.

Default: `IYPR` = 1.

MATSTR — Parameter specifying the Jacobian matrix structure (Input)
Set to:

Value	Description
0	The Jacobian matrices (whether `IUJAC` = 0 or 1) are to be stored in full storage mode.
1	The Jacobian matrices are to be stored in band storage mode. In this case, if `IUJAC` = 1, the partial derivative matrices have their entries for row *i* and column *j*, stored as array elements `D`(*i* – *j* + `MU` + 1, *j*). This occurs when `IRES`= 2 or 3 in `GCN`.
2	A user-defined matrix structure is used (see the documentation for `IRES = 6 or 7` for more details). If `MATSTR` = 2, `ISOLVE` and `IUJAC` are set to 1 internally.

Default: `MATSTR` = 0.

ISOLVE — Solve method. (Input)

Value	Description
0	DAESL solves the linear systems.
1	The user wishes to solve the linear system in routine GCN. See parameter GCN for details.

Default: ISOLVE = 0 for MATSTR = 0 or 1, ISOLVE = 1 for MATSTR = 2.

ML — Number of non-zero diagonals below the main diagonal in the Jacobian matrices when band storage mode is used. (Input)
ML is ignored if MATSTR ≠ 1.
Default: ML = NEQ-1.

MU — Number of non-zero diagonals above the main diagonal in the Jacobian matrices when band storage mode is used. (Input)
MU is ignored if MATSTR ≠ 1.
Default: MU = NEQ−1.

RTOL — Relative error tolerance for solver. (Input)
The program attempts to maintain a local error in Y(*i*) less than
RTOL*|Y(*i*)| + ATOL(*i*).
Default: RTOL = $\sqrt{\varepsilon}$, where **ε** is machine precision.

ATOL — Array of size NEQ containing absolute error tolerances. (Input)
See description of RTOL.
Default: ATOL(***i***) = 0.

H0 — Initial stepsize used by the solver. (Input)
If H0 = 0, the routine defines the initial stepsize.
Default: H0 = 0.

HMAX — Maximum stepsize used by the solver. (Input)
If HMAX=0, the routine defines the maximum stepsize.
Default: HMAX = 0.

MAXORD — Maximum order of the backward difference formulas used. (Input).
1 ≤ MAXORD ≤ 5.
Default: MAXORD = 5.

MAXSTEPS — Maximum number of steps taken from T to TEND. (Input).
Default: MAXSTEPS = 500.

TSTOP — Integration limit point. (Input)

For efficiency reasons, the code sometimes integrates past TEND and interpolates a solution at TEND. If a value for TSTOP is specified, the code will never integrate past T=TSTOP.

Default: No TSTOP value is specified.

FMAG — Order-of-magnitude estimate. (Input)

FMAG is used as an order-of-magnitude estimate of the magnitude of the functions F_i (see description of GCN), for convergence testing, if IYPR = 2. FMAG is ignored if IYPR=0 or 1.

Default: FMAG = 1.

FCN_DATA — A derived type, s_fcn_data, which may be used to pass additional information to/from the user-supplied subroutine. (Input/Output)

The derived type, s_fcn_data, is defined as:

```
type s_fcn_data
   real(kind(1e0)), pointer, dimension(:) :: rdata
   integer, pointer, dimension(:) :: idata
end type
```

in module mp_types. The double precision counterpart to s_fcn_data is named d_fcn_data. The user must include a use mp_types statement in the calling program to define this derived type.

Note that if this optional argument is present then FCN_DATA must also be defined as an optional argument in the user-supplied subroutine.

FORTRAN 90 Interface

Generic: CALL DAESL (T, TEND, IDO, Y, YPRIME, GCN [, …])

Specific: The specific interface names are S_DAESL and D_DAESL.

Description

Routine DAESL finds an approximation to the solution of a system of differential-algebraic equations $g(t, y, y') = 0$ with given initial data for y and y'. The routine uses BDF formulas, which are appropriate for stiff systems. DAESL is based on the code DASSL designed by Linda Petzold [1982], and has been modified by Hanson and Krogh [2008] *Solving Constrained Differential-Algebraic Systems Using Projections* to allow the inclusion of additional constraints, including conservation principles, after each time step. The modified code also provides a more robust algorithm to calculate initial y' values consistent with the given initial y values. This occurs when the initial y' are not known.

A differential-algebraic system of equations is said to have "index 0" if the Jacobian matrix of partial derivatives of the F_i with respect to the y_j' is nonsingular. Thus it is possible to solve for all the initial values of y_j' and put the system in the form of a standard ODE system. If it is possible to reduce the system to a system of index 0 by taking first derivatives of some of the equations, the system has index 1, otherwise the index is greater than 1. See Brenan [1989] for a definition of index. DAESL can generally only solve systems of index 0 or 1; other systems will usually have to be reduced to such a form through differentiation.

Examples

Example 1 – Method of Lines PDE Problem

This example solves the partial differential equation $U_t = U_{xx} + U$, with initial condition $U\left(x,0\right) = 1 + x$, and boundary conditions $U\left(0,t\right) = e^t$, $U\left(1,t\right) = 2e^t$ which has exact solution $U\left(x,t\right) = \left(1 + x\right)e^t$. If we approximate the U_{xx} term using finite differences, where

$x_i = \left(i - 1\right)h$, and $h = 1 / \left(n - 1\right)$, we get:

$$U\left(x_1,t\right) = e^t$$

$$U'(x_i,t) = \left[\, U(x_{i+1},t) - 2U(x_i,t) + U(x_{i-1},t) \right] / h^2 + U(x_i,t), \quad i = 2, \ \ldots\ , n-1$$

$$U\left(x_n,t\right) = 2e^t$$

If $Y_i(t) = U(x_i,t)$, the first and last equations are algebraic and the others are differential equations, so this is a system of differential-algebraic equations. The system has index = 1, since it could be transformed into an ODE system by differentiating the first and last equations. Note that the Jacobian matrices are banded (tridiagonal), with ML = MU = 1. We use this and specify the option for dealing with banded matrices in DAESL. The parameter h and the number of equations is passed to the evaluation routine, GCN, with the optional argument USER_DATA.

(Example daesl_ex1.f90)

```
      USE DAESL_INT
      USE MP_TYPES
      IMPLICIT NONE

!                                NEQ = Number of equations
      INTEGER, PARAMETER :: NEQ=101
      REAL T, Y(NEQ), YPRIME(NEQ), TEND, X, TRUE, HX, ERRMAX
      INTEGER NOUT, IDO, I, NSTEPS
      REAL, TARGET :: RPARAM(1)
      INTEGER, TARGET :: IPARAM(1)
      TYPE (S_FCN_DATA) USER_DATA
      EXTERNAL GCN

!                                Pass NEQ, HX to GCN
      HX = 1.0 / (NEQ-1)
      IPARAM(1) = NEQ
      RPARAM(1) = HX
```

```
      USER_DATA%RDATA=>RPARAM
      USER_DATA%IDATA=>IPARAM
!                               Initial values for y, initial guesses for y'
      DO I = 1, NEQ
        X = (I-1) * HX
        Y(I) = 1 + X
      END DO
      YPRIME = 0.0

      NSTEPS = 10
!                               Always set IDO=1 on first call
      IDO = 1
      DO I = 1, NSTEPS
!                               Output solution at T=0.1,0.2,...,1.0
        T = 0.1 * (I-1)
        TEND = 0.1 * I

!                               Set IDO = 3 on last call
        IF (I == NSTEPS) IDO = 3

!                               User-supplied Jacobian matrix (IUJAC=1)
!                               Banded Jacobian (MATSTR=1)
        CALL DAESL (T, TEND, IDO, Y, YPRIME, GCN, IYPR=1, IUJAC=1, &
               MATSTR=1, ML=1, MU=1, RTOL=1.0E-4, FCN_DATA=USER_DATA)
      END DO

      ERRMAX = 0.0
      DO I = 1, NEQ
         X = (I-1) * HX
         TRUE = (1+X) * EXP(T)
         ERRMAX = MAX(ERRMAX, ABS(Y(I) - TRUE))
      END DO

      CALL UMACH(2, NOUT)
      WRITE (NOUT, *) ' Max Error at T=1 is ', ERRMAX
      END


      SUBROUTINE GCN (T, Y, YPRIME, DELTA, D, LDD, IRES, FCN_DATA)
      USE MP_TYPES
      IMPLICIT NONE

      REAL T, Y(*), YPRIME(*), DELTA(*), D(LDD,*), HX
      INTEGER IRES, LDD, I, J, NEQ, MU
      TYPE (S_FCN_DATA), OPTIONAL, INTENT(INOUT) :: FCN_DATA

      NEQ = FCN_DATA%IDATA(1)
      HX = FCN_DATA%RDATA(1)
      MU = 1

      SELECT CASE (IRES)

!                               F_I defined here
      CASE(1)
        DELTA(1) = Y(1) - EXP(T)
        DO I = 2, NEQ-1
           DELTA(I) = -YPRIME(I) + (Y(I+1) - 2.0 * Y(I) + Y(I-1)) &
                      / HX**2 + Y(I)
        END DO
        DELTA(NEQ) = Y(NEQ) - 2.0 * EXP(T)

!                               D(I-J+MU+1,J) = D(F_I)/D(Y_J)
!                               in band storage mode
      CASE(2)
        D(MU+1,1) = 1.0
        DO I = 2, NEQ-1
```

```
            J = I-1
            D(I-J+MU+1, J) = 1.0 / HX**2
            J = I
            D(I-J+MU+1, J) = -2.0 / HX**2 + 1.0
            J = I+1
            D(I-J+MU+1, J) = 1.0 / HX**2
         END DO
         D(MU+1, NEQ) = 1.0

!                             D(I-J+MU+1,J) = D(F_I)/D(YPRIME_J)
       CASE(3)
         DO I = 2, NEQ-1
            D(MU+1, I) = -1.0
         END DO

       END SELECT
       END
```

Output

```
    Max Error at T=1 is  5.6743621E-5
```

Example 2 – Pendulum Problem

The first-order equations of motion of a point-mass *m* suspended on a massless wire of length *L* under the influence of gravity, *mg*, and wire tension, λ , in Cartesian coordinates (*p*,*q*) are

$$\begin{aligned} p' &= u \\ q' &= v \\ mu' &= -p\lambda \\ mv' &= -q\lambda - mg \\ p^2 + q^2 - L^2 &= 0 \end{aligned}$$

The problem above has an index number equal to 3, thus it cannot be solved with `DAESL` directly. Unfortunately, the fact that the index is greater than 1 is not obvious, but an attempt to solve it will generally produce an error message stating the corrector equation did not converge, or if `IYPR`=2 an error message stating that the index appears to be greater than 1 should be issued. The user then differentiates the last equation, which after replacing p' by *u* and q' by *v*, gives $pu + qv = 0$. This system still has index = 2 (again not obvious, the user discovers this by unsuccessfully trying to solve the new system) and the last equation must be differentiated again, to finally (after appropriate substitutions) give the equation of total energy balance:

$$m\left(u^2 + v^2\right) - mgq - L^2\lambda = 0$$

With initial conditions and appropriate definitions of the dependent variables, the system becomes:

$$p(0) = L,\ q(0) = u(0) = v(0) = \lambda(0) = 0$$

$$
\begin{aligned}
y_1 &= p \\
y_2 &= q \\
y_3 &= u \\
y_4 &= v \\
y_5 &= \lambda \\
F_1 &= y_3 - y_1{}' = 0 \\
F_2 &= y_4 - y_2{}' = 0 \\
F_3 &= -y_1 y_5 - m y_3{}' = 0 \\
F_4 &= -y_2 y_5 - mg - m y_4{}' = 0 \\
F_5 &= m\left(y_3{}^2 + y_4{}^2\right) - mgy_2 - L^2 y_5 = 0
\end{aligned}
$$

The initial conditions correspond to the pendulum starting in a horizontal position.

Since we have replaced the original constraint, $G_1 = p^2 + q^2 - L^2 = 0$, which requires that the pendulum length be *L*, by differentiating it twice, this constraint is no longer explicitly enforced, and if we try to solve the above system alone (ie, with `NCON` = 0), the pendulum length drifts substantially from *L* at larger times. `DAESL` therefore allows the user to add additional constraints, to be re-enforced after each time step, so we add this original constraint, as well as the intermediate constraint $G_2 = pu + qv = 0$. Using these two supplementary constraints, (`NCON` = 2), the pendulum length is constant.

(Example daesl_ex2.f90)

```
      USE DAESL_INT
      USE MP_TYPES
      IMPLICIT NONE

!              NEQ = Number of equations
!              NCON = Number of extra constraints
      INTEGER, PARAMETER :: NEQ=5, NCON = 2
      REAL, PARAMETER :: MASS=1.0, LENGTH=1.1, GRAVITY=9.806650

      REAL T, Y(NEQ), YPRIME(NEQ), TEND, ATOL(NEQ), TOL, LEN
      INTEGER NOUT, IDO, I, NSTEPS
      REAL, TARGET :: RPARAM(3)
      TYPE (S_FCN_DATA) USER_DATA
      EXTERNAL GCN

!              Pass Mass, Pendulum length and G as parameters
      RPARAM(1) = MASS
      RPARAM(2) = LENGTH
      RPARAM(3) = GRAVITY
      USER_DATA%RDATA=>RPARAM

!              Initial values for y, guesses for initial y'
      Y = 0.0
      Y(1) = LENGTH
```

```
      YPRIME = 0.0
      TOL = 1.0E-5
      ATOL = TOL

      CALL UMACH(2, NOUT)
      WRITE (NOUT, 5)

      NSTEPS = 5
!              Always set IDO=1 on first call
      IDO = 1
      DO I = 1, NSTEPS
!              Output solution at T=10,20,30,40,50
        T = 10.0 * (I-1)
        TEND = 10.0 * I

!              Set IDO = 3 on last call
        IF (I.EQ.NSTEPS) IDO = 3

!              User-supplied Jacobian matrix (IUJAC=1)
!              Use new algorithm to get compatible y'
        CALL DAESL (T, TEND, IDO, Y, YPRIME, GCN, NCON=NCON, RTOL=TOL, &
          ATOL=ATOL, IYPR=2, IUJAC=1, MAXSTEPS=50000, &
          FCN_DATA=USER_DATA)

!              LEN = pendulum length (should be constant)
        LEN = SQRT(Y(1)**2 + Y(2)**2)
        WRITE (NOUT, 10) T, Y(1), Y(2), LEN
      END DO

    5 FORMAT (8X,'T',14X,'Y(1)',11X,'Y(2)',11X,'Length',/)
   10 FORMAT (4F15.7)
      END


      SUBROUTINE GCN (T, Y, YPRIME, DELTA, D, LDD, IRES, FCN_DATA)
      USE MP_TYPES
      IMPLICIT NONE

!              Simple swinging pendulum problem
      REAL T, Y(*), YPRIME(*), DELTA(*), D(LDD,*), MASS, &
           LENGTH, GRAVITY, MG, LSQ
      INTEGER IRES, LDD
      TYPE (S_FCN_DATA), OPTIONAL, INTENT(INOUT) :: FCN_DATA

      MASS = FCN_DATA%RDATA(1)
      LENGTH = FCN_DATA%RDATA(2)
      GRAVITY = FCN_DATA%RDATA(3)
      MG = MASS * GRAVITY
      LSQ = LENGTH**2

      SELECT CASE (IRES)

!              F_I defined here
      CASE(1)
        DELTA(1) = Y(3) - YPRIME(1)
        DELTA(2) = Y(4) - YPRIME(2)
        DELTA(3) = -Y(1) * Y(5) - MASS * YPRIME(3)
        DELTA(4) = -Y(2) * Y(5) - MASS * YPRIME(4) - MG
        DELTA(5) = MASS * (Y(3)**2 + Y(4)**2) - MG * Y(2) - LSQ * Y(5)

!              D(I,J) = D(F_I)/D(Y_J)
      CASE(2)
        D(1, 3) = 1.0
        D(2, 4) = 1.0
        D(3, 1) = -Y(5)
```

```
          D(3, 5) = -Y(1)
          D(4, 2) = -Y(5)
          D(4, 5) = -Y(2)
          D(5, 2) = -MG
          D(5, 3) = MASS * 2.0 * Y(3)
          D(5, 4) = MASS * 2.0 * Y(4)
          D(5, 5) = -LSQ

!               D(I,J) = D(F_I)/D(YPRIME_J)
        CASE(3)
          D(1, 1)= -1.0
          D(2, 2)= -1.0
          D(3, 3)= -MASS
          D(4, 4)= -MASS


!               DELTA(I) = D(F_I)/DT
        CASE(4)
          DELTA(1:5) = 0.0

!               DELTA(I) = G_I
!               D(I,J) = D(G_I)/D(Y_J)
        CASE(5)
          DELTA(1) = Y(1)**2 + Y(2)**2 - LSQ
          DELTA(2) = Y(1) * Y(3) + Y(2) * Y(4)
          D(1, 1) = 2.0 * Y(1)
          D(1, 2) = 2.0 * Y(2)
          D(1, 3) = 0.0
          D(1, 4) = 0.0
          D(1, 5) = 0.0
          D(2, 1) = Y(3)
          D(2, 2) = Y(4)
          D(2, 3) = Y(1)
          D(2, 4) = Y(2)
          D(2, 5) = 0.0

        END SELECT
        END
```

Output

```
          T              Y(1)           Y(2)           Length

     10.0000000      1.0998126     -0.0203017      1.0999999
     20.0000000      1.0970103     -0.0810476      1.1000000
     30.0000000      1.0850314     -0.1808525      1.1000004
     40.0000000      1.0535675     -0.3162208      1.1000000
     50.0000000      0.9896186     -0.4802662      1.1000003
```

Example 3 – User Solves Linear System

Consider the system of ordinary differential equations, $y' = By$, where B is the bi-diagonal matrix with $(-1, -1/2, -1/3, \ldots, -1/(n-1), 0)$ on the main diagonal and with 1's along the first sub-diagonal. The initial condition is $y(0) = (1,0,0,\ldots,0)^T$, and since $y'(0) = By(0) = (-1,1,0,\ldots,0)^T$, $y'(0)$ is also known for this problem.

Since $B^T v = 0$, where $v_i = 1/(i-1)!$, v is an eigenvector of B^T corresponding to the eigenvalue 0. Thus

$$0 = v^T\left(y' - By\right) = v^T y' - \left(B^T v\right)^T y = v^T y' = \left(v^T y\right)'$$

so $v^T y(t)$ is constant. Since it has the value $v^T y(0) = v_1 = 1$ at $t = 0$, the constraint $v^T y(t) = 1$ is satisfied for all t. This constraint is imposed in this example.

This example also illustrates how the user can solve his/her own linear systems (`MATSTR` = 2). Normally, when `IRES` = 6, the matrix

$$A = \frac{\partial g}{\partial y} + cj\frac{\partial g}{\partial y'}$$

is computed, saved and possibly factored, using a sparse matrix factorization routine of the user's choice. Then when `IRES` = 7, the system Ax = `DELTA` is solved, using the matrix B saved and factored earlier, and the solution is returned in `DELTA`. In this case, B is just a bidiagonal matrix, so there is no need to save or factor A when `IRES` = 6, since a bi-diagonal system can be solved directly using forward substitution, when `IRES` = 7.

(Example daesl_ex3.f90)

```
      USE DAESL_INT
      USE MP_TYPES
      IMPLICIT NONE

!              NEQ = Number of equations
      INTEGER, PARAMETER :: NEQ=100
      REAL T, Y(NEQ), YPRIME(NEQ), TEND, ATOL(NEQ), CON
      INTEGER NOUT, IDO, I, NSTEPS
      REAL, TARGET :: RPARAM(NEQ)
      INTEGER, TARGET :: IPARAM(1)
      TYPE (S_FCN_DATA) USER_DATA
      EXTERNAL GCN

!              Pass NEQ and A^T eigenvector V to GCN
      IPARAM(1) = NEQ
      RPARAM(1) = 1.0
      DO I = 2, NEQ
         RPARAM(I) = RPARAM(I-1) / FLOAT(I-1)
      END DO
      USER_DATA%RDATA=>RPARAM
      USER_DATA%IDATA=>IPARAM

!              Initial values for y, y'
      Y = 0.0
      Y(1) = 1.0

      YPRIME = 0.0
      YPRIME(1) = -1.0
      YPRIME(2) =  1.0

      ATOL = 1.0E-4
      NSTEPS = 10

!              Always set IDO=1 on first call
      IDO = 1
      DO I = 1, NSTEPS
!              Output solution at T=1,2,...,10
        T = I-1
        TEND = I
```

```
!              Set IDO = 3 on last call
        IF (I == NSTEPS) IDO = 3
!              User-defined Jacobian matrix structure (MATSTR=2)
        CALL DAESL (T, TEND, IDO, Y, YPRIME, GCN, IYPR=0, MATSTR=2, &
                    NCON=1, ATOL=ATOL, FCN_DATA=USER_DATA)
      END DO

!              Check if solution satisfies constraint
      CON = 0.0
      DO I = 1, NEQ
         CON = CON + RPARAM(I) * Y(I)
      END DO

      CALL UMACH(2, NOUT)
      WRITE (NOUT, *) ' V dot Y =', CON
      END


      SUBROUTINE GCN (T, Y, YPRIME, DELTA, D, LDD, IRES, FCN_DATA)
      USE MP_TYPES
      IMPLICIT NONE

      REAL T, Y(*), YPRIME(*), DELTA(*), D(LDD,*), CON, CJ
      INTEGER IRES, LDD, I, NEQ
      SAVE CJ
      TYPE (S_FCN_DATA), OPTIONAL, INTENT(INOUT) :: FCN_DATA

      NEQ = FCN_DATA%IDATA(1)
      SELECT CASE (IRES)

!              F_I defined here
      CASE(1)
        DELTA(1) = YPRIME(1) + Y(1)
        DO I = 2, NEQ-1
           DELTA(I) = YPRIME(I) - Y(I-1) + Y(I) / FLOAT(I)
        END DO
        DELTA(NEQ) = YPRIME(NEQ) - Y(NEQ-1)

!              Constraint is V dot Y = 1
      CASE(5)
        CON = -1.0
        DO I = 1, NEQ
           CON = CON + FCN_DATA%RDATA(I) * Y(I)
           D(1,I) = FCN_DATA%RDATA(I)
        END DO
        DELTA(1) = CON

!              Normally, compute matrix A = dF/dY + CJ*dF/dY'
!              = -B + CJ*I here.  Only CJ needs to be saved
!              in this case, however, since B is bidiagonal,
!              so A*x=DELTA can be solved (IRES=7) without
!              saving or factoring B.
      CASE(6)
        CJ = DELTA(1)
!              If CJ > 0 not close to zero, A is nonsingular,
!              so set IRES = 0.
        IF (CJ >= 1.0E-4) IRES = 0

!              Solve A*x=DELTA and return x in DELTA.
      CASE(7)
        DELTA(1) = DELTA(1) / (1.0 + CJ)
        DO I = 2, NEQ-1
           DELTA(I) = (DELTA(I) + DELTA(I-1)) / (1.0 / FLOAT(I) + CJ)
        END DO
        DELTA(NEQ) = (DELTA(NEQ) + DELTA(NEQ-1)) / CJ
```

```
        END SELECT
        END
```

Output

```
    V dot Y = 1.0
```

DASPG

Deprecated Routine: `DASPG` is a deprecated routine and has been replaced with `DAESL`. To view the deprecated documentation, see `daspg.pdf` on the IMSL website. You can also access a local copy in your IMSL documentation directory at pdf\deprecated_routines\math\daspg.pdf.

IVOAM

Solves an initial-value problem for a system of ordinary differential equations of order one or two using a variable order Adams method.

Required Arguments

IDO — Flag indicating the state of the computation. (Input/Output)

IDO	State
1	Initial entry input value.
2	Normal re-entry input value. On output, if IDO = 2 then the integration is finished. If the integrator is called with a new value for TEND, the integration continues. If the integrator is called with TEND unchanged, an error message is issued.
3	Input value to use on final call to release workspace.
>3	Output value that indicates that a fatal error has occurred.

The initial call is made with IDO = 1. The routine then sets IDO = 2, and this value is used for all but the last call that is made with IDO = 3. This final call is only used to release workspace which was automatically allocated by the initial call with IDO = 1.

***FCN* —** User-supplied subroutine to evaluate functions.
The usage is CALL FCN (IDO, T, Y, HIDRVS [, …]), where

Required Arguments

IDO — Flag indicating the state of the computation. (Input)
This flag corresponds to the IDO argument described above. If FCN has complicated subexpressions, which depend only weakly or not at all on Y then these subexpressions need only be computed when IDO = 1 and their values then reused when IDO = 2.

T — Independent variable, *t*. (Input)

Y — Array of length *k* containing the dependent variable values, *y*, and first derivatives, if any. *k* will be the sum of the orders of the equations in the system of equations to solve. (Input)

HIDRVS — Array of length *n* = NEQ, where n is the number of equations in the system to solve, containing the values of the highest order derivatives evaluated at (*t*, *y*). (Output)

IVOAM uses size(HIDRVS) to set the default value of NEQ unless the optional argument NEQ is used.

Optional Arguments

`FCN_DATA` — A derived type, `s_fcn_data`, which may be used to pass additional integer or floating point information to or from the user-supplied subroutine. (Input/Output)

For a detailed description of this argument see `FCN_DATA` below.

`FCN` must be declared `EXTERNAL` in the calling program.

T — Independent variable, *t*. (Input/Output)
On input, `T` contains the initial independent variable value. On output, `T` is replaced by `TEND` unless error conditions arise. See `IDO` for details. (Input/Output)

TEND — Value of $t = tend$ where the solution is required. (Input)

Y — Array of length *k* containing the dependent variables, $y(t)$, and first derivatives, if any. (Input/Output)
k will be the sum of the orders of the equations in the system of equations to solve. On input, `Y` contains the initial values, $y(t_0)$ and $y'(t_0)$ (if needed). On output, `Y` contains the approximate solution, $y(t)$. For example, for a system of first order equations, `Y`(*i*) is the *i*-th dependent variable. For a system of second order equations, `Y`(*2i-1*) is the *i*-th dependent variable and `Y`(*2i*) is the derivative of the *i*-th dependent variable. For systems of equations in which one or more equations is of order 2, optional argument `KORDER` must be used to denote the order of each equation so that the derivatives in `Y` can be identified. By default it is assumed that all equations are of order 1 and `Y` contains only dependent variables.

HIDRVS — Array of length n = `NEQ`, where `n` is the number of equations in the system to solve, containing the highest order derivatives at the point `Y`. (Output)
`IVOAM` uses `size (HIDRVS)` to set the default value of `NEQ` unless the optional argument `NEQ` is used.

Optional Arguments

NEQ — Number of differential equations in the system of equations to solve. (Input)
Default: `NEQ` = size (`HIDRVS`).

KORDER — An array of length `NEQ` specifying the orders of the equations in the system of equations to solve. The elements of `KORDER` can be 1 or 2. `KORDER` must be used with argument `Y` to define systems of mixed or higher order. (Input)
Default: `KORDER` = (1,1,1 …,1).

EQNERR — An array of length `NEQ` specifying the error tolerance for each equation. (Input)
Let *e(i)* be the error tolerance for equation *i*. Then

Value	Explanation
e(i) > *0*	Implies an absolute error tolerance of *e(i)* is to be used for equation *i*.
e(i) = *0*	Implies that the default absolute error tolerance (defined below) is to be used for equation *i*.
e(i) < *0*	Implies a relative error test is to be performed for equation *i*. In this case, the base error tolerance used will be |*e(i)*| and the relative error factor used will be (15/16 * |*e(i)*|). Thus the actual absolute error tolerance used will be |*e(i)*| * (15/16 * |*e(i)*|).

Default: An absolute error tolerance of 1.E-5 is used for single precision and 1.D-10 for double precision for all equations.

HINC — Factor used for increasing the stepsize. (Input)

One should set `HINC` such that 9/8 <= `HINC` <= 4.

Default: `HINC` = 2.0.

HDEC — Factor used for decreasing the stepsize. (Input)

One should set `HDEC` such that 1/4 <= `HDEC` <= 7/8.

Default: `HDEC` = 0.5.

HMIN — Absolute value of the minimum stepsize permitted. (Input)

Default: `HMIN` = 10.0/`amach`(2) for single precision and 10.0/`dmach`(2) for double precision.

HMAX — Absolute value of the maximum stepsize permitted. (Input)

Default: `HMAX` = `amach`(2) for single precision and `dmach`(2) for double precision.

FCN_DATA – A derived type, `s_fcn_data`, which may be used to pass additional information to/from the user-supplied subroutine. (Input/Output)

The derived type, `s_fcn_data`, is defined as:

```
type s_fcn_data
   real(kind(1e0)), pointer, dimension(:) :: rdata
   integer, pointer, dimension(:) :: idata
end type
```

in module `mp_types`. The double precision counterpart to `s_fcn_data` is named `d_fcn_data`. The user must include a `use mp_types` statement in the calling program to define this derived type.

Note that if this optional argument is present then `FCN_DATA` must also be defined as an optional argument in the user-supplied subroutine.

Fortran 90 Interface

Generic: `CALL IVOAM (IDO, FCN, T, TEND, Y, HIDRVS [, …])`

Specific: The specific interface names are `S_IVOAM` and `D_IVOAM`.

Description

Routine `IVOAM` is based on the JPL Library routine `SIVA`. `IVOAM` uses a variable order Adams method to solve the initial value problem

$$\left.\begin{array}{l} \frac{dy_i}{dt} = f_i\left(t, y_1, y_2, \ldots, y_{NEQ}\right) \\ y_i\left(t_0\right) = \eta_i \end{array}\right\}, \quad i = 1, 2, \ldots, NEQ$$

or more generally

$$z_i^{(d_i)} = f_i\left(t, y\right), \; y\left(t_0\right) = \eta_0, \quad i = 1,2, \ldots, NEQ,$$

where *y* is the vector

$$\left(z_1, z_1', \ldots, z_1^{(d_1 - 1)}, z_2, \ldots, z_{NEQ}^{(d_{NEQ} - 1)}\right),$$

$z_i^{(k)}$ is the k^{th} derivative of z_i with respect to *t*, d_i is the order of the i^{th} differential equation, and η is a vector with the same dimension as *y*.

Note that the systems of equations solved by `IVOAM` can be of order one, order two, or mixed order one and two.

Comments

Informational errors

Type	Code	Description
3	1	The requested error tolerance is too small.
3	2	The stepsize has been reduced too rapidly. The integrator is going to do a restart.

Examples

Example 1

In this example a system of two equations of order two is solved.

$$Y_1'' = -Y_1 / \left(\left(Y_1^2 + Y_2^2 \right)^{\frac{3}{2}} \right)$$

$$Y_2'' = -Y_2 / \left(\left(Y_1^2 + Y_2^2 \right)^{\frac{3}{2}} \right)$$

The initial conditions are

$$Y_1(0) = 1.0,\ Y_1'(0) = 0.0,\ Y_2(0) = 0.0,\ Y_2'(0) = 1.0$$

Since the system is of order two, optional argument `KORDER` must be used to specify the orders of the equations. Also, because the system is of order two, `Y`(1) contains the first dependent variable, `Y`(2) contains the derivative of the first dependent variable, `Y`(3) contains the second dependent variable, and `Y`(4) contains the derivative of the second dependent variable.

```
      USE IVOAM_INT
      USE UMACH_INT
      USE CONST_INT

      IMPLICIT   NONE
      INTEGER    IDO, IEND, NOUT, KORDER(2)
      REAL       T, TEND, Y(4), HIDRVS(2), DELTA

      EXTERNAL   FCN
!                                  Initialize
      IDO   = 1
      T     = 0.0
      Y(1)  = 1.0
      Y(2)  = 0.0
      Y(3)  = 0.0
      Y(4)  = 1.0
      KORDER = 2
!                                  Write title
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99997)
!                                  Integrate ODE
      IEND = 0
      DELTA = CONST('PI')
      DELTA = 2.0*DELTA
      DO
         IEND = IEND + 1
         TEND = T + DELTA
         IF(TEND .GT. 20.0) TEND = 20.0
         CALL IVOAM (IDO, FCN, T, TEND, Y, HIDRVS, KORDER=KORDER)
         IF (IEND .LE. 4) THEN
            WRITE (NOUT,99998) T, Y(1), Y(2), HIDRVS(1)
            WRITE (NOUT,99999) Y(3), Y(4), HIDRVS(2)
```

```
!                                  Finish up
            IF (IEND .EQ. 4) IDO = 3
            CYCLE
         END IF
         EXIT
      END DO
99997 FORMAT (11X, 'T', 12X, 'Y1/Y2', 9X, 'Y1P/Y2P', 7X, 'Y1PP/Y2PP')
99998 FORMAT (4F15.4)
99999 FORMAT (15X, 3F15.4)
      END

      SUBROUTINE FCN (IDO, T, Y, HIDRVS)
      INTEGER    IDO
      REAL       T, Y(*), HIDRVS(*)
      REAL       TP

      TP = Y(1)*Y(1) + Y(3)*Y(3)
      TP = 1.0E0/(TP*SQRT(TP))
      HIDRVS(1) = -Y(1)*TP
      HIDRVS(2) = -Y(3)*TP
      RETURN
      END
```

Output

```
    T             Y1/Y2         Y1P/Y2P       Y1PP/Y2PP
  6.2832          1.0000        -0.0000        -1.0000
                  0.0000         1.0000         0.0000
 12.5664          1.0000        -0.0000        -1.0000
                  0.0000         1.0000        -0.0000
 18.8496          1.0000        -0.0000        -1.0000
                  0.0000         1.0000        -0.0000
 20.0000          0.4081        -0.9129        -0.4081
                  0.9129         0.4081        -0.9129
```

Example 2

This contrived example illustrates how to use `IVOAM` to solve a system of equations of mixed order.

The height, $y(t)$, of an object of mass m above the surface of the Earth can be modelled using Newton's second law as:

$$my'' = -mg - ky'$$

or

$$y'' = -g - (k/m)y' \quad (1)$$

where $-mg$ is the downward force of gravity and $-ky'$ is the force due to air resistance, in a direction opposing the velocity. If the object is a meteor, the mass, m, and air resistance, k, will decrease as the meteor burns up in the atmosphere. The mass is proportional to r^3 (r = radius) and the air resistance, presumably dependent on the surface area, may be assumed to be proportional to r^2, so that $k/m = k_0/r$. The rate at which the meteor's radius decreases as it burns up may depend on r, on the velocity y', and, since the density of the atmosphere depends on y, on y itself. However, we will construct a very simple model where the rate is just proportional to the square of the velocity,

$$r' = -c_0(y')^2 \quad (2)$$

We solve (1) and (2), with $k_0 = 0.005$, $c_0 = 10^{-8}$, $g = 9.8$ and initial conditions $y(0) = 100{,}000$ meters, $y'(0) = -1000$ meters/second, $r(0) = 1$ meter.

```
      USE IVOAM_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    IDO, IEND, NOUT, KORDER(2)
      REAL       T, TEND, Y(3), HIDRVS(2), DELTA, EQNERR(2)
      EXTERNAL   FCN
!                                 Initialize
      IDO  = 1
      T    = 0.0
      Y(1) = 100000.0
      Y(2) = -1000.0
      Y(3) = 1.0
      KORDER(1) = 2
      KORDER(2) = 1
      EQNERR = .003
!                                 Write title
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99997)
!                                 Integrate ODE
      IEND = 0
      DELTA = 10.0
      DO
         IEND = IEND + 1
         TEND = T + DELTA
         IF(TEND .GT. 50.0) TEND = 50.0
         CALL IVOAM (IDO, FCN, T, TEND, Y, HIDRVS, &
                     KORDER=KORDER, EQNERR=EQNERR)
         IF (IEND .LE. 5) THEN
            WRITE (NOUT,99998) T, Y(1), Y(2), HIDRVS(1)
            WRITE (NOUT,99999) Y(3), HIDRVS(2)
!                                 Finish up
            IF (IEND .EQ. 5) IDO = 3
            CYCLE
         END IF
         EXIT
      END DO
99997 FORMAT (11X, 'T', 10X, 'Y1/Y2', 11X, 'Y1P', 11X, 'Y1PP/Y2PP')
99998 FORMAT (4F15.4)
99999 FORMAT (2(15X, F15.4))
      END

      SUBROUTINE FCN (IDO, T, Y, HIDRVS)
      INTEGER    IDO
      REAL       T, Y(*), HIDRVS(*)

      HIDRVS(1) = -9.8 - .005/y(3)*y(2)
      HIDRVS(2) = -1.0E-8 * y(2)*y(2)
      RETURN
      END
```

Output

```
        T           Y1/Y2            Y1P            Y1PP/Y2PP
    10.0000      89773.0391     -1044.0096          -3.9701
                     0.8954                          -0.0109
    20.0000      79150.9844     -1078.6334          -2.9083
                     0.7826                          -0.0116
    30.0000      68240.9453     -1101.0380          -1.5031
                     0.6635                          -0.0121
    40.0000      57184.9062     -1106.9635           0.4253
                     0.5413                          -0.0121
    50.0000      46178.1367     -1089.8292           3.1700
                     0.4201                          -0.0119
```

Introduction to Subroutine PDE_1D_MG

The section describes an algorithm and a corresponding integrator subroutine `PDE_1D_MG` for solving a system of partial differential equations

$$u_{\mathrm{t}} \equiv \frac{\partial u}{\partial t} = f\left(u,x,t\right),\ x_{\mathrm{L}} < x < x_{\mathrm{R}},\ t > t_0$$

Equation 1

This software is a one-dimensional solver. It requires initial and boundary conditions in addition to values of u_t. The integration method is noteworthy due to the maintenance of grid lines in the space variable, *x*. Details for choosing new grid lines are given in Blom and Zegeling, (1994). The class of problems solved with `PDE_1D_MG` is expressed by equations:

$$\begin{aligned}&\sum_{k=1}^{NPDE} C_{j,k}\left(x,t,u,u_x\right)\frac{\partial u^k}{\partial t} = x^{-m}\frac{\partial}{\partial x}\left(x^m R_j\left(x,t,u,u_x\right)\right) - Q_j\left(x,t,u,u_x\right),\\ &j = 1, \ldots, NPDE, \quad x_L < x < x_{R,} \quad t > t_0, \quad m \in \left\{0,1,2\right\}\end{aligned}$$

Equation 2

The vector

$$u \equiv \left[u' \ldots, u^{NPDE}\right]^T$$

is the solution. The integer value NPDE ≥ 1 is the number of differential equations. The functions R_j and Q_j can be regarded, in special cases, as flux and source terms. The functions

$$u,\ C_{j,k},\ R_j, \text{ and } Q_j$$

are expected to be continuous. Allowed values

$$m = 0,\ m = 1, \text{ and } m = 2$$

are for problems in Cartesian, cylindrical or polar, and spherical coordinates. In the two cases

$m > 0$, the interval

$$[x_L, x_R]$$

must not contain $x = 0$ as an interior point.

The boundary conditions have the master equation form

$$\beta_j(x,t)R_j(x,t,u,u_x) = \gamma_j(x,t,u,u_x),$$
$$\text{at } x = x_L \text{ and } x = x_R, \quad j = 1, \ldots, NPDE$$

Equation 3

In the boundary conditions the

$$\beta_j \text{ and } \gamma_j$$

are continuous functions of their arguments. In the two cases $m > 0$ and an endpoint occurs at 0, the finite value of the solution at $x = 0$ must be ensured. This requires the specification of the solution at $x = 0$, or implies that

$$R_j|_{x=x_L} = 0$$

or

$$R_j|_{x=x_R} = 0$$

The initial values satisfy

$$u(x,t_0) = u_0(x), \quad x \in [x_L, x_R]$$

where u_0 is a piece-wise continuous vector function of x with *NPDE* components.

The user must pose the problem so that mathematical definitions are known for the functions

$$C_{k,j}, R_j, Q_j, \beta_j, \gamma_j, \text{ and } u_0$$

These functions are provided to the routine `PDE_1D_MG` in the form of three subroutines. Optionally, this information can be provided by *reverse communication*. These forms of the interface are explained below and illustrated with examples. Users may turn directly to the examples if they are comfortable with the description of the algorithm.

PDE_1D_MG

more...

Invokes a module, with the statement `USE PDE_1D_MG`, near the second line of the program unit. The integrator is provided with single or double precision arithmetic, and a generic named interface is provided. We do not recommend using 32-bit floating point arithmetic here. The routine is called within the following loop, and is entered with each value of `IDO`. The loop continues until a value of `IDO` results in an exit.

```
IDO=1
DO
   CASE(IDO == 1) {Do required initialization steps}
   CASE(IDO == 2) {Save solution, update T0 and TOUT }
       IF{Finished with integration} IDO=3
   CASE(IDO == 3) EXIT {Normal}
   CASE(IDO == 4) EXIT {Due to errors}
   CASE(IDO == 5) {Evaluate initial data}
   CASE(IDO == 6) {Evaluate differential equations}
   CASE(IDO == 7) {Evaluate boundary conditions}
   CASE(IDO == 8) {Prepare to solve banded system}
   CASE(IDO == 9) {Solve banded system}
   CALL PDE_1D_MG (T0, TOUT, IDO, U, &
   initial_conditions,&
   pde_system_definition,&
   boundary_conditions, IOPT)
END DO
```

The arguments to `PDE_1D_MG` are *required* or *optional*.

Required Arguments

T0—(Input/Output)

This is the value of the independent variable t where the integration of u_t begins. It is set to the value `TOUT` on return.

TOUT—(Input)

This is the value of the independent variable t where the integration of u_t ends. Note: Values of `T0 < TOUT` imply integration in the forward direction, while values of `T0 > TOUT` imply integration in the backward direction. Either direction is permitted.

IDO—(Input/Output)

This in an integer flag that directs program control and user action. Its value is used for initialization, termination, and for directing user response during reverse communication:

`IDO = 1` This value is assigned by the user for the start of a new problem. Internally it causes allocated storage to be reallocated, conforming to the problem size. Various initialization steps are performed.

`IDO = 2` This value is assigned by the routine when the integrator has successfully reached the end point, `TOUT`.

`IDO = 3` This value is assigned by the user at the end of a problem. The routine is called by the user with this value. Internally it causes termination steps to be performed.

`IDO = 4` This value is assigned by the integrator when a type `FATAL` or `TERMINAL` error condition has occurred, and error processing is set **NOT** to **STOP** for these types of errors. It is not necessary to make a final call to the integrator with **`IDO=3`** in this case.

Values of `IDO` = 5,6,7,8,9 are reserved for applications that provide problem information or linear algebra computations using reverse communication. When problem information is provided using reverse communication, the differential equations, boundary conditions and initial data must all be given. The absence of optional subroutine names in the calling sequence directs the routine to use reverse communication. In the module `PDE_1D_MG_INT`, scalars and arrays for evaluating results are named below. The names are preceded by the prefix "`s_pde_1d_mg_`" or "`d_pde_1d_mg_`", depending on the precision. We use the prefix "`?_pde_1d_mg_`", for the appropriate choice.

`IDO = 5` This value is assigned by the integrator, requesting data for the initial conditions. Following this evaluation the integrator is re-entered.

(Optional) Update the grid of values in array locations $U(NPDE + 1, j)$ $j = 2, \ldots, N$. This grid is returned to the user equally spaced, but can be updated as desired, provided the values are increasing.

(Required) Provide initial values for all components of the system at the grid of values $U(NPDE + 1, j)$ $j = 1, \ldots, N$. If the optional step of updating the initial grid is performed, then the initial values are evaluated at the updated grid.

`IDO = 6` This value is assigned by the integrator, requesting data for the differential equations. Following this evaluation the integrator is re-entered. Evaluate the terms of the system of Equation 2. A default value of $m = 0$ is assumed, but this can be changed to one of the other choices, $m = 1$ or $m = 2$. Use the optional argument `IOPT(:)` for that purpose. Put the values in the arrays as indicated.

The assign-to equality, $a := b$, used here and below, is read "the expression b is evaluated and then assigned to the location a."

$$
\begin{aligned}
&x \equiv ?\_pde\_1d\_mg\_x \\
&t \equiv ?\_pde\_1d\_mg\_t \\
&u^j \equiv ?\_pde\_1d\_mg\_u(j) \\
&\frac{\partial u^j}{\partial x} = u_x^j \equiv ?\_pde\_1d\_mg\_dudx\left(j\right) \\
&?\_pde\_1d\_mg\_c(j,k) := C_{j,k}\left(x,t,u,u_x\right) \\
&?\_pde\_1d\_mg\_r\left(j\right) := r_j\left(x,t,u,u_x\right) \\
&?\_pde\_1d\_mg\_q\left(j\right) := q_j\left(x,t,u,u_x\right) \\
&j,k = 1,...NPDE
\end{aligned}
$$

If any of the functions cannot be evaluated, set `pde_1d_mg_ires=3`. Otherwise do not change its value.

`IDO = 7` This value is assigned by the integrator, requesting data for the boundary conditions, as expressed in Equation 3. Following the evaluation the integrator is re-entered.

$$
\begin{aligned}
&x \equiv ?\_pde\_1d\_mg\_x \\
&t \equiv ?\_pde\_1d\_mg\_t \\
&u^j \equiv ?\_pde\_1d\_mg\_u(j) \\
&\frac{\partial u^j}{\partial x} = u_x^j \equiv ?\_pde\_1d\_mg\_dudx\left(j\right) \\
&?\_pde\_1d\_mg\_beta\left(j\right) := \beta_j\left(x,t,u,u_x\right) \\
&?\_pde\_1d\_mg\_gamma\left(j\right) := \gamma_j\left(x,t,u,u_x\right) \\
&j = 1,...NPDE
\end{aligned}
$$

The value $x \in \{x_L, x_R\}$, and the logical flag `pde_1d_mg_LEFT=.TRUE.` for $x = x_L$. It has the value `pde_1d_mg_LEFT=.FALSE.` for $x = x_R$. If any of the functions cannot be evaluated, set `pde_1d_mg_ires=3`. Otherwise do not change its value.

`IDO = 8` This value is assigned by the integrator, requesting the calling program to prepare for solving a banded linear system of algebraic equations. This value will occur only when the option for “reverse communication solving” is set in the array `IOPT(:)`, with option `PDE_1D_MG_REV_COMM_FACTOR_SOLVE`. The matrix data for this system is in *Band Storage Mode*, described in the *Reference Material* for the IMSL Fortran Numerical Libraries.

`PDE_1D_MG_IBAND`	Half band-width of linear system
`PDE_1D_MG_LDA`	The value `3*PDE_1D_MG_IBAND+1`, with $NEQ = (NPDE + 1)N$

?_PDE_1D_MG_A	Array of size PDE_1D_MG_LDA by NEQ holding the problem matrix in *Band Storage Mode*
PDE_1D_MG_PANIC_FLAG	Integer set to a non-zero value only if the linear system is detected as singular

IDO = 9 This value is assigned by the integrator , requesting the calling program to solve a linear system with the matrix defined as noted with IDO=8.

?_PDE_1D_MG_RHS	Array of size NEQ holding the linear system problem right-hand side
PDE_1D_MG_PANIC_FLAG	Integer set to a non-zero value only if the linear system is singular
?_PDE_1D_MG_SOL	Array of size NEQ to receive the solution, after the solving step

U (1:NPDE+1,1:N) —(Input/Output)

This assumed-shape array specifies *Input* information about the problem size and boundaries. The dimension of the problem is obtained from $NPDE + 1 = size(U,1)$. The number of grid points is obtained by $N = \text{size}(U,2)$. Limits for the variable x are assigned as input in array locations, $U(NPDE + 1, 1) = x_L$, $U(NPDE + 1, N) = x_R$. It is not required to define $U(NPDE + 1, j)$, $j = 2, \ldots, N-1$. At completion, the array U(1:NPDE,1:N) contains the approximate solution value $U_i(x_j(TOUT),TOUT)$ in location U(I,J). The grid value $x_j(TOUT)$ is in location U(NPDE+1,J). Normally the grid values are equally spaced as the integration starts. Variable spaced grid values can be provided by defining them as *Output* from the subroutine initial_conditions or during reverse communication, IDO=5.

Optional Arguments

initial_conditions—(Input)

The name of an external subroutine, written by the user, when using forward communication. If this argument is not used, then reverse communication is used to provide the problem information. The routine gives the initial values for the system at the starting independent variable value T0. This routine can also provide a non-uniform grid at the initial value.

```
SUBROUTINE initial_conditions (NPDE,N,U)
   Integer NPDE,N
   REAL(kind(T0)) U(:,)
END SUBROUTINE
```

(Optional) Update the grid of values in array locations $U(NPDE) + 1, j)$, $j = 2, \ldots, N-1$. This grid is input equally spaced, but can be updated as desired, provided the values are increasing.

(Required) Provide initial values $U(:, j)$, $j = 1, \ldots, N$ for all components of the system at the grid of values $U(NPDE) + 1, j)$, $j = 1, \ldots, N$. If the optional step of updating the initial grid is performed, then the initial values are evaluated at the updated grid.

pde_system_definition—(Input)

The name of an external subroutine, written by the user, when using forward communication. It gives the differential equation, as expressed in Equation 2.

```
SUBROUTINE pde_system_definition (t, x, NPDE, r, dudx, c, q, r, IRES)
    Integer NPDE, IRES
    REAL(kind(T0)) t, x, u(:), dudx(:)
    REAL(kind(T0)) c(:,:), q(:), r(:)
END SUBROUTINE
```

Evaluate the terms of the system of equations. A default value of $m = 0$ is assumed, but this can be changed to one of the other choices $m = 1$ or 2. Use the optional argument `IOPT(:)` for that purpose. Put the values in the arrays as indicated.

$$u^j \equiv u(j)$$
$$\frac{\partial u^j}{\partial x} = u_x^j \equiv dudx(j)$$
$$c(j,k) := C_{j,k}(x,t,u,u_x)$$
$$r(j) := r_j(x,t,u,u_x)$$
$$q(j) := q_j(x,t,u,u_x)$$
$$j,k = 1,...NPDE$$

If any of the functions cannot be evaluated, set `IRES=3`. Otherwise do not change its value.

boundary_conditions—(Input)

The name of an external subroutine, written by the user when using forward communication. It gives the boundary conditions, as expressed in Equation 2.

```
SUBROUTINE BOUNDARY_CONDITIONS(T,BETA,GAMMA,U,DUDX,NPDE,LEFT,IRES)
        real(kind(1d0)),intent(in)::t
    real(kind(1d0)),intent(out),dimension(:)::BETA, GAMMA
    real(kind(1d0)),intent(in),dimension(:)::U,DUDX
    integer,intent(in)::NPDE
    logical,intent(in)::LEFT
    integer,intent(out)::IRES
END SUBROUTINE
```

$$u^j \equiv u(j)$$
$$\frac{\partial u^j}{\partial x} = u_x^j \equiv dudx(j)$$
$$beta(j) := \beta_j(x,t,u,u_x)$$
$$gamma(j) := \gamma_j(x,t,u,u_x)$$
$$j = 1,...NPDE$$

The value $x \in \{x_L, x_R\}$, and the logical flag `LEFT=.TRUE.` for $x = x_L$. The flag has the value `LEFT=.FALSE.` for $x = x_R$.

IOPT—(Input)

Derived type array `s_options` or `d_options`, used for passing optional data to `PDE_1D_MG`. See the section *Optional Data* in the Introduction for an explanation of the derived type and its use. It is necessary to invoke a module, with the statement `USE ERROR_OPTION_PACKET`, near the second line of the program unit. Examples 2-8 use this optional argument. The choices are as follows:

Packaged Options for **PDE_1D_MG**		
Option Prefix = ?	Option Name	Option Value
s_, d_	PDE_1D_MG_CART_COORDINATES	1
s_, d_	PDE_1D_MG_CYL_COORDINATES	2
s_, d_	PDE_1D_MG_SPH_COORDINATES	3
s_, d_	PDE_1D_MG_TIME_SMOOTHING	4
s_, d_	PDE_1D_MG_SPATIAL_SMOOTHING	5
s_, d_	PDE_1D_MG_MONITOR_REGULARIZING	6
s_, d_	PDE_1D_MG_RELATIVE_TOLERANCE	7
s_, d_	PDE_1D_MG_ABSOLUTE_TOLERANCE	8
s_, d_	PDE_1D_MG_MAX_BDF_ORDER	9
s_, d_	PDE_1D_MG_REV_COMM_FACTOR_SOLVE	10
s_, d_	PDE_1D_MG_NO_NULLIFY_STACK	11

`IOPT(IO) = PDE_1D_MG_CART_COORDINATES`

Use the value $m = 0$ in Equation 2. This is the default.

`IOPT(IO) = PDE_1D_MG_CYL_COORDINATES`

Use the value $m = 1$ in Equation 2. The default value is $m = 0$.

`IOPT(IO) = PDE_1D_MG_SPH_COORDINATES`

Use the value $m = 2$ in Equation 2. The default value is $m = 0$.

`IOPT(IO) = ?_OPTIONS(PDE_1D_MG_TIME_SMOOTHING,TAU)`

This option resets the value of the parameter $\tau \geq 0$ described above.
The default value is $\tau = 0$.

`IOPT(IO) = ?_OPTIONS(PDE_1D_MG_SPATIAL_SMOOTHING,KAP)`

This option resets the value of the parameter $\kappa \geq 0$, described above.
The default value is $\kappa = 2$

`IOPT(IO) = ?_OPTIONS(PDE_1D_MG_MONITOR_REGULARIZING,ALPH)`

This option resets the value of the parameter $\alpha \geq 0$, described above.

The default value is $\alpha = 0.01$.

`IOPT(IO) = ?_OPTIONS(PDE_1D_MG_RELATIVE_TOLERANCE,RTOL)`

This option resets the value of the relative accuracy parameter used in `DASPG`.

The default value is `RTOL=1E-2` for single precision and `RTOL=1D-4` for double precision.

`IOPT(IO) = ?_OPTIONS(PDE_1D_MG_ABSOLUTE_TOLERANCE,ATOL)`

This option resets the value of the absolute accuracy parameter used in `DASPG`. The default value is `ATOL=1E-2` for single precision and`ATOL=1D-4` for double precision.

`IOPT(IO) = PDE_1D_MG_MAX_BDF_ORDER`

`IOPT(IO+1) = MAXBDF`

Reset the maximum order for the `BDF` formulas used in `DASPG`. The default value is `MAXBDF=2`. The new value can be any integer between 1 and 5. Some problems will benefit by making this change. We used the default value due to the fact that `DASPG` may cycle on its selection of order and step-size with orders higher than value 2.

`IOPT(IO) = PDE_1D_MG_REV_COMM_FACTOR_SOLVE`

The calling program unit will solve the banded linear systems required in the stiff differential-algebraic equation integrator. Values of **IDO=8, 9** will occur only when this optional value is used.

`IOPT(IO) = PDE_1D_MG_NO_NULLIFY_STACK`

To maintain an efficient interface, the routine `PDE_1D_MG` collapses the subroutine call stack with `CALL_E1PSH("NULLIFY_STACK")`. This implies that the overhead of maintaining the stack will be eliminated, which may be important with reverse communication. It does not eliminate error processing. However, precise information of which routines have errors will not be displayed. To see the full call chain, this option should be used. Following completion of the integration, stacking is turned back on with `CALL_E1POP("NULLIFY_STACK")`.

FORTRAN 90 Interface

Generic: `CALL PDE_1D_MG (T0, TOUT, IDO, [,…])`

Specific: The specific interface names are `S_PDE_1D_MG` and `D_PDE_1D_MG`.

Description

The equation

$$u_t = f(u, x, t),\ x_L < x < x_R,\ t > t_0,$$

is approximated at *N* time-dependent grid values

$$x_L = x_0 < \ \dots \ < x_i(t) < x_{i+1}(t) < \ \dots \ < x_N = x_R$$

Using the total differential

$$\frac{du}{dt} = u_t + u_x \frac{dx}{dt}$$

transforms the differential equation to

$$\frac{du}{dt} - u_x \frac{dx}{dt} = u_t = f(u,x,t)$$

Using central divided differences for the factor u_x leads to the system of ordinary differential equations in implicit form

$$\frac{dU_i}{dt} - \frac{(U_{i+1} - U_{i-1})}{(x_{i+1} - x_{i-1})} \frac{dx_i}{dt} = F_i, \quad t > t_0, \quad i = 1, \ \dots\ , N$$

The terms U_i, F_i respectively represent the approximate solution to the partial differential equation and the value of $f(u,x,t)$ at the point $(x,t) = (x_i(t),t)$. The truncation error is second-order in the space variable, x. The above ordinary differential equations are underdetermined, so additional equations are added for the variation of the time-dependent grid points. It is necessary to discuss these equations, since they contain parameters that can be adjusted by the user. Often it will be necessary to modify these parameters to solve a difficult problem. For this purpose the following quantities are defined:

$$\begin{aligned}
&\Delta x_i = x_{i+1} - x_i, \quad n_i = (\Delta x_i)^{-1} \\
&\mu_i = n_i - \kappa(\kappa + 1)(n_{i+1} - 2n_i + n_{i-1}), \quad 0 \le i \le N \\
&n_{-1} \equiv n_0, \quad n_{N+1} \equiv n_N
\end{aligned}$$

> The three-tiered equal sign, used here and below, is read "$a \equiv b$, or a and b are exactly the same object or value."

The values n_i are the so-called point concentration of the grid, and $\kappa \ge 0$ denotes a spatial smoothing parameter. Now the grid points are defined implicitly so that

$$\frac{\mu_{i-1} + \tau \frac{d\mu_{i-1}}{dt}}{M_{i-1}} = \frac{\mu_i + \tau \frac{d\mu_1}{dt}}{M_i}, 1 \le i \le N$$

where $\tau \ge 1$ is a time-smoothing parameter. Choosing τ very large results in a fixed grid. Increasing the value of τ from its default avoids the error condition where grid lines cross. The divisors are

$$M_i^2 = \alpha + NPDE^{-1} \sum_{j=1}^{NPDE} \frac{(U_{i+1}^j - U_i^j)^2}{(\Delta x_i)^2}$$

The value κ determines the level of clustering or spatial smoothing of the grid points. Decreasing κ from its default decrease the amount of spatial smoothing. The parameters M_i approximate arc length and help determine the shape of the grid or x_i-distribution. The parameter τ prevents the grid movement from adjusting immediately to new values of the M_i, thereby avoiding oscillations in the grid that cause large relative errors. This is important when applied to solutions with steep gradients.

The discrete form of the differential equation and the smoothing equations are combined to yield the implicit system of differential equations.

$$A(Y)\frac{dY}{dt} = L(Y),$$
$$Y = \left[U_1^1, \ \dots , U_1^{NPDE}, x_1, \ \dots , U_j^1, \ \dots , U_j^{NPDE} x_j, \ \dots \right]^T$$

This is frequently a stiff differential-algebraic system. It is solved using the integrator `DASPG` and its subroutines, including `D2SPG`. These are documented in this chapter. Note that `DASPG` is restricted to use within `PDE_1D_MG` until the routine exits with the flag `IDO = 3`. If `DASPG` is needed during the evaluations of the differential equations or boundary conditions, use of a second processor and inter-process communication is required. The only options for `DASPG` set by `PDE_1D_MG` are the Maximum BDF Order, and the absolute and relative error values, `ATOL` and `RTOL`. Users may set other options using the Options Manager. This is described in routine `DASPG` and generally in *Chapter 11* of this manual.

Remarks on the Examples

Due to its importance and the complexity of its interface, this subroutine is presented with several examples. Many of the program features are exercised. The problems complete without any change to the optional arguments, except where these changes are required to describe or to solve the problem.

In many applications the solution to a PDE is used as an auxiliary variable, perhaps as part of a larger design or simulation process. The truncation error of the approximate solution is commensurate with piece-wise linear interpolation on the grid of values, at each output point.

Example 1 - Electrodynamics Model

This example is from Blom and Zegeling (1994). The system is

$$
\begin{aligned}
&u_t = \varepsilon p u_{xx} - g(u - v)\\
&v_t = p v_{xx} + g(u - v),\\
&\text{where } g(z) = \exp(\eta z/3) - \exp(-2\eta z/3)\\
&0 \le x \le 1, 0 \le t \le 4\\
&u_x = 0 \text{ and } v = 0 \text{ at } x = 0\\
&u = 1 \text{ and } v_x = 0 \text{ at } x = 1\\
&\varepsilon = 0.143,\ p = 0.1743,\ \eta = 17.19
\end{aligned}
$$

We make the connection between the model problem statement and the example:

$$
\begin{aligned}
&C = I_2\\
&m = 0,\ R_1 = \varepsilon p u_x,\ R_2 = p v_x\\
&Q_1 = g(u - v),\ Q_2 = -Q_1
\end{aligned}
$$

The boundary conditions are

$$
\begin{aligned}
&\beta_1 = 1,\ \beta_2 = 0,\ \gamma_1 = 0,\ \gamma_2 = v, \text{ at } x = x_L = 0\\
&\beta_1 = 0,\ \beta_2 = 1,\ \gamma_1 = u - 1,\ \gamma_2 = 0, \text{ at } x = x_R = 1
\end{aligned}
$$

Rationale: Example 1

This is a non-linear problem with sharply changing conditions near $t = 0$. The default settings of integration parameters allow the problem to be solved. The use of `PDE_1D_MG` with forward communication requires three subroutines provided by the user to describe the initial conditions, differential equations, and boundary conditions.

```
      program PDE_EX1
! Electrodynamics Model:
        USE PDE_1d_mg_int
        IMPLICIT NONE

        INTEGER, PARAMETER :: NPDE=2, N=51, NFRAMES=5
        INTEGER I, IDO

! Define array space for the solution.
        real(kind(1d0)) U(NPDE+1,N), T0, TOUT
        real(kind(1d0)) :: ZERO=0D0, ONE=1D0, &
          DELTA_T=10D0, TEND=4D0
        EXTERNAL IC_01, PDE_01, BC_01

! Start loop to integrate and write solution values.
        IDO=1
        DO
           SELECT CASE (IDO)

! Define values that determine limits.
           CASE (1)
              T0=ZERO
              TOUT=1D-3
              U(NPDE+1,1)=ZERO;U(NPDE+1,N)=ONE
              OPEN(FILE='PDE_ex01.out',UNIT=7)
              WRITE(7, "(3I5, 4F10.5)") NPDE, N, NFRAMES,&
```

```
                U(NPDE+1,1), U(NPDE+1,N), T0, TEND
! Update to the next output point.
! Write solution and check for final point.
           CASE (2)

              WRITE(7,"(F10.5)")TOUT
              DO I=1,NPDE+1
                WRITE(7,"(4E15.5)")U(I,:)
              END DO
              T0=TOUT;TOUT=TOUT*DELTA_T
              IF(T0 >= TEND) IDO=3
              TOUT=MIN(TOUT, TEND)

! All completed.  Solver is shut down.
           CASE (3)
              CLOSE(UNIT=7)
              EXIT

           END SELECT

! Forward communication is used for the problem data.
           CALL PDE_1D_MG (T0, TOUT, IDO, U,&
             initial_conditions= IC_01,&
             PDE_system_definition= PDE_01,&
             boundary_conditions= BC_01)

        END DO
     END

     SUBROUTINE IC_01(NPDE, NPTS, U)
! This is the initial data for Example 1.
        IMPLICIT NONE
        INTEGER NPDE, NPTS
        REAL(KIND(1D0)) U(NPDE+1,NPTS)
        U(1,:)=1D0;U(2,:)=0D0
     END SUBROUTINE

     SUBROUTINE PDE_01(T, X, NPDE, U, DUDX, C, Q, R, IRES)
! This is the differential equation for Example 1.
        IMPLICIT NONE
        INTEGER NPDE, IRES
        REAL(KIND(1D0)) T, X, U(NPDE), DUDX(NPDE),&
          C(NPDE,NPDE), Q(NPDE), R(NPDE)
        REAL(KIND(1D0)) :: EPS=0.143D0, P=0.1743D0,&
          ETA=17.19D0, Z, TWO=2D0, THREE=3D0

        C=0D0;C(1,1)=1D0;C(2,2)=1D0
        R=P*DUDX;R(1)=R(1)*EPS
        Z=ETA*(U(1)-U(2))/THREE
        Q(1)=EXP(Z)-EXP(-TWO*Z)
        Q(2)=-Q(1)

     END SUBROUTINE

     SUBROUTINE BC_01(T, BTA, GAMA, U, DUDX, NPDE, LEFT, IRES)
! These are the boundary conditions for Example 1.
        IMPLICIT NONE
        INTEGER NPDE, IRES
        LOGICAL LEFT
        REAL(KIND(1D0)) T, BTA(NPDE), GAMA(NPDE),&
          U(NPDE), DUDX(NPDE)

        IF(LEFT) THEN
           BTA(1)=1D0;BTA(2)=0D0
           GAMA(1)=0D0;GAMA(2)=U(2)
        ELSE
```

```
            BTA(1)=0D0;BTA(2)=1D0
            GAMA(1)=U(1)-1D0;GAMA(2)=0D0
          END IF
        END SUBROUTINE
```

Example 2 - Inviscid Flow on a Plate

This example is a first order system from Pennington and Berzins, (1994). The equations are

$$
\begin{aligned}
&u_t = -v_x \\
&uu_t = -vu_x + w_{xx} \\
&w = u_x, \text{ implying that } uu_t = -vu_x + u_{xx} \\
&u(0,t) = v(0,t) = 0,\ u(\infty,t) = u(x_R,t) = 1,\ t \geq 0 \\
&u(x,0) = 1,\ v(x,0) = 0,\ x \geq 0
\end{aligned}
$$

Following elimination of *w*, there remain *NPDE* = 2 differential equations. The variable *t* is not time, but a second space variable. The integration goes from *t* = 0 to *t* = 5. It is necessary to truncate the variable *x* at a finite value, say $x_{max} = x_R = 25$. In terms of the integrator, the system is defined by letting *m* = 0 and

$$C = \left\{C_{jk}\right\} = \begin{bmatrix} 1 & 0 \\ u & 0 \end{bmatrix},\ R = \begin{bmatrix} -v \\ u_x \end{bmatrix},\ Q = \begin{bmatrix} 0 \\ vu_x \end{bmatrix}$$

The boundary conditions are satisfied by

$$
\begin{aligned}
&\beta = 0,\ \gamma = \begin{bmatrix} u - \exp(-20t) \\ v \end{bmatrix},\ \text{at } x = x_L \\
&\beta = 0,\ \gamma = \begin{bmatrix} u - 1 \\ v_x \end{bmatrix},\ \text{at } x = x_R
\end{aligned}
$$

We use *N* = 10 + 51 = 61 grid points and output the solution at steps of $\Delta t = 0.1$.

Rationale: Example 2

This is a non-linear boundary layer problem with sharply changing conditions near *t* = 0. The problem statement was modified so that boundary conditions are continuous near *t* = 0. Without this change the underlying integration software, `DASPG`, cannot solve the problem. The continuous blending function *u* = *exp*(-20*t*) is arbitrary and artfully chosen. This is a mathematical change to the problem, required because of the stated discontinuity at *t* = 0. Reverse communication is used for the problem data. No additional user-written subroutines are required when using reverse communication. We also have chosen 10 of the initial grid points to be concentrated near $x_L = 0$, anticipating rapid change in the solution near that point. Optional changes are made to use a pure absolute error tolerance and non-zero time-smoothing.

```
      program PDE_1D_MG_EX02
```

```
! Inviscid Flow Over a Plate
        USE PDE_1d_mg_int
        USE ERROR_OPTION_PACKET
        IMPLICIT NONE

        INTEGER, PARAMETER :: NPDE=2, N1=10, N2=51, N=N1+N2
        INTEGER I, IDO, NFRAMES
! Define array space for the solution.
        real(kind(1d0)) U(NPDE+1,N), T0, TOUT, DX1, DX2, DIF
        real(kind(1d0)) :: ZERO=0D0, ONE=1D0, DELTA_T=1D-1,&
          TEND=5D0, XMAX=25D0
        real(kind(1d0)) :: U0=1D0, U1=0D0, TDELTA=1D-1, TOL=1D-2
        TYPE(D_OPTIONS) IOPT(3)
! Start loop to integrate and record solution values.
        IDO=1
        DO
           SELECT CASE (IDO)
! Define values that determine limits and options.
           CASE (1)
              T0=ZERO
              TOUT=DELTA_T
              U(NPDE+1,1)=ZERO;U(NPDE+1,N)=XMAX
              OPEN(FILE='PDE_ex02.out',UNIT=7)
              NFRAMES=NINT((TEND+DELTA_T)/DELTA_T)
              WRITE(7, "(3I5, 4D14.5)") NPDE, N, NFRAMES,&
                U(NPDE+1,1), U(NPDE+1,N), T0, TEND
              DX1=XMAX/N2;DX2=DX1/N1
              IOPT(1)=D_OPTIONS(PDE_1D_MG_RELATIVE_TOLERANCE,ZERO)
              IOPT(2)=D_OPTIONS(PDE_1D_MG_ABSOLUTE_TOLERANCE,TOL)
              IOPT(3)=D_OPTIONS(PDE_1D_MG_TIME_SMOOTHING,1D-3)

! Update to the next output point.
! Write solution and check for final point.
           CASE (2)
              T0=TOUT
              IF(T0 <= TEND) THEN
                 WRITE(7,"(F10.5)")TOUT
                 DO I=1,NPDE+1
                    WRITE(7,"(4E15.5)")U(I,:)
                 END DO
                 TOUT=MIN(TOUT+DELTA_T,TEND)
                 IF(T0 == TEND)IDO=3
              END IF

! All completed.  Solver is shut down.
           CASE (3)

              CLOSE(UNIT=7)
              EXIT

! Define initial data values.
           CASE (5)
              U(:NPDE,:)=ZERO;U(1,:)=ONE
              DO I=1,N1
                 U(NPDE+1,I)=(I-1)*DX2
              END DO
              DO I=N1+1,N
                 U(NPDE+1,I)=(I-N1)*DX1
              END DO
              WRITE(7,"(F10.5)")T0
              DO I=1,NPDE+1
                 WRITE(7,"(4E15.5)")U(I,:)
              END DO

! Define differential equations.
           CASE (6)
```

```
                D_PDE_1D_MG_C=ZERO
                D_PDE_1D_MG_C(1,1)=ONE
                D_PDE_1D_MG_C(2,1)=D_PDE_1D_MG_U(1)

                D_PDE_1D_MG_R(1)=-D_PDE_1D_MG_U(2)
                D_PDE_1D_MG_R(2)= D_PDE_1D_MG_DUDX(1)

                D_PDE_1D_MG_Q(1)= ZERO
                D_PDE_1D_MG_Q(2)= &
                  D_PDE_1D_MG_U(2)*D_PDE_1D_MG_DUDX(1)
! Define boundary conditions.
             CASE (7)
                D_PDE_1D_MG_BETA=ZERO
                IF(PDE_1D_MG_LEFT) THEN
                   DIF=EXP(-20D0*D_PDE_1D_MG_T)
! Blend the left boundary value down to zero.
                   D_PDE_1D_MG_GAMMA=(/D_PDE_1D_MG_U(1)-DIF,D_PDE_1D_MG_U(2)/)
                ELSE
                   D_PDE_1D_MG_GAMMA=(/D_PDE_1D_MG_U(1)-ONE,D_PDE_1D_MG_DUDX(2)/)
                END IF
             END SELECT

! Reverse communication is used for the problem data.
             CALL PDE_1D_MG (T0, TOUT, IDO, U, IOPT=IOPT)
          END DO
       end program
```

Example 3 - Population Dynamics

This example is from Pennington and Berzins (1994). The system is

$$u_t = -u_x - I(t)u,\ x_L = 0 \le x \le a = x_R,\ t \ge 0$$

$$I(t) = \int_0^a u(x,t)\,dx$$

$$u(x,0) = \frac{\exp(-x)}{2-\exp(-a)}$$

$$u(0,t) = g\left(\int_0^a b(x,I(t))\,u(x,t)\,dx, t\right), \text{ where}$$

$$b(x,y) = \frac{xy\exp(-x)}{(y+1)^2}, \text{ and}$$

$$g(z,t) =$$

$$\frac{4z\left(2-2\exp(-a)+\exp(-t)\right)^2}{\left(1-\exp(-a)\right)\left(1-\left(1+2a\right)\exp(-2a)\right)\left(1-\exp(-a)+\exp(-t)\right)}$$

This is a notable problem because it involves the unknown

$$u(x,t) = \frac{\exp(-x)}{1 - \exp(-a) + \exp(-t)}$$

across the entire domain. The software can solve the problem by introducing two dependent algebraic equations:

$$v_1(t) = \int_0^a u(x,t)\,dx,$$
$$v_2(t) = \int_0^a x\exp(-x)\,u(x,t)\,dx$$

This leads to the modified system

$$u_t = -u_x - v_1 u,\ 0 \le x \le a,\ t \ge 0$$
$$u(0,t) = \frac{g(1,t)v_1 v_2}{(v_1+1)^2}$$

In the interface to the evaluation of the differential equation and boundary conditions, it is necessary to evaluate the integrals, which are computed with the values of $u(x,t)$ on the grid. The integrals are approximated using the trapezoid rule, commensurate with the truncation error in the integrator.

Rationale: Example 3

This is a non-linear integro-differential problem involving non-local conditions for the differential equation and boundary conditions. Access to evaluation of these conditions is provided using reverse communication. It is not possible to solve this problem with forward communication, given the current subroutine interface. Optional changes are made to use an absolute error tolerance and non-zero time-smoothing. The time-smoothing value $\tau = 1$ prevents grid lines from crossing.

```
      program PDE_1D_MG_EX03
! Population Dynamics Model.
        USE PDE_1d_mg_int
        USE ERROR_OPTION_PACKET
        IMPLICIT NONE
        INTEGER, PARAMETER :: NPDE=1, N=101
        INTEGER IDO, I, NFRAMES
! Define array space for the solution.
        real(kind(1d0)) U(NPDE+1,N), MID(N-1), T0, TOUT, V_1, V_2
        real(kind(1d0)) :: ZERO=0D0, HALF=5D-1, ONE=1D0,&
          TWO=2D0, FOUR=4D0, DELTA_T=1D-1,TEND=5D0, A=5D0
        TYPE(D_OPTIONS) IOPT(3)
! Start loop to integrate and record solution values.
        IDO=1
        DO
           SELECT CASE (IDO)
! Define values that determine limits.
           CASE (1)
              T0=ZERO
              TOUT=DELTA_T
              U(NPDE+1,1)=ZERO;U(NPDE+1,N)=A
```

```
                OPEN(FILE='PDE_ex03.out',UNIT=7)
                NFRAMES=NINT((TEND+DELTA_T)/DELTA_T)
                WRITE(7, "(3I5, 4D14.5)") NPDE, N, NFRAMES,&
                  U(NPDE+1,1), U(NPDE+1,N), T0, TEND
                IOPT(1)=D_OPTIONS(PDE_1D_MG_RELATIVE_TOLERANCE,ZERO)
                IOPT(2)=D_OPTIONS(PDE_1D_MG_ABSOLUTE_TOLERANCE,1D-2)
                IOPT(3)=D_OPTIONS(PDE_1D_MG_TIME_SMOOTHING,1D0)
! Update to the next output point.
! Write solution and check for final point.
             CASE (2)
                T0=TOUT
                IF(T0 <= TEND) THEN
                  WRITE(7,"(F10.5)")TOUT
                  DO I=1,NPDE+1
                    WRITE(7,"(4E15.5)")U(I,:)
                  END DO
                  TOUT=MIN(TOUT+DELTA_T,TEND)
                  IF(T0 == TEND)IDO=3
                END IF
! All completed.  Solver is shut down.
             CASE (3)
                CLOSE(UNIT=7)
                EXIT
! Define initial data values.
             CASE (5)
                U(1,:)=EXP(-U(2,:))/(TWO-EXP(-A))
                WRITE(7,"(F10.5)")T0
                DO I=1,NPDE+1
                  WRITE(7,"(4E15.5)")U(I,:)
                END DO
! Define differential equations.
             CASE (6)
                D_PDE_1D_MG_C(1,1)=ONE
                D_PDE_1D_MG_R(1)=-D_PDE_1D_MG_U(1)
! Evaluate the approximate integral, for this t.
                V_1=HALF*SUM((U(1,1:N-1)+U(1,2:N))*&
                             (U(2,2:N) - U(2,1:N-1)))
                D_PDE_1D_MG_Q(1)=V_1*D_PDE_1D_MG_U(1)
! Define boundary conditions.
             CASE (7)
                IF(PDE_1D_MG_LEFT) THEN
! Evaluate the approximate integral, for this t.
! A second integral is needed at the edge.
                V_1=HALF*SUM((U(1,1:N-1)+U(1,2:N))*&
                             (U(2,2:N) - U(2,1:N-1)))
                MID=HALF*(U(2,2:N)+U(2,1:N-1))
                V_2=HALF*SUM(MID*EXP(-MID)*&
                (U(1,1:N-1)+U(1,2:N))*(U(2,2:N)-U(2,1:N-1)))
                   D_PDE_1D_MG_BETA=ZERO
D_PDE_1D_MG_GAMMA=G(ONE,D_PDE_1D_MG_T)*V_1*V_2/(V_1+ONE)**2-&
                     D_PDE_1D_MG_U
                ELSE
                   D_PDE_1D_MG_BETA=ZERO
                   D_PDE_1D_MG_GAMMA=D_PDE_1D_MG_DUDX(1)
                END IF
              END SELECT
! Reverse communication is used for the problem data.
             CALL PDE_1D_MG (T0, TOUT, IDO, U, IOPT=IOPT)
          END DO
CONTAINS
          FUNCTION G(z,t)
          IMPLICIT NONE
            REAL(KIND(1d0)) Z, T, G
            G=FOUR*Z*(TWO-TWO*EXP(-A)+EXP(-T))**2
            G=G/((ONE-EXP(-A))*(ONE-(ONE+TWO*A)*&
              EXP(-TWO*A))*(1-EXP(-A)+EXP(-T)))
```

```
        END FUNCTION
      end program
```

Example 4 - A Model in Cylindrical Coordinates

This example is from Blom and Zegeling (1994). The system models a reactor-diffusion problem:

$$T_z = r^{-1}\frac{\partial\left(\beta r T_r\right)}{\partial r} + \gamma \exp\left(\frac{T}{1+\varepsilon T}\right)$$

$$T_r\left(0,z\right) = 0,\ T\left(1,z\right) = 0,\ z > 0$$

$$T\left(r,0\right) = 0,\ 0 \le r < 1$$

$$\beta = 10^{-4},\ \gamma = 1,\ \varepsilon = 0.1$$

The axial direction z is treated as a time coordinate. The radius r is treated as the single space variable.

Rationale: Example 4

This is a non-linear problem in cylindrical coordinates. Our example illustrates assigning $m = 1$ in Equation 2. We provide an optional argument that resets this value from its default, $m = 0$. Reverse communication is used to interface with the problem data.

```
      program PDE_1D_MG_EX04
! Reactor-Diffusion problem in cylindrical coordinates.
        USE pde_1d_mg_int
        USE error_option_packet
        IMPLICIT NONE
        INTEGER, PARAMETER :: NPDE=1, N=41
        INTEGER IDO, I, NFRAMES
! Define array space for the solution.
        real(kind(1d0)) T(NPDE+1,N), Z0, ZOUT
        real(kind(1d0)) :: ZERO=0D0, ONE=1D0, DELTA_Z=1D-1,&
          ZEND=1D0, ZMAX=1D0, BTA=1D-4, GAMA=1D0, EPS=1D-1
        TYPE(D_OPTIONS) IOPT(1)
! Start loop to integrate and record solution values.
        IDO=1
        DO
           SELECT CASE (IDO)
! Define values that determine limits.
           CASE (1)
              Z0=ZERO
              ZOUT=DELTA_Z
              T(NPDE+1,1)=ZERO;T(NPDE+1,N)=ZMAX
              OPEN(FILE='PDE_ex04.out',UNIT=7)
              NFRAMES=NINT((ZEND+DELTA_Z)/DELTA_Z)
              WRITE(7, "(3I5, 4D14.5)") NPDE, N, NFRAMES,&
                T(NPDE+1,1), T(NPDE+1,N), Z0, ZEND
              IOPT(1)=PDE_1D_MG_CYL_COORDINATES
! Update to the next output point.
! Write solution and check for final point.
           CASE (2)
              IF(Z0 <= ZEND) THEN
                WRITE(7,"(F10.5)")ZOUT
                DO I=1,NPDE+1
                  WRITE(7,"(4E15.5)")T(I,:)
```

```
                  END DO
                  ZOUT=MIN(ZOUT+DELTA_Z,ZEND)
                  IF(Z0 == ZEND)IDO=3
                END IF
! All completed.  Solver is shut down.
             CASE (3)
                CLOSE(UNIT=7)
                EXIT
! Define initial data values.
             CASE (5)
                T(1,:)=ZERO
                WRITE(7,"(F10.5)")Z0
                DO I=1,NPDE+1
                  WRITE(7,"(4E15.5)")T(I,:)
                END DO
! Define differential equations.
             CASE (6)
                D_PDE_1D_MG_C(1,1)=ONE
                D_PDE_1D_MG_R(1)=BTA*D_PDE_1D_MG_DUDX(1)
                D_PDE_1D_MG_Q(1)= -GAMA*EXP(D_PDE_1D_MG_U(1)/&
                  (ONE+EPS*D_PDE_1D_MG_U(1)))
! Define boundary conditions.
             CASE (7)
                IF(PDE_1D_MG_LEFT) THEN
                   D_PDE_1D_MG_BETA=ONE; D_PDE_1D_MG_GAMMA=ZERO
                ELSE
                   D_PDE_1D_MG_BETA=ZERO; D_PDE_1D_MG_GAMMA=D_PDE_1D_MG_U(1)
                END IF
             END SELECT
! Reverse communication is used for the problem data.
! The optional derived type changes the internal model
! to use cylindrical coordinates.
             CALL PDE_1D_MG (Z0, ZOUT, IDO, T, IOPT=IOPT)
          END DO
       end program
```

Example 5 - A Flame Propagation Model

This example is presented more fully in Verwer, *et al*., (1989). The system is a normalized problem relating mass density $u(x,t)$ and temperature $v(x,t)$:

$$u_t = u_{xx} - uf(v)$$
$$v_t = v_{xx} + uf(v),$$
$$\text{where } f(z) = \gamma \exp(-\beta / z),\ \beta = 4, \gamma = 3.52 \times 10^6$$
$$0 \le x \le 1,\ 0 \le t \le 0.006$$
$$u(x,0) = 1,\ v(x,0) = 0.2$$
$$u_x = v_x = 0,\ x = 0$$
$$u_x = 0,\ v = b(t),\ x = 1, \text{ where}$$
$$b(t) = 1.2,\ \mathit{for}\ t \ge 2 \times 10^{-4}, \text{ and}$$
$$= 0.2 + 5 \times 10^3 t, \text{ for } 0 \le t \le 2 \times 10^{-4}$$

Rationale: Example 5

This is a non-linear problem. The example shows the model steps for replacing the banded solver in the software with one of the user's choice. Reverse communication is used for the interface to the problem data and the linear solver. Following the computation of the matrix factorization in DL2CRB, we declare the system to be singular when the reciprocal of the condition number is smaller than the working precision. This choice is not suitable for all problems. Attention must be given to detecting a singularity when this option is used.

```
      program PDE_1D_MG_EX05
! Flame propagation model
        USE pde_1d_mg_int
        USE ERROR_OPTION_PACKET
        USE Numerical_Libraries, ONLY :&
         dl2crb, dlfsrb
        IMPLICIT NONE

        INTEGER, PARAMETER :: NPDE=2, N=40, NEQ=(NPDE+1)*N
        INTEGER I, IDO, NFRAMES, IPVT(NEQ)

! Define array space for the solution.
        real(kind(1d0)) U(NPDE+1,N), T0, TOUT
! Define work space for the banded solver.
        real(kind(1d0)) WORK(NEQ), RCOND
        real(kind(1d0)) :: ZERO=0D0, ONE=1D0, DELTA_T=1D-4,&
          TEND=6D-3, XMAX=1D0, BTA=4D0, GAMA=3.52D6
        TYPE(D_OPTIONS) IOPT(1)
! Start loop to integrate and record solution values.
        IDO=1
        DO
           SELECT CASE (IDO)

! Define values that determine limits.
           CASE (1)
              T0=ZERO
              TOUT=DELTA_T
              U(NPDE+1,1)=ZERO; U(NPDE+1,N)=XMAX
              OPEN(FILE='PDE_ex05.out',UNIT=7)
              NFRAMES=NINT((TEND+DELTA_T)/DELTA_T)
              WRITE(7, "(3I5, 4D14.5)") NPDE, N, NFRAMES,&
                U(NPDE+1,1), U(NPDE+1,N), T0, TEND
```

```
                IOPT(1)=PDE_1D_MG_REV_COMM_FACTOR_SOLVE
! Update to the next output point.
! Write solution and check for final point.
             CASE (2)
               T0=TOUT
                IF(T0 <= TEND) THEN
                  WRITE(7,"(F10.5)")TOUT
                  DO I=1,NPDE+1
                    WRITE(7,"(4E15.5)")U(I,:)
                  END DO
                  TOUT=MIN(TOUT+DELTA_T,TEND)
                  IF(T0 == TEND)IDO=3
                END IF

! All completed.  Solver is shut down.
             CASE (3)
                CLOSE(UNIT=7)
                EXIT

! Define initial data values.
             CASE (5)
                U(1,:)=ONE; U(2,:)=2D-1
                WRITE(7,"(F10.5)")T0
                DO I=1,NPDE+1
                  WRITE(7,"(4E15.5)")U(I,:)
                END DO
! Define differential equations.
             CASE (6)
                D_PDE_1D_MG_C=ZERO
                D_PDE_1D_MG_C(1,1)=ONE; D_PDE_1D_MG_C(2,2)=ONE

                D_PDE_1D_MG_R=D_PDE_1D_MG_DUDX

                D_PDE_1D_MG_Q(1)=  D_PDE_1D_MG_U(1)*F(D_PDE_1D_MG_U(2))
                D_PDE_1D_MG_Q(2)= -D_PDE_1D_MG_Q(1)
! Define boundary conditions.
             CASE (7)
                IF(PDE_1D_MG_LEFT) THEN
                   D_PDE_1D_MG_BETA=ZERO;D_PDE_1D_MG_GAMMA=D_PDE_1D_MG_DUDX
                ELSE
                   D_PDE_1D_MG_BETA(1)=ONE
                   D_PDE_1D_MG_GAMMA(1)=ZERO
                   D_PDE_1D_MG_BETA(2)=ZERO
                   IF(D_PDE_1D_MG_T >= 2D-4) THEN
                     D_PDE_1D_MG_GAMMA(2)=12D-1
                   ELSE
                     D_PDE_1D_MG_GAMMA(2)=2D-1+5D3*D_PDE_1D_MG_T
                   END IF
                   D_PDE_1D_MG_GAMMA(2)=D_PDE_1D_MG_GAMMA(2)-&
                    D_PDE_1D_MG_U(2)
                END IF
             CASE(8)
! Factor the banded matrix.  This is the same solver used
! internally but that is not required.  A user can substitute
! one of their own.
               call dl2crb (neq, d_pde_1d_mg_a, pde_1d_mg_lda, &
               pde_1d_mg_iband, pde_1d_mg_iband, d_pde_1d_mg_a, &
               pde_1d_mg_lda, ipvt, rcond, work)
               IF(rcond <= EPSILON(ONE)) pde_1d_mg_panic_flag = 1
             CASE(9)
! Solve using the factored banded matrix.
               call dlfsrb(neq, d_pde_1d_mg_a, pde_1d_mg_lda, &
               pde_1d_mg_iband, pde_1d_mg_iband, ipvt, &
               d_pde_1d_mg_rhs, 1, d_pde_1d_mg_sol)
             END SELECT
```

```
! Reverse communication is used for the problem data.
            CALL PDE_1D_MG (T0, TOUT, IDO, U, IOPT=IOPT)
         END DO
CONTAINS
         FUNCTION F(Z)
         IMPLICIT NONE
         REAL(KIND(1D0)) Z, F
           F=GAMA*EXP(-BTA/Z)
         END FUNCTION
      end program
```

Example 6 - A 'Hot Spot' Model

This example is presented more fully in Verwer, *et al*., (1989). The system is a normalized problem relating the temperature $u(x,t)$, of a reactant in a chemical system. The formula for $h(z)$ is equivalent to their example.

$$u_t = u_{xx} + h(u),$$

$$\text{where} \quad h(z) = \tfrac{R}{a\delta}(1 + a - z)exp(-\delta(1/z - 1)),$$

$$a = 1,\ \delta = 20,\ R = 5$$

$$0 \le x \le 1,\ 0 \le t \le 0.29$$

$$u(x,0) = 1$$

$$u_x = 0,\ x = 0$$

$$u = 1,\ x = 1$$

Rationale: Example 6

This is a non-linear problem. The output shows a case where a rapidly changing front, or hot-spot, develops after a considerable way into the integration. This causes rapid change to the grid. An option sets the maximum order BDF formula from its default value of 2 to the theoretical stable maximum value of 5.

```
         USE pde_1d_mg_int
         USE error_option_packet
         IMPLICIT NONE

         INTEGER, PARAMETER :: NPDE=1, N=80
         INTEGER I, IDO, NFRAMES

! Define array space for the solution.
         real(kind(1d0)) U(NPDE+1,N), T0, TOUT
         real(kind(1d0)) :: ZERO=0D0, ONE=1D0, DELTA_T=1D-2,&
           TEND=29D-2, XMAX=1D0, A=1D0, DELTA=2D1, R=5D0
         TYPE(D_OPTIONS) IOPT(2)
! Start loop to integrate and record solution values.
         IDO=1
         DO
            SELECT CASE (IDO)

! Define values that determine limits.
            CASE (1)
               T0=ZERO
               TOUT=DELTA_T
               U(NPDE+1,1)=ZERO; U(NPDE+1,N)=XMAX
               OPEN(FILE='PDE_ex06.out',UNIT=7)
```

```
                NFRAMES=(TEND+DELTA_T)/DELTA_T
                WRITE(7, "(3I5, 4D14.5)") NPDE, N, NFRAMES,&
                  U(NPDE+1,1), U(NPDE+1,N), T0, TEND
! Illustrate allowing the BDF order to increase
! to its maximum allowed value.
                IOPT(1)=PDE_1D_MG_MAX_BDF_ORDER
                  IOPT(2)=5
! Update to the next output point.
! Write solution and check for final point.
             CASE (2)
                T0=TOUT
                IF(T0 <= TEND) THEN
                  WRITE(7,"(F10.5)")TOUT
                  DO I=1,NPDE+1
                    WRITE(7,"(4E15.5)")U(I,:)
                  END DO
                  TOUT=MIN(TOUT+DELTA_T,TEND)
                  IF(T0 == TEND)IDO=3
                END IF
! All completed.  Solver is shut down.
             CASE (3)
                CLOSE(UNIT=7)
                EXIT

! Define initial data values.
             CASE (5)
                U(1,:)=ONE
                WRITE(7,"(F10.5)")T0
                DO I=1,NPDE+1
                  WRITE(7,"(4E15.5)")U(I,:)
                END DO
! Define differential equations.
             CASE (6)
                D_PDE_1D_MG_C=ONE
                D_PDE_1D_MG_R=D_PDE_1D_MG_DUDX
                D_PDE_1D_MG_Q= - H(D_PDE_1D_MG_U(1))

! Define boundary conditions.
             CASE (7)
                IF(PDE_1D_MG_LEFT) THEN
                   D_PDE_1D_MG_BETA=ZERO
                   D_PDE_1D_MG_GAMMA=D_PDE_1D_MG_DUDX
                ELSE

                   D_PDE_1D_MG_BETA=ZERO
                   D_PDE_1D_MG_GAMMA=D_PDE_1D_MG_U(1)-ONE
                END IF
             END SELECT

! Reverse communication is used for the problem data.
             CALL PDE_1D_MG (T0, TOUT, IDO, U, IOPT=IOPT)
          END DO
CONTAINS
          FUNCTION H(Z)
          real(kind(1d0)) Z, H
            H=(R/(A*DELTA))*(ONE+A-Z)*EXP(-DELTA*(ONE/Z-ONE))
          END FUNCTION
       end program
```

Example 7 - Traveling Waves

This example is presented more fully in Verwer, *et al*., (1989). The system is a normalized problem relating the interaction of two waves, $u(x,t)$ and $v(x,t)$ moving in opposite directions. The waves meet and reduce in amplitude, due to the non-linear terms in the equation. Then they separate and travel onward, with reduced amplitude.

$$
\begin{aligned}
&u_t = -u_x - 100uv,\\
&v_t = v_x - 100uv,\\
&-0.5 \le x \le 0.5,\ 0 \le t \le 0.5\\
&u(x,0) = 0.5(1+\cos(10\pi x)),\ x \in [-0.3, -0.1],\ \text{and}\\
&\quad = 0,\ \text{otherwise},\\
&v(x,0) = 0.5(1+\cos(10\pi x)),\ x \in [0.1, 0.3],\ \text{and}\\
&\quad = 0,\ \text{otherwise},\\
&u = v = 0 \text{ at both ends, } t \ge 0
\end{aligned}
$$

Rationale: Example 7

This is a non-linear system of first order equations.

```
      program PDE_1D_MG_EX07
 ! Traveling Waves
         USE pde_1d_mg_int
         USE error_option_packet
         IMPLICIT NONE

         INTEGER, PARAMETER :: NPDE=2, N=50
         INTEGER I, IDO, NFRAMES

 ! Define array space for the solution.
         real(kind(1d0)) U(NPDE+1,N), TEMP(N), T0, TOUT
         real(kind(1d0)) :: ZERO=0D0, HALF=5D-1, &
           ONE=1D0, DELTA_T=5D-2,TEND=5D-1, PI
         TYPE(D_OPTIONS) IOPT(5)
 ! Start loop to integrate and record solution values.
         IDO=1
         DO
            SELECT CASE (IDO)

 ! Define values that determine limits.
            CASE (1)
               T0=ZERO
               TOUT=DELTA_T
               U(NPDE+1,1)=-HALF; U(NPDE+1,N)=HALF
               OPEN(FILE='PDE_ex07.out',UNIT=7)
               NFRAMES=(TEND+DELTA_T)/DELTA_T
               WRITE(7, "(3I5, 4D14.5)") NPDE, N, NFRAMES,&
                 U(NPDE+1,1), U(NPDE+1,N), T0, TEND
               IOPT(1)=D_OPTIONS(PDE_1D_MG_TIME_SMOOTHING,1D-3)
               IOPT(2)=D_OPTIONS(PDE_1D_MG_RELATIVE_TOLERANCE,ZERO)
               IOPT(3)=D_OPTIONS(PDE_1D_MG_ABSOLUTE_TOLERANCE,1D-3)
               IOPT(4)=PDE_1D_MG_MAX_BDF_ORDER
                 IOPT(5)=3
 ! Update to the next output point.
 ! Write solution and check for final point.
```

```
            CASE (2)
               T0=TOUT
               IF(T0 <= TEND) THEN
                 WRITE(7,"(F10.5)")TOUT
                 DO I=1,NPDE+1
                   WRITE(7,"(4E15.5)")U(I,:)
                 END DO
                 TOUT=MIN(TOUT+DELTA_T,TEND)
                 IF(T0 == TEND)IDO=3
               END IF

! All completed.  Solver is shut down.
            CASE (3)
               CLOSE(UNIT=7)
               EXIT

! Define initial data values.
            CASE (5)
               TEMP=U(3,:)
               U(1,:)=PULSE(TEMP); U(2,:)=U(1,:)
               WHERE (TEMP < -3D-1 .or. TEMP > -1D-1) U(1,:)=ZERO
               WHERE (TEMP <  1D-1 .or. TEMP >  3D-1) U(2,:)=ZERO
               WRITE(7,"(F10.5)")T0
               DO I=1,NPDE+1
                 WRITE(7,"(4E15.5)")U(I,:)
               END DO

! Define differential equations.
            CASE (6)
               D_PDE_1D_MG_C=ZERO
               D_PDE_1D_MG_C(1,1)=ONE; D_PDE_1D_MG_C(2,2)=ONE

               D_PDE_1D_MG_R=D_PDE_1D_MG_U
               D_PDE_1D_MG_R(1)=-D_PDE_1D_MG_R(1)

               D_PDE_1D_MG_Q(1)= 100D0*D_PDE_1D_MG_U(1)*D_PDE_1D_MG_U(2)
               D_PDE_1D_MG_Q(2)= D_PDE_1D_MG_Q(1)

! Define boundary conditions.
            CASE (7)
               D_PDE_1D_MG_BETA=ZERO;D_PDE_1D_MG_GAMMA=D_PDE_1D_MG_U

            END SELECT

! Reverse communication is used for the problem data.
            CALL PDE_1D_MG (T0, TOUT, IDO, U, IOPT=IOPT)
         END DO
CONTAINS
         FUNCTION PULSE(Z)
         real(kind(1d0)) Z(:), PULSE(SIZE(Z))
           PI=ACOS(-ONE)
           PULSE=HALF*(ONE+COS(10D0*PI*Z))
         END FUNCTION
      end program
```

Example 8 - Black-Scholes

The value of a European “call option,” $c(s,t)$, with exercise price *e* and expiration date *T*, satisfies the “asset-or-nothing payoff ” $c(s,T) = s, s \geq e; = 0, s < e$. Prior to expiration $c(s,t)$ is estimated by the Black-Scholes differential equation

$$c_t + \frac{\sigma^2}{2}s^2 c_{ss} + rsc_s - rc \equiv c_t + \frac{\sigma^2}{2}\left(s^2 c_s\right)_s + \left(r - \sigma^2\right)sc_s - rc = 0$$

The parameters in the model are the risk-free interest rate, *r*, and the stock volatility, σ. The boundary conditions are $c\left(0,t\right) = 0$ and $c_s\left(s,t\right) \approx 1, s \to \infty$. This development is described in Wilmott, *et al*. (1995), pages 41-57. There are explicit solutions for this equation based on the Normal Curve of Probability. The normal curve, and the solution itself, can be efficiently computed with the IMSL function ANORDF, IMSL (1994), page 186. With numerical integration the equation itself or the payoff can be readily changed to include other formulas, $c\left(s,T\right)$, and corresponding boundary conditions. We use

$$e = 100,\ r = 0.08,\ T\text{–}t = 0.25,\ \sigma^2 = 0.04,\ s_L = 0, \text{ and } s_R = 150$$

Rationale: Example 8

This is a linear problem but with initial conditions that are discontinuous. It is necessary to use a positive time-smoothing value to prevent grid lines from crossing. We have used an absolute tolerance of 10^{-3}. In $US, this is one-tenth of a cent.

```
      program PDE_1D_MG_EX08
! Black-Scholes call price
        USE pde_1d_mg_int
        USE error_option_packet
        IMPLICIT NONE

        INTEGER, PARAMETER :: NPDE=1, N=100
        INTEGER I, IDO, NFRAMES

! Define array space for the solution.
        real(kind(1d0)) U(NPDE+1,N), T0, TOUT, SIGSQ, XVAL
        real(kind(1d0)) :: ZERO=0D0, HALF=5D-1, ONE=1D0, &
          DELTA_T=25D-3, TEND=25D-2, XMAX=150, SIGMA=2D-1, &
          R=8D-2, E=100D0
        TYPE(D_OPTIONS) IOPT(5)
! Start loop to integrate and record solution values.
        IDO=1
        DO
           SELECT CASE (IDO)

! Define values that determine limits.
           CASE (1)
              T0=ZERO
              TOUT=DELTA_T
              U(NPDE+1,1)=ZERO; U(NPDE+1,N)=XMAX
              OPEN(FILE='PDE_ex08.out',UNIT=7)
              NFRAMES=NINT((TEND+DELTA_T)/DELTA_T)
              WRITE(7, "(3I5, 4D14.5)") NPDE, N, NFRAMES,&
                U(NPDE+1,1), U(NPDE+1,N), T0, TEND
                SIGSQ=SIGMA**2
! Illustrate allowing the BDF order to increase
! to its maximum allowed value.
              IOPT(1)=PDE_1D_MG_MAX_BDF_ORDER
                IOPT(2)=5
              IOPT(3)=D_OPTIONS(PDE_1D_MG_TIME_SMOOTHING,5D-3)
              IOPT(4)=D_OPTIONS(PDE_1D_MG_RELATIVE_TOLERANCE,ZERO)
              IOPT(5)=D_OPTIONS(PDE_1D_MG_ABSOLUTE_TOLERANCE,1D-2)
! Update to the next output point.
```

```
! Write solution and check for final point.
           CASE (2)
              T0=TOUT
              IF(T0 <= TEND) THEN
                WRITE(7,"(F10.5)")TOUT
                DO I=1,NPDE+1
                  WRITE(7,"(4E15.5)")U(I,:)
                END DO
                TOUT=MIN(TOUT+DELTA_T,TEND)
                IF(T0 == TEND)IDO=3
              END IF
! All completed.  Solver is shut down.
           CASE (3)
              CLOSE(UNIT=7)
              EXIT

! Define initial data values.
           CASE (5)
              U(1,:)=MAX(U(NPDE+1,:)-E,ZERO)  ! Vanilla European Call
              U(1,:)=U(NPDE+1,:)              ! Asset-or-nothing Call
              WHERE(U(1,:) <= E) U(1,:)=ZERO  ! on these two lines
              WRITE(7,"(F10.5)")T0
              DO I=1,NPDE+1
                WRITE(7,"(4E15.5)")U(I,:)
              END DO
! Define differential equations.
           CASE (6)
              XVAL=D_PDE_1D_MG_X
              D_PDE_1D_MG_C=ONE
              D_PDE_1D_MG_R=D_PDE_1D_MG_DUDX*XVAL**2*SIGSQ*HALF
              D_PDE_1D_MG_Q=-(R-SIGSQ)*XVAL*D_PDE_1D_MG_DUDX+R*D_PDE_1D_MG_U
! Define boundary conditions.
           CASE (7)
              IF(PDE_1D_MG_LEFT) THEN
                 D_PDE_1D_MG_BETA=ZERO
                 D_PDE_1D_MG_GAMMA=D_PDE_1D_MG_U
              ELSE

                 D_PDE_1D_MG_BETA=ZERO
                 D_PDE_1D_MG_GAMMA=D_PDE_1D_MG_DUDX(1)-ONE
              END IF
           END SELECT

! Reverse communication is used for the problem data.
           CALL PDE_1D_MG (T0, TOUT, IDO, U, IOPT=IOPT)
        END DO

     end program
```

Example 9 - Electrodynamics, Parameters Studied with MPI

MPI REQUIRED

For a detailed description of MPI Requirements see *Dense Matrix Parallelism Using MPI* in *Chapter 10* of this manual.

This example, described above in Example 1, is from Blom and Zegeling (1994). The system parameters ε, ρ, and η, are varied, using uniform random numbers. The intervals studied are $0.1 \le \varepsilon \le 0.2$, $0.1 \le \rho \le 0.2$, and $10 \le \eta \le 20$. Using $N = 21$ grid values and other program options, the elapsed time, parameter values, and the value $v(x,t)|_{x=1,\ t=4}$ are sent to the root node. This information is written on a file. The final summary includes the minimum value of $v(x,t)|_{x=1,\ t=4}$ and the maximum and average time per integration, per node.

Rationale: Example 9

This is a non-linear simulation problem. Using at least two integrating processors and MPI allows more values of the parameters to be studied in a given time than with a single processor. This code is valuable as a study guide when an application needs to estimate timing and other output parameters. The simulation time is controlled at the root node. An integration is started, after receiving results, within the first `SIM_TIME` seconds. The elapsed time will be longer than `SIM_TIME` by the slowest processor's time for its last integration.

```
      program PDE_1D_MG_EX09
! Electrodynamics Model, parameter study.
        USE PDE_1d_mg_int
        USE MPI_SETUP_INT
        USE RAND_INT
        USE SHOW_INT
        IMPLICIT NONE
        INCLUDE "mpif.h"
        INTEGER, PARAMETER :: NPDE=2, N=21
        INTEGER I, IDO, IERROR, CONTINUE, STATUS(MPI_STATUS_SIZE)
        INTEGER, ALLOCATABLE :: COUNTS(:)
! Define array space for the solution.
        real(kind(1d0)) :: U(NPDE+1,N), T0, TOUT
        real(kind(1d0)) :: ZERO=0D0, ONE=1D0,DELTA_T=10D0, TEND=4D0
! SIM_TIME is the number of seconds to run the simulation.
        real(kind(1d0)) :: EPS, P, ETA, Z, TWO=2D0, THREE=3D0, SIM_TIME=60D0
        real(kind(1d0)) :: TIMES, TIMEE, TIMEL, TIME, TIME_SIM, V_MIN, &
        DATA(5)
        real(kind(1d0)), ALLOCATABLE :: AV_TIME(:), MAX_TIME(:)
        TYPE(D_OPTIONS) IOPT(4), SHOW_IOPT(2)
        TYPE(S_OPTIONS) SHOW_INTOPT(2)
        MP_NPROCS=MP_SETUP(1)
        MPI_NODE_PRIORITY=(/(I-1,I=1,MP_NPROCS)/)
! If NP_NPROCS=1, the program stops.  Change
! MPI_ROOT_WORKS=.TRUE. if MP_NPROCS=1.
        MPI_ROOT_WORKS=.FALSE.
        IF(.NOT. MPI_ROOT_WORKS .and. MP_NPROCS == 1) STOP
        ALLOCATE(AV_TIME(MP_NPROCS), MAX_TIME(MP_NPROCS), COUNTS(MP_NPROCS))
! Get time start for simulation timing.
        TIME=MPI_WTIME()
        IF(MP_RANK == 0) OPEN(FILE='PDE_ex09.out',UNIT=7)
 SIMULATE: DO
! Pick random parameter values.
           EPS=1D-1*(ONE+rand(EPS))
           P=1D-1*(ONE+rand(P))
           ETA=10D0*(ONE+rand(ETA))
! Start loop to integrate and communicate solution times.
           IDO=1
! Get time start for each new problem.
           DO
              IF(.NOT. MPI_ROOT_WORKS .and. MP_RANK == 0) EXIT
              SELECT CASE (IDO)
```

```
! Define values that determine limits.
                CASE (1)
                   T0=ZERO
                   TOUT=1D-3
                   U(NPDE+1,1)=ZERO;U(NPDE+1,N)=ONE
                   IOPT(1)=PDE_1D_MG_MAX_BDF_ORDER
                   IOPT(2)=5
                   IOPT(3)=D_OPTIONS(PDE_1D_MG_RELATIVE_TOLERANCE,1D-2)
                   IOPT(4)=D_OPTIONS(PDE_1D_MG_ABSOLUTE_TOLERANCE,1D-2)

                   TIMES=MPI_WTIME()
! Update to the next output point.
! Write solution and check for final point.
                CASE (2)
                   T0=TOUT;TOUT=TOUT*DELTA_T
                   IF(T0 >= TEND) IDO=3
                   TOUT=MIN(TOUT, TEND)
! All completed.  Solver is shut down.
                CASE (3)
                   TIMEE=MPI_WTIME()
                   EXIT
! Define initial data values.
                CASE (5)
                   U(1,:)=1D0;U(2,:)=0D0
! Define differential equations.
                CASE (6)
                   D_PDE_1D_MG_C=0D0;D_PDE_1D_MG_C(1,1)=1D0;D_PDE_1D_MG_C(2,2)=1D0
                   D_PDE_1D_MG_R=P*D_PDE_1D_MG_DUDX
                   D_PDE_1D_MG_R(1)=D_PDE_1D_MG_R(1)*EPS
                   Z=ETA*(D_PDE_1D_MG_U(1)-D_PDE_1D_MG_U(2))/THREE
                   D_PDE_1D_MG_Q(1)=EXP(Z)-EXP(-TWO*Z)
                   D_PDE_1D_MG_Q(2)=-D_PDE_1D_MG_Q(1)
! Define boundary conditions.
                CASE (7)
                   IF(PDE_1D_MG_LEFT) THEN
                      D_PDE_1D_MG_BETA(1)=1D0;D_PDE_1D_MG_BETA(2)=0D0
                      D_PDE_1D_MG_GAMMA(1)=0D0;D_PDE_1D_MG_GAMMA(2)=D_PDE_1D_MG_U(2)
                   ELSE
                      D_PDE_1D_MG_BETA(1)=0D0;D_PDE_1D_MG_BETA(2)=1D0
                      D_PDE_1D_MG_GAMMA(1)=D_PDE_1D_MG_U(1)- &
                      1D0;D_PDE_1D_MG_GAMMA(2)=0D0
                   END IF
                END SELECT
! Reverse communication is used for the problem data.
                CALL PDE_1D_MG (T0, TOUT, IDO, U)
             END DO
             TIMEL=TIMEE-TIMES
             DATA=(/EPS, P, ETA, U(2,N), TIMEL/)
             IF(MP_RANK > 0) THEN
! Send parameters and time to the root.
                CALL MPI_SEND(DATA, 5, MPI_DOUBLE_PRECISION,0, MP_RANK, &
                MP_LIBRARY_WORLD, IERROR)
! Receive back a "go/stop" flag.
                CALL MPI_RECV(CONTINUE, 1, MPI_INTEGER, 0, MPI_ANY_TAG, &
                MP_LIBRARY_WORLD, STATUS, IERROR)
! If root notes that time is up, it sends node a quit flag.
                IF(CONTINUE == 0) EXIT SIMULATE
             ELSE
! If root is working, record its result and then stand ready
! for other nodes to send.
                IF(MPI_ROOT_WORKS) WRITE(7,*) MP_RANK, DATA
! If all nodes have reported, then quit.
                IF(COUNT(MPI_NODE_PRIORITY >= 0) == 0) EXIT SIMULATE
! See if time is up. Some nodes still must report.
                IF(MPI_WTIME()-TIME >= SIM_TIME) THEN
                   CONTINUE=0
```

```
                ELSE
                   CONTINUE=1
                END IF
! Root receives simulation data and finds which node sent it.
                IF(MP_NPROCS > 1) THEN
                   CALL MPI_RECV(DATA, 5, MPI_DOUBLE_PRECISION, &
                   MPI_ANY_SOURCE, MPI_ANY_TAG, MP_LIBRARY_WORLD, &
                   STATUS, IERROR)
                   WRITE(7,*) STATUS(MPI_SOURCE), DATA
! If time at the root has elapsed, nodes receive signal to stop.
! Send the reporting node the "go/stop" flag.
! Mark if a node has been stopped.
                   CALL MPI_SEND(CONTINUE, 1, MPI_INTEGER, &
                   STATUS(MPI_SOURCE), &0, MP_LIBRARY_WORLD, IERROR)
                   IF (CONTINUE == 0) MPI_NODE_PRIORITY(STATUS(MPI_SOURCE)+1)&
                   =- MPI_NODE_PRIORITY(STATUS(MPI_SOURCE)+1)-1
                END IF
                IF (CONTINUE == 0) MPI_NODE_PRIORITY(1)=-1
             END IF
          END DO SIMULATE
          IF(MP_RANK == 0) THEN
             ENDFILE(UNIT=7);REWIND(UNIT=7)
! Read the data. Find extremes and averages.
             MAX_TIME=ZERO;AV_TIME=ZERO;COUNTS=0;V_MIN=HUGE(ONE)
             DO
                READ(7,*, END=10) I, DATA
                COUNTS(I+1)=COUNTS(I+1)+1
                AV_TIME(I+1)=AV_TIME(I+1)+DATA(5)
                IF(MAX_TIME(I+1) < DATA(5)) MAX_TIME(I+1)=DATA(5)
                V_MIN=MIN(V_MIN, DATA(4))
             END DO
10           CONTINUE
             CLOSE(UNIT=7)
! Set printing Index to match node numbering.
             SHOW_IOPT(1)= SHOW_STARTING_INDEX_IS
             SHOW_IOPT(2)=0
             SHOW_INTOPT(1)=SHOW_STARTING_INDEX_IS
             SHOW_INTOPT(2)=0
             CALL SHOW(MAX_TIME,"Maximum Integration Time, per process:",IOPT=SHOW_IOPT)
             AV_TIME=AV_TIME/MAX(1,COUNTS)
             CALL SHOW(AV_TIME,"Average Integration Time, per process:",IOPT=SHOW_IOPT)
             CALL SHOW(COUNTS,"Number of Integrations",IOPT=SHOW_INTOPT)
             WRITE(*,"(1x,A,F6.3)") "Minimum value for v(x,t),at x=1,t=4:  ",V_MIN
          END IF
          MP_NPROCS=MP_SETUP("Final")
       end program
```

MMOLCH

more...

Solves a system of partial differential equations of the form $u_t = f(x, t, u, u_x, u_{xx})$ using the method of lines. The solution is represented with cubic Hermite polynomials.

Note: `MMOLCH` replaces deprecated function `MOLCH`.

Required Arguments

IDO — Flag indicating the state of the computation. (Input/Output)

IDO	State
1	Initial entry
2	Normal reentry
3	Final call, release workspace

Normally, the initial call is made with `IDO` = 1. The routine then sets `IDO` = 2, and this value is then used for all but the last call that is made with `IDO` = 3.

FCNUT — User-supplied `subroutine` to evaluate the function u_t. The usage is `CALL FCNUT (NPDES, X, T, U, UX, UXX, UT [,…])` where

Required Arguments

`NPDES` — Number of equations. (Input)

`X` — Space variable, *x*. (Input)

`T` — Time variable, *t*. (Input)

`U` — Array of length `NPDES` containing the dependent variable values, *u*. (Input)

`UX` — Array of length `NPDES` containing the first derivatives u_x. (Input)

`UXX` — Array of length `NPDES` containing the second derivative u_{xx}. (Input)

`UT` — Array of length `NPDES` containing the computed derivatives, u_t. (Output)

Optional Arguments

FCN_DATA — A derived type, s_fcn_data, which may be used to pass additional integer or floating point information to or from the user-supplied subroutine. For a detailed description of this argument see FCN_DATA below. (Input/Output)

FCNUT must be declared EXTERNAL in the calling program.

FCNBC — User-supplied subroutine to evaluate the boundary conditions. The boundary conditions accepted by MMOLCH are $\alpha_k u_k + \beta_k u_x = \gamma_k(t)$. Users must supply the values α_k and β_k, and functions $\gamma_k(t)$. The usage is CALL FCNBC (NPDES, X, T, ALPHA, BETA, GAMMA [, …]), where

Required Arguments

NPDES – Number of equations. (Input)

X — Space variable, *x*. This value directs which boundary condition to compute. (Input)

T — Time variable, *t*. (Input)

ALPHA — Array of length NPDES containing the α_k values. (Output)

BETA — Array of length NPDES containing the β_k values. (Output)

GAMMA — Array of length NPDES containing the values of $\gamma_k(t)$. (Output)

Optional Arguments

FCN_DATA — A derived type, s_fcn_data, which may be used to pass additional integer or floating point information to or from the user-supplied subroutine. For a detailed description of this argument see FCN_DATA below. (Input/Output)

FCNBC must be declared EXTERNAL in the calling program.

T — Independent variable, *t*. (Input/Output)

On input, T supplies the initial time, t_0. On output, T is set to the value to which the integration has been updated. Normally, this new value is TEND.

TEND — Value of $t = tend$ at which the solution is desired. (Input)

XBREAK — Array of length NX containing the break points for the cubic Hermite splines used in the *x* discretization. (Input)

The points in the array XBREAK must be strictly increasing. The values XBREAK(1) and XBREAK(NX) are the endpoints of the interval.

Y — Array of size NPDES by NX containing the solution. (Input/Output)

The array Y contains the solution as $Y(k, i) = u_k(x, t)$ at x = XBREAK(*i*). On input, Y contains the initial values. On output, Y contains the computed solution. The user can optionally supply the derivative values, $u_x(x, t_0)$. The user allocates twice the space for Y to pass this information. The optional derivative information is input as

$$\mathrm{Y}\left(k,i+\mathrm{NX}\right) = \frac{\partial u_k}{\partial x}\left(x,t_0\right)$$

at x = XBREAK(*i*). The array Y contains the optional derivative values as output:

$$\mathrm{Y}(k,i+\mathrm{NX}) = \frac{\partial u_k}{\partial x}(x,tend)$$

at x = XBREAK(i). To signal that this information is provided, set INPDER = 1.

Optional Arguments

NPDES — Number of differential equations. (Input)
Default: NPDES = size (Y,1).

NX — Number of mesh points or lines. (Input)
Default: NX = size (XBREAK,1).

TOL — Differential equation error tolerance. (Input)
An attempt is made to control the local error in such a way that the global error is proportional to TOL.
Default: TOL = 100 * machine precision.

HINIT — Initial step size in the t integration. (Input)
This value must be nonnegative. If HINIT is zero, an initial step size of $0.001|tend-t_0|$ will be arbitrarily used. The step will be applied in the direction of integration.
Default: HINIT = 0.0.

INPDER — Set INPDER = 1 if the user is supplying the derivative values, $u_{\boldsymbol{x}}(x, t_0)$, in the array Y. (Input)
Default: INPDER = 0.

FCN_DATA — A derived type, s_fcn_data, which may be used to pass additional information to/from the user-supplied function. (Input/Output)
The derived type, s_fcn_data, is defined as:

```
type s_fcn_data
   real(kind(1e0)), pointer, dimension(:) :: rdata
   integer, pointer, dimension(:) :: idata
end type
```

in module mp_types. The double precision counterpart to s_fcn_data is named d_fcn_data. The user must include a use mp_types statement in the calling program to define this derived type.

FORTRAN 90 Interface

Generic: CALL MMOLCH (IDO, FCNUT, FCNBC, T, TEND, XBREAK, Y [, …])

Specific: The specific interface names are S_MMOLCH and D_MMOLCH.

Description

Let M = `NPDES`, N = `NX` and x_i = `XBREAK(I)`. The routine `MMOLCH` uses the method of lines to solve the partial differential equation system

$$\frac{\partial u_k}{\partial t} = f_k\left(x,t,u_1, \ldots u_M, \frac{\partial u_1}{\partial x}, \ldots \frac{\partial u_M}{\partial x}, \frac{\partial^2 u_1}{\partial x^2}, \ldots \frac{\partial^2 u_M}{\partial x^2}\right)$$

with the initial conditions

$$u_k = u_k(x) \text{ at } t = t_0$$

and the boundary conditions

$$\alpha_k u_k + \beta_k \frac{\partial u_k}{\partial x} = \gamma_k(t) \text{ at } x = x_1 \text{ and at } x = x_N$$

for $k = 1, \ldots, M$.

Cubic Hermite polynomials are used in the x variable approximation so that the trial solution is expanded in the series

$$\hat{u}_k(x,t) = \sum_{i=1}^{N}\left(a_{i,k}(t)\phi_i(x) + b_{i,k}(t)\psi_i(x)\right)$$

where $\phi_i(x)$ and $\Psi_i(x)$ are the standard basis functions for the cubic Hermite polynomials with the knots $x_1 < x_2 < \ldots < x_N$. These are piecewise cubic polynomials with continuous first derivatives. At the breakpoints, they satisfy

$$\phi_i(x_l) = \delta_{il} \quad \psi_i(x_l) = 0$$
$$\frac{d\phi_i}{dx}(x_l) = 0 \quad \frac{d\psi_i}{dx}(x_l) = \delta_{il}$$

According to the collocation method, the coefficients of the approximation are obtained so that the trial solution satisfies the differential equations at the two Gaussian points in each subinterval,

$$p_{2j-1} = x_j + \frac{3-\sqrt{3}}{6}\left(x_{j+1} - x_j\right)$$
$$p_{2j} = x_j + \frac{3+\sqrt{3}}{6}\left(x_{j+1} + x_j\right)$$

for $j = 1, \ldots, N$. The collocation approximation to the differential equation is

$$\sum_{i=1}^{N} \frac{da_{i,k}}{dt}\phi_i\left(p_j\right) + \frac{db_{i,k}}{dt}\psi_i\left(p_j\right) =$$
$$f_k\left(p_j, t, \hat{u}_1(p_j), \ \ldots, \hat{u}_M(p_j), \ \ldots, (\hat{u}_1)_{xx}(p_j), \ \ldots, (\hat{u}_M)_{xx}(p_j)\right)$$

for $k = 1, \ldots, M$ and $j = 1, \ldots, 2(N - 1)$.

This is a system of $2M(N - 1)$ ordinary differential equations in $2MN$ unknown coefficient functions, $a_{i,k}$ and $b_{i,k}$.

This system can be written in the matrix-vector form as $A\frac{dc}{dt} = F\left(t,c\right)$ with $c(t_0) = c_0$ where c is a vector of coefficients of length $2MN$ and c_0 holds the initial values of the coefficients. The last $2M$ equations are obtained from the boundary conditions.

If $\alpha_k = \beta_k = 0$, it is assumed that no boundary condition is desired for the k-th unknown at the left endpoint. A similar comment holds for the right endpoint. Thus, collocation is done at the endpoint. This is generally a useful feature for systems of first-order partial differential equations.

The input/output array `Y` contains the values of the $a_{i,k}$. The initial values of the $b_{i,k}$ are obtained by using the IMSL cubic spline routine `CSINT` (see *Chapter 3, "Interpolation and Approximation"*) to construct functions

$$\hat{u}_k\left(x, t_0\right)$$

such that

$$\hat{u}_k\left(x_i, t_0\right) = a_{i,k}$$

The IMSL routine `CSDER`, (see *Chapter 3, "Interpolation and Approximation"*), is used to approximate the values

$$\frac{d\hat{u}_k}{dx}\left(x_i, t_0\right) \equiv b_{i,k}$$

If `INPDER` = 1, the user should provide the initial values of $b_{i,k}$.

The order of matrix A is $2MN$ and its maximum bandwidth is $6M-1$. The band structure of the Jacobian of F with respect to c is the same as the band structure of A. This system is solved using a modified version of `IVPAG`. Numerical Jacobians are used exclusively. The algorithm is unchanged. Gear's BDF method is used as the default because the system is typically stiff. For more details, see Sewell (1982).

We now present three examples of PDEs that illustrate how users can interface their problems with IMSL PDE solving software. The examples are small and not indicative of the complexities that most practitioners will face in their applications. A set of seven sample application problems, some of them with more than one equation, is given in Sincovec and Madsen (1975). Two further examples are given in Madsen and Sincovec (1979).

Comments

Informational errors

Type	Code	Description
4	1	After some initial success, the integration was halted by repeated error test failures.
4	2	On the next step, `X` + `H` will equal `X`. Either `TOL` is too small or the problem is stiff.
4	3	After some initial success, the integration was halted by a test on `TOL`.
4	4	Integration was halted after failing to pass the error test even after reducing the step size by a factor of `1.0E` + 10. `TOL` may be too small.
4	5	Integration was halted after failing to achieve corrector convergence even after reducing the step size by a factor of `1.0E` + 10. `TOL` may be too small.

Examples

Example 1

The normalized linear diffusion PDE, $u_t = u_{xx}$, $0 \le x \le 1$, $t > 0$, is solved. The initial values are $u(x, 0) = u_0 = 1$. There is a “zero-flux” boundary condition at $x = 1$, namely $u_x(1, t) = 0$, $(t > 0)$. The boundary value of $u(0, t)$ is abruptly changed from u_0 to the value 0, for $t > 0$.

When the boundary conditions are discontinuous, or incompatible with the initial conditions such as in this example, it may be important to use double precision.

```
      USE MMOLCH_INT
      USE WRRRN_INT
      IMPLICIT    NONE

      INTEGER, PARAMETER ::  NPDES=1, NX=8

      INTEGER            ::  I, IDO, J, NSTEP
      REAL               ::  HINIT, T, TEND, TOL
      REAL               ::  XBREAK(NX), Y(NPDES,NX), U0
      CHARACTER          ::  TITLE*19

      EXTERNAL    FCNBC, FCNUT
!                                SET BREAKPOINTS AND INITIAL CONDITIONS
      U0 = 1.0
      DO I=1,NX
         XBREAK(I) = FLOAT(I-1)/FLOAT(NX-1)
         Y(1,I)    = U0
      END DO
!                                SET PARAMETERS FOR MMOLCH
      TOL    = 10.e-4
      HINIT  = 0.01*TOL
      T      = 0.0
      IDO    = 1
```

```
      NSTEP  = 10
      DO J=1,NSTEP
         TEND = FLOAT(J)/FLOAT(NSTEP)
!                                SOLVE THE PROBLEM
         CALL MMOLCH (IDO, FCNUT, FCNBC, T, TEND, XBREAK, Y, TOL=TOL, &
           HINIT=HINIT)
!                                PRINT RESULTS
         WRITE (TITLE,'(A,F4.2)') 'Solution at T =', TEND
         CALL WRRRN (TITLE, Y)
      END DO
!                                LAST CALL, TO RELEASE WORKSPACE
      IDO = 3
      CALL MMOLCH (IDO, FCNUT, FCNBC, T, TEND, XBREAK, Y, TOL=TOL, &
        HINIT=HINIT)
      STOP
      END

      SUBROUTINE FCNUT (NPDES, X, T, U, UX, UXX, UT)

      INTEGER    NPDES
      REAL       X, T, U(*), UX(*), UXX(*), UT(*)
!                                DEFINE THE PDE
      UT(1) = UXX(1)
      RETURN
      END

      SUBROUTINE FCNBC (NPDES, X, T, ALPHA, BTA, GAM)

      INTEGER    NPDES
      REAL       X, T, ALPHA(*), BTA(*), GAM(*)
!                                DEFINE THE BOUNDARY CONDITIONS
      IF (X .EQ. 0.0) THEN
!                                THESE ARE FOR X=0
         ALPHA(1) = 1.0
         BTA(1) = 0.0
         GAM(1) = 0.0
      ELSE
!                                THESE ARE FOR X=1
         ALPHA(1) = 0.0
         BTA(1) = 1.0
         GAM(1) = 0.0
      END IF
      RETURN
      END
```

Output

```
                         Solution at T =0.10
       1         2         3         4         5         6         7         8
  0.0000    0.2507    0.4771    0.6617    0.7972    0.8857    0.9341    0.9493

                         Solution at T =0.20
       1         2         3         4         5         6         7         8
  0.0000    0.1762    0.3424    0.4893    0.6100    0.6992    0.7538    0.7721

                         Solution at T =0.30
       1         2         3         4         5         6         7         8
  0.0000    0.1356    0.2642    0.3793    0.4751    0.5471    0.5916    0.6067

                         Solution at T =0.40
       1         2         3         4         5         6         7         8
  0.0000    0.1057    0.2060    0.2960    0.3711    0.4276    0.4626    0.4745

                         Solution at T =0.50
       1         2         3         4         5         6         7         8
  0.0000    0.0825    0.1610    0.2313    0.2900    0.3341    0.3616    0.3708

                         Solution at T =0.60
       1         2         3         4         5         6         7         8
  0.0000    0.0645    0.1258    0.1808    0.2267    0.2612    0.2826    0.2899

                         Solution at T =0.70
       1         2         3         4         5         6         7         8
  0.0000    0.0504    0.0983    0.1413    0.1772    0.2041    0.2209    0.2266

                         Solution at T =0.80
       1         2         3         4         5         6         7         8
  0.0000    0.0394    0.0769    0.1105    0.1385    0.1597    0.1728    0.1772

                         Solution at T =0.90
       1         2         3         4         5         6         7         8
  0.0000    0.0309    0.0602    0.0865    0.1084    0.1249    0.1352    0.1387

                         Solution at T =1.00
       1         2         3         4         5         6         7         8
  0.0000    0.0242    0.0471    0.0677    0.0849    0.0979    0.1059    0.1086
```

Example 2

In this example, using MMOLCH, we solve the linear normalized diffusion PDE $u_t = u_{xx}$ but with an optional usage that provides values of the derivatives, u_x, of the initial data. Due to errors in the numerical derivatives computed by spline interpolation, more precise derivative values are required when the initial data is $u(x, 0) = 1 + \cos[(2n-1)\pi x]$, $n > 1$. The boundary conditions are “zero flux” conditions $u_x(0, t) = u_x(1, t) = 0$ for $t > 0$.

```
      USE MMOLCH_INT
      USE CONST_INT
      USE WRRRN_INT
      USE PGOPT_INT
      IMPLICIT    NONE

      INTEGER, PARAMETER  :: NPDES=1, NX=10
      INTEGER             :: I, IDO, J, NSTEP, N, IPAGE
      REAL                :: HINIT, T, TEND, TOL, XBREAK(NX)
      REAL                :: Y(NPDES,2*NX), PI, ARG1
      CHARACTER           :: TITLE*36
```

```
      EXTERNAL    FCNBC, FCNUT
      REAL        FLOAT

      N    = 5
      PI   = CONST('pi')
      DO I=1,NX
         XBREAK(I) = FLOAT(I-1)/FLOAT(NX-1)
         ARG1 = (2.*N-1)*PI
!                                SET FUNCTION VALUES
         Y(1,I)    = 1. + COS(ARG1*XBREAK(I))
!                                SET FIRST DERIVATIVE VALUES
         Y(1,I+NX) = -ARG1*SIN(ARG1*XBREAK(I))
      END DO
!                                SET PARAMETERS FOR MMOLCH
      TOL    = 10.0e-4
      HINIT  = 0.01*TOL
!                                OUTPUT AT STEPS OF 0.001
      TEND   = 0.
      T      = 0.0
      IDO    = 1
      NSTEP  = 10
      DO J=1,NSTEP
         TEND = TEND + 0.001
!                                SOLVE THE PROBLEM
         CALL MMOLCH (IDO, FCNUT, FCNBC, T, TEND, XBREAK, Y, NPDES=NPDES, &
           NX=NX, HINIT=HINIT, TOL=TOL, INPDER=1)
!                                PRINT RESULTS
         IPAGE = 70
         CALL PGOPT(-1, IPAGE)
         WRITE (TITLE,'(A,F5.3)') 'Solution and derivatives at T =', T
         CALL WRRRN (TITLE, Y)
      END DO
!                                LAST CALL, TO RELEASE WORKSPACE
      IDO = 3
      CALL MMOLCH (IDO, FCNUT, FCNBC, T, TEND, XBREAK, Y, NPDES=NPDES, &
        NX=NX, HINIT=HINIT, TOL=TOL, INPDER=1)
      END

      SUBROUTINE FCNUT (NPDES, X, T, U, UX, UXX, UT)

      INTEGER    NPDES
      REAL       X, T, U(*), UX(*), UXX(*), UT(*)
!                                DEFINE THE PDE
      UT(1) = UXX(1)
      RETURN
      END

      SUBROUTINE FCNBC (NPDES, X, T, ALPHA, BTA, GAM)

      INTEGER    NPDES
      REAL       X, T, ALPHA(*), BTA(*), GAM(*)
!                                DEFINE THE BOUNDARY CONDITIONS
      ALPHA(1) = 0.0
      BTA(1) = 1.0
      GAM(1) = 0.0
      RETURN
      END
```

Output

```
                 Solution and derivatives at T =0.001
      1       2       3       4       5       6       7       8       9
  1.482   0.518   1.482   0.518   1.482   0.518   1.482   0.518   1.482
```

```
      10       11       12       13       14       15       16       17       18
   0.518    0.000    0.000    0.000    0.000   -0.000    0.000   -0.000    0.000

      19       20
  -0.000   -0.000

                  Solution and derivatives at T =0.002
       1        2        3        4        5        6        7        8        9
   1.235    0.765    1.235    0.765    1.235    0.765    1.235    0.765    1.235

      10       11       12       13       14       15       16       17       18
   0.765    0.000    0.000    0.000    0.000   -0.000    0.000   -0.000    0.000

      19       20
  -0.000    0.000

                  Solution and derivatives at T =0.003
       1        2        3        4        5        6        7        8        9
   1.114    0.886    1.114    0.886    1.114    0.886    1.114    0.886    1.114

      10       11       12       13       14       15       16       17       18
   0.886    0.000    0.000    0.000    0.000   -0.000    0.000   -0.000    0.000

      19       20
  -0.000   -0.000

                  Solution and derivatives at T =0.004
       1        2        3        4        5        6        7        8        9
   1.055    0.945    1.055    0.945    1.055    0.945    1.055    0.945    1.055

      10       11       12       13       14       15       16       17       18
   0.945    0.000    0.000    0.000    0.000   -0.000   -0.000    0.000    0.000

      19       20
  -0.000   -0.000

                  Solution and derivatives at T =0.005
       1        2        3        4        5        6        7        8        9
   1.027    0.973    1.027    0.973    1.027    0.973    1.027    0.973    1.027

      10       11       12       13       14       15       16       17       18
   0.973    0.000   -0.000    0.000    0.000    0.000   -0.000   -0.000    0.000

      19       20
  -0.000   -0.000

                  Solution and derivatives at T =0.006
       1        2        3        4        5        6        7        8        9
   1.013    0.987    1.013    0.987    1.013    0.987    1.013    0.987    1.013

      10       11       12       13       14       15       16       17       18
   0.987    0.000    0.000    0.000   -0.000    0.000    0.000   -0.000    0.000

      19       20
  -0.000   -0.000

                  Solution and derivatives at T =0.007
       1        2        3        4        5        6        7        8        9
   1.006    0.994    1.006    0.994    1.006    0.994    1.006    0.994    1.006

      10       11       12       13       14       15       16       17       18
   0.994    0.000    0.000    0.000   -0.000    0.000    0.000   -0.000   -0.000

      19       20
  -0.000   -0.000
```

```
                    Solution and derivatives at T =0.008
      1       2       3       4       5       6       7       8       9
  1.003   0.997   1.003   0.997   1.003   0.997   1.003   0.997   1.003

     10      11      12      13      14      15      16      17      18
  0.997   0.000   0.000   0.000  -0.000  -0.000   0.000   0.000  -0.000

     19      20
 -0.000  -0.000

                    Solution and derivatives at T =0.009
      1       2       3       4       5       6       7       8       9
  1.002   0.998   1.002   0.998   1.002   0.998   1.002   0.998   1.002

     10      11      12      13      14      15      16      17      18
  0.998   0.000   0.000   0.000  -0.000  -0.000  -0.000   0.000  -0.000

     19      20
 -0.000   0.000

                    Solution and derivatives at T =0.010
      1       2       3       4       5       6       7       8       9
  1.001   0.999   1.001   0.999   1.001   0.999   1.001   0.999   1.001

     10      11      12      13      14      15      16      17      18
  0.999   0.000   0.000   0.000  -0.000  -0.000  -0.000   0.000  -0.000

     19      20
 -0.000  -0.000
```

Example 3

In this example, we consider the linear normalized hyperbolic PDE, $u_{tt} = u_{xx}$, the “vibrating string” equation. This naturally leads to a system of first order PDEs. Define a new dependent variable $u_t = v$. Then, $v_t = u_{xx}$ is the second equation in the system. We take as initial data $u(x,0) = \sin(\pi x)$ and $u_t(x, 0) = v(x, 0) = 0$. The ends of the string are fixed so $u(0, t) = u(1, t) = v(0, t) = v(1, t) = 0$. The exact solution to this problem is $u(x, t) = \sin(\pi x) \cos(\pi t)$. Residuals are computed at the output values of t for $0 < t \le 2$. Output is obtained at 200 steps in increments of 0.01.

Even though the sample code `MMOLCH` gives satisfactory results for this PDE, users should be aware that for *nonlinear problems*, “shocks” can develop in the solution. The appearance of shocks may cause the code to fail in unpredictable ways. See Courant and Hilbert (1962), pages 488-490, for an introductory discussion of shocks in hyperbolic systems.

```
      USE MMOLCH_INT
      USE UMACH_INT
      USE CONST_INT

      IMPLICIT    NONE

      INTEGER, PARAMETER  :: NPDES=2, NX=10
      INTEGER             :: I, IDO, J, NOUT, NSTEP
      REAL                :: HINIT, T, TEND, TOL, XBREAK(NX)
      REAL                :: Y(NPDES,2*NX), PI, ERROR, ERRU
      CHARACTER           :: TITLE*36

      EXTERNAL    FCNBC, FCNUT
      REAL        FLOAT
```

```
      CALL UMACH (2,NOUT)
!                                  SET BREAKPOINTS AND INITIAL CONDITIONS
      PI    = CONST('pi')
      DO I=1,NX
         XBREAK(I) = FLOAT(I-1)/FLOAT(NX-1)
!                                  SET FUNCTION VALUES
         Y(1,I)     = SIN(PI*XBREAK(I))
         Y(2,I)     = 0.
!                                  SET FIRST DERIVATIVE VALUES
         Y(1,I+NX) = PI*COS(PI*XBREAK(I))
         Y(2,I+NX) = 0.
      END DO
!                                  SET PARAMETERS FOR MMOLCH
      TOL    = 10.0e-4
      HINIT  = 0.01*TOL
!                                  OUTPUT AT STEPS OF 0.01
      TEND   = 0.
      T      = 0.0
      IDO    = 1
      NSTEP  = 200
      DO J=1,NSTEP
         TEND = TEND + 0.01
!                                  SOLVE THE PROBLEM
         CALL MMOLCH (IDO, FCNUT, FCNBC, T, TEND, XBREAK, Y, &
           HINIT=HINIT, TOL=TOL, INPDER=1)
!                                  COMPUTE MAXIMUM ERROR
         ERRU = 0.0
         DO I=1,NX
            ERROR = Y(1,I) - SIN(PI*XBREAK(I))*COS(PI*TEND)
            ERRU = AMAX1(ERRU,ABS(ERROR))
         END DO
      END DO
!                                  PRINT ERROR
         WRITE (NOUT, *) ' Maximum error in u(x,t): ', ERRU
!                                  LAST CALL, TO RELEASE WORKSPACE
      IDO = 3
      CALL MMOLCH (IDO, FCNUT, FCNBC, T, TEND, XBREAK, Y, &
        HINIT=HINIT, TOL=TOL, INPDER=1)
      END

      SUBROUTINE FCNUT (NPDES, X, T, U, UX, UXX, UT)

      INTEGER    NPDES
      REAL       X, T, U(*), UX(*), UXX(*), UT(*)
!                                  DEFINE THE PDEs
      UT(1) = U(2)
      UT(2) = UXX(1)
      RETURN
      END

      SUBROUTINE FCNBC (NPDES, X, T, ALPHA, BTA, GAM)

      INTEGER    NPDES
      REAL       X, T, ALPHA(*), BTA(*), GAM(*)
!                                  DEFINE THE BOUNDARY CONDITIONS
      ALPHA(1) = 1.0
      BTA(1) = 0.0
      GAM(1) = 0.0
      ALPHA(2) = 1.0
      BTA(2) = 0.0
      GAM(2) = 0.0
      RETURN
      END
```

Output

```
Maximum error in u(x,t):  5.49525E-3
```

MOLCH

Deprecated Routine: `MOLCH` is a deprecated routine and has been replaced with `MMOLCH`. To view the deprecated documentation, see `molch.pdf` on the IMSL website. You can also access a local copy in your IMSL documentation directory at pdf\deprecated_routines\math\molch.pdf.

FEYNMAN_KAC

more...

Solves the generalized Feynman-Kac PDE on a rectangular grid using a finite element Galerkin method. Initial and boundary conditions are provided. The solution is represented by a series of C^2 Hermite quintic splines.

Required Arguments

XGRID — Rank-1 array containing the set of breakpoints that define the end points for the Hermite quintic splines. (Input)
Let m = size(XGRID). The points in XGRID must be in strictly increasing order, and $m \geq 2$.

TGRID — Rank-1 array containing the set of time points (in time-remaining units) at which an approximate solution is computed. (Input)
Let n = size(TGRID). The points in TGRID must be strictly positive and in strictly increasing order and $n \geq 1$.

NLBC — The number of left boundary conditions. (Input)
$1 \leq$ NLBC ≤ 3.

NRBC — The number of right boundary conditions. (Input)
$1 \leq$ NRBC ≤ 3.

FKCOEF — User-supplied FUNCTION to evaluate the coefficients σ, σ', μ and κ of the Feynman-Kac PDE. The usage is FKCOEF (X, TX, IFLAG [, …]), where

Function Return Value

FKCOEF — Value of the coefficient function. Which value is computed depends on the input value for IFLAG, see description of IFLAG.

Required Arguments

X — Point in the x-space at which the coefficient is to be evaluated. (Input)

TX — Time point at which the coefficient is to be evaluated. (Input)

IFLAG — Flag related to the coefficient that has to be computed (Input/Output).
On entry, IFLAG indicates which coefficient is to be computed. The following table shows which value has to be returned by FKCOEF for all possible values of IFLAG:

IFLAG	Computed coefficient
1	$\sigma' = \frac{\partial\sigma(x,t)}{\partial x}$
2	σ
3	μ
4	κ

One indicates when a coefficient does not depend on t by setting IFLAG = 0 after the coefficient is defined. If there is time dependence, the value of IFLAG should not be changed. This action will usually yield a more efficient algorithm because some finite element matrices do not have to be reassembled for each t value.

Optional Arguments

FCN_DATA — A derived type, s_fcn_data, which may be used to pass additional integer or floating point information to or from the user-supplied function. For a detailed description of this argument see FCN_DATA below. (Input/Output)

FKCOEF must be declared EXTERNAL in the calling program.

FKINITCOND — User-supplied FUNCTION to evaluate the initial condition function $p(x)$ in the Feynman-Kac PDE. The usage is FKINITCOND (X [, …]), where

Function Return Value

FKINITCOND — Value of the initial condition function $p(x)$.

Required Arguments

X — Point in the x-space at which the initial condition is to be evaluated. (Input)

Optional Arguments

FCN_DATA — A derived type, s_fcn_data, which may be used to pass additional integer or floating point information to or from the user-supplied function. For a detailed description of this argument see FCN_DATA below. (Input/Output)

FKINITCOND must be declared EXTERNAL in the calling program.

FKBC — User-supplied subroutine to evaluate the coefficients for the left and right boundary conditions the Feynman-Kac PDE must satisfy. There are NLBC conditions specified at the left end, x_{min}, and NRBC conditions at the right end, x_{max}. The boundary conditions can be vectors of dimension 1, 2 or 3 and are defined by

$$a(x,t)f + b(x,t)f_x + c(x,t)f_{xx} = d(x,t), \quad x = x_{\min} \text{ or } x = x_{\max}$$

The usage is FKBC (TX, IFLAG, BCCOEFS [, …]) where

Required Arguments

TX — Time point at which the coefficients are to be evaluated. (Input)

IFLAG — Flag related to the boundary conditions that have to be computed (Input/Output).
On input, IFLAG indicates whether the coefficients for the left or right boundary conditions have to be computed:

IFLAG	Computed boundary conditions
1	Left end, x = x_{min}
2	Right end, x = x_{max}

If there is no time dependence for one of the boundaries then set IFLAG = 0 after the array BCCOEFS is defined for either end point. This can avoid unneeded continued computation of the finite element matrices.

BCCOEFS — Array of size 3 × 4 containing the coefficients of the left or right boundary conditions in its first NLBC or NRBC rows, respectively. (Output)
The coefficients for $x_{\min}$ are stored row-wise according to the following matrix-scheme:

$$\begin{pmatrix} a_1(x_{\min},t), & b_1(x_{\min},t), & c_1(x_{\min},t), & d_1(x_{\min},t) \\ a_{NLBC}(x_{\min},t), & b_{\mathrm{NLBC}}(x_{\min},t), & c_{NLBC}(x_{\min},t), & d_{NLBC}(x_{\min},t) \end{pmatrix}$$

The coefficients for x_{max} are stored similarly.

Optional Arguments

FCN_DATA — A derived type, s_fcn_data, which may be used to pass additional integer or floating point information to or from the user-supplied subroutine. For a detailed description of this argument see FCN_DATA below. (Input/Output)

FKBC must be declared EXTERNAL in the calling program.

Y — Array of size (3**m*) by (*n*+1) containing the coefficients of the Hermite representation of the approximate solution for the Feynman-Kac PDE at time points (in time-remaining units)
0, TGRID(1), …, TGRID(*n*). (Output)
For t = TGRID(j), j = 1, …, *n*, the coefficients are stored in columns 1, …, *n* of array Y and the approximate solution is given by

$$f(x,t) = \sum_{\mathtt{i}=1}^{3*m} \mathtt{Y}(\mathtt{i},\mathtt{j})\beta_{\mathtt{i}}(x)$$

The coefficients of the representation for the initial data are given in column 0 of array `Y` and are defined by

$$p(x) = \sum_{\mathtt{i}=1}^{3*m} \mathtt{Y}(\mathtt{i},0)\beta_{\mathtt{i}}(x)$$

The starting coefficients `Y(i,0)`, `i` = 1, …, *m* are estimated using least-squares.

After the integrations, use `Y(:,0)` and `Y(:,j)` as input argument `COEFFS` to function `HQSVAL` to obtain an array of values for *f*(*x*, *t*) or its partials f_x, f_{xx}, f_{xxx} at time points `t` = 0 and `t` = `TGRID(j)`, `j`=1, …, *n*, respectively.

The expressions for the basis functions $\beta_i(x)$ are represented piece-wise and can be found in Hanson, R. (2008) "*Integrating Feynman-Kac Equations Using Hermite Quintic Finite Elements*".

YPRIME — Array of size (3*m) by (*n* + 1) containing the first derivatives of the coefficients of the Hermite representation of the approximate solution for the Feynman-Kac PDE at time points (in time-remaining units) 0, `TGRID(1)`, …, `TGRID(n)`. (Output)
For *t* = 0 and *t* = `TGRID(j)`, `j`=1, …, *n* , the derivatives of the coefficients are stored in column 0 and columns 1 to *n* of array `YPRIME`, respectively. The columns in `YPRIME` represent

$$f_t(x,\bar{t}) = \sum_{i=1}^{3*m} \mathtt{YPRIME}(i,j)\beta_i(x) \text{ for } \bar{t} = \mathtt{TGRID(j)},\ j = 1,\ \ldots,\ n,$$

and

$$f_t(x,\bar{t}) = \sum_{\mathtt{i}=1}^{3*m} \mathtt{YPRIME}(\mathtt{i},0)\beta_{\mathtt{i}}(x) \text{ for } \bar{t} = 0.$$

After the integrations, use `YPRIME(:,j)` as input argument `COEFFS` to function `HQSVAL` to obtain an array of values for the partials $f_t, f_{tx}, f_{txx}, f_{txxx}$ at time points *t* = `TGRID(j)`, *j* = 1, …, *n*, and `YPRIME(:,0)` for the partials at *t* = 0.

Optional Arguments

FKINIT — User-supplied `subroutine` that allows for adjustment of initial data or as an opportunity for output during the integration steps.

The usage is `CALL FKINIT` (`XGRID`, `TGRID`, `TX`, `YPRIME`, `Y`, `ATOL`, `RTOL`, `[, …]`) where

Required Arguments

`XGRID` — Array of size *m* containing the set of breakpoints that define the end points for the Hermite quintic splines. (Input)

`TGRID` — Array of size *n* containing the set of time points (in time-remaining units) at which an approximate solution is computed. (Input)

`TX` — Time point for the evaluation. (Input)
Possible values are 0 (the initial or "terminal" time point) and all values in array `TGRID`.

`YPRIME` — Array of length `3*`*m* containing the derivatives of the Hermite quintic spline coefficients at time point `TX`. (Input)

`Y` — Array of length `3*` *m* containing the Hermite quintic spline coefficients at time point `TX`. (Input/Output)
For the initial time point `TX` = 0 this array can be used to reset the Hermite quintic spline coefficients to user defined values. For all other values of `TX` array `Y` is an input array.

`ATOL` — Array of length `3*`*m* containing absolute error tolerances used in the integration routine that determines the Hermite quintic spline coefficients and its derivatives. (Input/Output)

`RTOL` — Array of length `3*`*m* containing relative error tolerances used in the integration routine that determines the Hermite quintic spline coefficients and its derivatives. (Input/Output)

Optional Arguments

`FCN_DATA` — A derived type, `s_fcn_data`, which may be used to pass additional integer or floating point information to or from the user-supplied function. For a detailed description of this argument see `FCN_DATA` below. (Input/Output)

`FKINIT` must be declared `EXTERNAL` in the calling program.

FKFORCE — User-supplied `subroutine` that computes local contributions

$$\varphi_t^i := \int_{x_i}^{x_{i+1}} \varphi\left(f,x,t\right)\hat{\beta}\left(x\right)dx \quad \text{and} \quad \frac{\partial \varphi_t^i}{\partial y} := \int_{x_i}^{x_{i+1}} \frac{\partial \varphi(f,x,t)}{\partial f}\hat{\beta}\left(x\right)^T\hat{\beta}\left(x\right)dx$$

The usage is `CALL FKFORCE` (`I`, `T`, `WIDTH`, `Y`, `XLOCAL`, `QW`, `U`, `PHI`, `DPHI` `[, …]`) where

Required Arguments

`I` — Index related to the integration interval (`XGRID(I)`, `XGRID(I+1)`). (Input)

`T` — Time point at which the local contributions are computed. (Input)

WIDTH — Width of the integration interval I, WIDTH=XGRID(I+1)-XGRID(I). (Input)

Y — Array of length 3*m containing the coefficients of the Hermite quintic spline representing the solution of the Feynman-Kac PDE at time point T. (Input)
For each

$$x \in \left[x_i, x_{i+1}\right],\ h_i = x_{i+1} - x_i,\ z = \left(x - x_i\right) / h_i,\quad i = 1,\ \dots,\ m-1$$

the approximate solution is locally defined by

$$f(x,t) = f_i b_0(z) + f_{i+1} b_0(1-z) + h_i f_i' b_1(z)$$
$$-h_i f'_{i+1} b_1(1-z) + h_i^2 f''_i b_2(z) + h_i^2 f''_{i+1} b_2(1-z).$$

Here, the functions $b_0(z), b_1(z), b_2(z)$ are basis polynomials of order 5 and

$$f_i := f\left(x_i, t\right), f'_i := f_x\left(x_i, t\right), f''_i := f_{xx}\left(x_i, t\right)$$

The values

$$y_{3i-2} = f_i,\ y_{3i-1} = f'_i,\ y_{3i} = f''_i,\quad i = 1,\ \dots,\ m$$

are stored as successive triplets in array Y.

XLOCAL — Array containing the Gauss-Legendre points translated and normalized to the interval [XGRID(I),XGRID(I+1)]. (Input)
The size of the array is equal to the degree of the Gauss-Legendre polynomials used for constructing the finite element matrices.

QW — Array containing the Gauss-Legendre weights. (Input)
The size of the array is equal to the degree of the Gauss-Legendre polynomials used for constructing the finite element matrices.

U — Array of size size (XLOCAL) × 12 containing the basis function values that define $\hat{\beta}(x)$ at the Gauss-Legendre points XLOCAL. (Input)
Let

$$x \in \left[x_I, x_{I+1}\right], h_I := x_{I+1} - x_I, z(x) := \left(x - x_I\right) / h_I$$

Using the local approximation in the I-th interval, defined by

$$f\left(x,t\right) = \sum_{k=-2}^{3} y_{3I+k} \beta_{3I+k}\left(x\right)$$

and setting

$$u_{j,k} := \texttt{U}(\texttt{j,k}), \quad x_j := \texttt{XLOCAL(j)}, \text{ and } z(x_j) := z_j,$$

vector $\hat{\beta}(x_j) = \left(\hat{\beta}_1(x_j), \ldots, \hat{\beta}_6(x_j)\right)$ is defined as

$$\begin{aligned}\hat{\beta}(x_j) &:= \left(\beta_{3I-2}(x_j), \ldots, \beta_{3I+3}(x_j)\right)^T \\ &:= \left(b_0(z_j), h_I b_1(z_j), h_I^2 b_2(z_j), b_0(1-z_j), -h_I b_1(1-z_j), h_I^2 b_2(1-z_j)\right)^T \\ &:= \left(u_{j,1}, u_{j,2}, u_{j,3}, u_{j,7}, u_{j,8}, u_{j,9}\right)^T.\end{aligned}$$

`PHI` — Array of size 6 containing a Gauss-Legendre approximation for the local contribution $\varphi_t^I := \int_{XGRID(I)}^{XGRID(I+1)} \phi(f,x,t)\hat{\beta}(x)\,dx$, where t = `T` and $\hat{\beta}(x) := \left(\beta_{3I-2}(x), \ldots, \beta_{3I+3}(x)\right)^T$. (Output)

Setting $NDEG$`:=SIZE(XLOCAL)` and x_j = `XLOCAL(j)`, array `PHI` contains elements

$$\texttt{PHI(i)} = \texttt{WIDTH} * \sum_{j=1}^{\texttt{NDEG}} \texttt{QW}(j)\hat{\beta}_i(x_j)\varphi(f,x_j,t)$$

for i = 1, …, 6.

`DPHI` — Array of size 6 × 6, a Gauss-Legendre approximation for the Jacobian of the local contribution φ_t^I at time point t = `T`, (Output)

$$\frac{\partial \varphi_t^I}{\partial y} := \int_{\texttt{XGRID(I)}}^{\texttt{XGRID(I+1)}} \frac{\partial \phi(f,x,t)}{\partial f}\hat{\beta}(x)\hat{\beta}^T(x)\,dx$$

The approximation to this symmetric matrix is stored row-wise, i.e.

$$\texttt{DPHI(i,j)} = \texttt{WIDTH} * \sum_{k=1}^{\texttt{NDEG}} \texttt{QW}(\texttt{k})\hat{\beta}_i(x_k)\hat{\beta}_j(x_k)\frac{\partial \phi}{\partial f}\Big|_{x=\texttt{XLOCAL}(\texttt{k}),\ t=T}$$

for i, j = 1, …, 6.

Optional Arguments

`FCN_DATA` — A derived type, `s_fcn_data`, which may be used to pass additional integer or floating point information to or from the user-supplied subroutine. For a detailed description of this argument see `FCN_DATA` below. (Input/Output)

`FKFORCE` must be declared `EXTERNAL` in the calling program.

If subroutine `FKFORCE` is not used as an optional argument then it is assumed that the forcing term ϕ in the Feynman-Kac equation is identically zero.

ATOL — Array of non-negative values containing absolute error tolerances used in the computation of each column of solution array `Y` via integration routine `DASPH`. (Input)

The size of array `ATOL` can be 1 or 3 × m. In the first case, `ATOL(1:1)` is applied to all solution

components, in the latter each component of ATOL is assigned to the corresponding solution component allowing for individual control of the error tolerances. At least one entry in arrays ATOL or RTOL must be greater than 0.
Default: ATOL(1:1) = 1.0e-3 for single and 1.0d-5 for double precision.

RTOL — Array of non-negative values containing relative error tolerances used in the computation of each column of solution array Y via integration routine DASPH. (Input)
The size of array RTOL can be 1 or $3 \times m$. In the first case, RTOL(1:1) is applied to all solution components, in the latter each component of RTOL is assigned to the corresponding solution component allowing for individual control of the error tolerances. At least one entry in arrays ATOL or RTOL must be greater than 0.
Default: RTOL(1:1) = 1.0e-3 for single and 1.0d-5 for double precision.

NDEG — Degree of the Gauss-Legendre formulas used for constructing the finite element matrices. (Input)
NDEG ≥ 6.
Default: NDEG = 6.

RINITSTEPSIZE — Starting step size for the integration. (Input)
RINITSTEPSIZE must be strictly negative since the integration is internally done from T = 0 to T = TGRID(n) in a negative direction.
Default: Program defined initial stepsize.

MAXBDFORDER — Maximum order of the backward differentiation formulas (BDF) used in the integrator DASPH. (Input)
1 ≤ MAXBDFORDER ≤ 5.
Default: MAXBDFORDER = 5.

RMAXSTEPSIZE — Maximum step size the integrator may take. (Input)
RMAXSTEPSIZE must be strictly positive.
Default: RMAXSTEPSIZE = AMACH(2), the largest possible machine number.

MAXIT — Maximum number of internal integration steps between two consecutive time points in TGRID. (Input)
MAXIT must be strictly positive.
Default: MAXIT = 500000.

IMETHSTEPCTRL — Indicates which step control algorithm is used in the integration. (Input)
If IMETHSTEPCTRL = 0, then the step control method of Söderlind is used. If IMETHSTEPCTRL = 1, then the method used by the original Petzold code SASSL is used.

IMETHSTEPCTRL	Method used
0	Method of Söderlind..
1	Method from Petzold code SASSL.

Default: IMETHSTEPCTRL = 0.

TBARRIER — Time barrier past which the integration routine DASPH will not go during integration. (Input)

TBARRIER ≥ TGRID(n).

Default: TBARRIER = TGRID(n).

ISTATE — Array of size 5 whose entries flag the state of computation for the matrices and vectors required in the integration. (Output)

For each entry, a zero indicates that no computation has been done or that there is a time dependence. A one indicates that the entry has been computed and there is no time dependence.The ISTATE entries are as follows:

I	ISTATE(I)
1	State of computation of Mass matrix, M.
2	State of computation of Stiffness matrix, N.
3	State of computation of Bending matrix, R.
4	State of computation of Weighted mass matrix, K.
5	State of computation of initial data.

NVAL — Array of size 3 summarizing the number of evaluations required during the integration. (Output)

I	NVAL(I)
1	Number of residual function evaluationsof the DAE used in the model.
2	Number of factorizations of the differential matrix associated with solving the DAE.
3	Number of linear system solve steps using the differential matrix.

ITDEPEND — Logical array of size 7 indicating time dependence of the coefficients, boundary conditions and forcing term ϕ in the Feynman-Kac equation. (Output)

If `ITDEPEND(I)=.FALSE.` then argument `I` is not time dependent. If `ITDEPEND(I) =.TRUE.` then argument `I` is time dependent.

`I`	**ITDEPEND(`I`)**
1	Time dependence of σ'.
2	Time dependence of σ.
3	Time dependence of μ.
4	Time dependence of κ.
5	Time dependence of left boundary conditions.
6	Time dependence of right boundary conditions.
7	Time dependence of ϕ.

FCN_DATA — A derived type, `s_fcn_data`, which may be used to pass additional information to/from the user-supplied function. (Input/Output)

The derived type, `s_fcn_data`, is defined as:

```
type s_fcn_data
   real(kind(1e0)), pointer, dimension(:) :: rdata
   integer, pointer, dimension(:) :: idata
end type
```

in module `mp_types`. The double precision counterpart to `s_fcn_data` is named `d_fcn_data`. The user must include a `use mp_types` statement in the calling program to define this derived type.

Note that if user-supplied data are required in one of the user-defined functions or subroutines available for routine `FEYNMAN_KAC` then these data must be defined via `FCN_DATA`.

FORTRAN 90 Interface

Generic: `CALL FEYNMAN_KAC (XGRID, TGRID, NLBC, NRBC, FKCOEF, FKINITCOND, FKBC, Y, YPRIME [, …])`

Specific: The specific interface names are `S_FEYNMAN_KAC` and `D_FEYNMAN_KAC`.

Description

The generalized Feynman-Kac differential equation has the form

$$f_t + \mu(x,t) f_x + \frac{\sigma^2(x,t)}{2} f_{xx} - \kappa(x,t) f = \phi(f,x,t)$$

where the initial data satisfies

$$f(x,T) = p(x)$$

The derivatives are $f_t = \frac{\partial f}{\partial t}, f_x = \frac{\partial f}{\partial x}$ etc.

`FEYNMAN_KAC` uses a finite element Galerkin method over the rectangle

$$[x_{\min}, x_{\max}] \times [\overline{T}, T]$$

in (x,t) to compute the approximate solution. The interval $[x_{\min}, x_{\max}]$ is decomposed with a grid

$$(x_{\min} =)x_1 < x_2 < \ \dots \ < x_m(= x_{\max})$$

On each subinterval the solution is represented by

$$\begin{aligned} f(x,t) &= f_i b_0(z) + f_{i+1} b_0(1-z) + h_i f_i' b_1(z) \\ &\quad - h_i f'_{i+1} b_1(1-z) + h_i^2 f''_i b_2(z) + h_i^2 f''_{i+1} b_2(1-z). \end{aligned}$$

The values $f_i, f_i', f_i'', f_{i+1}, f'_{i+1}, f''_{i+1}$ are time-dependent coefficients associated with each interval. The basis functions b_0, b_1, b_2 are given for $x \in [x_i, x_{i+1}], h_i := x_{i+1} - x_i, z(x) := (x - x_i)/h_i \in [0,1]$,

by

$$\begin{aligned} b_0(z) &= -6z^5 + 15z^4 - 10z^3 + 1 = (1-z)^3(6z^2 + 3z + 1) \\ b_1(z) &= -3z^5 + 8z^4 - 6z^3 + z = (1-z)^3 z(3z+1) \\ b_2(z) &= \tfrac{1}{2}(-z^5 + 3z^4 - 3z^3 + z^2) = \tfrac{1}{2}(1-z)^3 z^2 \end{aligned}$$

The Galerkin principle is then applied. Using the provided initial and boundary conditions leads to an index 1 differential-algebraic equation (DAE) for the time-dependent coefficients

$$y_{3i-2} := f_i,\ y_{3i-1} := f_i',\ y_{3i} := f_i'', \quad i = 1, \ \dots, m$$

This system is integrated using the variable order, variable step algorithm `DASPH`. Solution values and their time derivatives are returned at a grid preceding time *T*, expressed in units of time remaining.

More mathematical details are found in Hanson, R. (2008) "*Integrating Feynman-Kac Equations Using Hermite Quintic Finite Elements*".

Examples

Example 1 – A Diffusion Model For Call Options

In Beckers (1980) there is a model for a Stochastic Differential Equation of option pricing. The idea is a "constant elasticity of variance diffusion (or CEV) class"

$$dS = \mu S dt + \sigma S^{\alpha/2} dW, \quad 0 \le \alpha < 2$$

The Black-Scholes model is the limiting case $\alpha \to 2$. A numerical solution of this diffusion model yields the price of a call option. Various values of the strike price *K*, time values σ, and power coefficient α are used to evaluate the option price at values of the underlying price. The sets of parameters in the computation are:

1. power α = {2.0,1.0,0.0}
2. strike price K = {15.0,20.0,25.0}
3. volatility σ = {0.2,0.3,0.4}
4. times until expiration = {1/12,4/12,7/12}
5. underlying prices = {19.0,20.0,21.0}
6. interest rate r = 0.05
7. $x_{min} = 0$, $x_{max} = 60$
8. $nx = 121$, $n = 3 \times nx = 363$

With this model the Feynman-Kac differential equation is defined by identifying:

$$x: \quad S$$

$$\sigma(x,t): \quad \sigma x^{\alpha/2}; \quad \frac{\partial\sigma}{\partial x} = \frac{a\sigma}{2}x^{\alpha/2-1}$$

$$\mu(x,t): \quad rx$$

$$\kappa(x,t): \quad r$$

$$\phi(f,x,t) \equiv 0$$

The payoff function is the “vanilla option”, $p(x) = \max(x-K,0)$.

(Example feynman_kac_ex1.f90)

```
! Compute Constant Elasticity of Variance Model for Vanilla Call
      use feynman_kac_int
      use hqsval_int
      use mp_types
      use umach_int

      implicit none

! The set of strike prices
      real(kind(1e0)) :: ks(3)=(/15.0e0,20.0e0,25.0e0/)
! The set of sigma values
      real(kind(1e0)) :: sigma(3) = (/0.2e0, 0.3e0, 0.4e0/)
! The set of model diffusion powers
      real(kind(1e0)) :: alpha(3) = (/2.0e0,1.0e0,0.0e0/)
! Time values for the options
      integer, parameter :: nt = 3
      real(kind(1e0)) :: time(nt)=(/1.e0/12., 4.e0/12., 7.e0/12./)
! Values of the underlying where evaluation are made
      integer, parameter :: nv = 3, nlbc = 3, nrbc = 3
      real(kind(1e0)) :: xs(nv) = (/19.0e0,20.0e0,21.0e0/)
! Value of the interest rate and continuous dividend
      real(kind(1e0)) :: r = 0.05e0, dividend = 0.0e0
! Values of the min and max underlying values modeled
      real(kind(1e0)) :: x_min = 0.0e0, x_max = 60.0e0

! Define parameters for the integration step.
      integer, parameter :: nx = 121, nint = nx-1, n = 3*nx
      real(kind(1e0)) :: xgrid(nx), y(n,0:nt), yprime(n,0:nt),&
                         dx, f(nv,nt)
      type(s_fcn_data) fcn_data
      integer :: nout
      real(kind(1e0)), external :: fkcoef, fkinitcond
      external fkbc

      integer :: i,i1,i2,i3,j
! Allocate space inside the derived type for holding
! data values. These are for the evaluation routines.
      allocate(fcn_data % rdata (6))
! Define an equally-spaced grid of points for the underlying price
      dx = (x_max-x_min)/real(nint)
      xgrid(1) = x_min
      xgrid(nx) = x_max
      do i = 2,nx-1
        xgrid(i) = xgrid(i-1) + dx
      end do
```

```
      call umach(2, nout)
      write(nout,'(T05,A)') "Constant Elasticity of Variance Model "//&
                            "for Vanilla Call"
      write(nout,'(T10,"Interest Rate ", F7.3, T38,"Continuous '//&
                   'Dividend ", F7.3  )') r, dividend
      write(nout,'(T10,"Minimum and Maximum Prices of Underlying ",'//&
                   '2F7.2)') x_min, x_max
      write(nout,'(T10,"Number of equally spaced spline knots ",I4,'//&
                   '/T10,"Number of unknowns ",I4)')&
                   nx-1,n
      write(nout,'(/T10,"Time in Years Prior to Expiration ",2X,'//&
                   '3F7.4)') time
      write(nout,'(T10,"Option valued at Underlying Prices  ",'//&
                   '3F7.2)') xs

      do i1 = 1,3        ! Loop over power
        do i2=1,3      ! Loop over volatility
          do i3=1,3  ! Loop over strike price
! Pass data through into evaluation routines.
            fcn_data % rdata =&
               (/ks(i3),x_max,sigma(i2),alpha(i1),r,dividend/)
            call feynman_kac (xgrid, time, nlbc, nrbc, fkcoef,&
                              fkinitcond, fkbc, y, yprime,&
                              FCN_DATA = fcn_data)
! Evaluate solution at vector of points XS(:), at each time value
! prior to expiration.
            do i=1,nt
              f(:,i) = hqsval (xs, xgrid, y(:,i))
            end do
            write(nout,'(/T05,"Strike=",F5.2," Sigma=", F5.2,'//&
              '" Alpha=", F5.2,/(T25," Call Option Values ",'//&
              'X,3F7.4))') ks(I3),sigma(I2),&
              alpha(i1),(f(i,:),i=1,nv)
          end do !i3 - Strike price loop
        end do !i2 - Sigma loop
      end do !i1 - Alpha loop
      end

! These functions and routines define the coefficients, payoff
! and boundary conditions.
      function fkcoef (X, TX, iflag, fcn_data)
        use mp_types
        implicit none
        real(kind(1e0)), intent(in) :: X, TX
        integer, intent(inout) :: iflag
         type(s_fcn_data), optional :: fcn_data
         real(kind(1e0)) :: fkcoef
         real(kind(1e0)) :: sigma, interest_rate, alpha, dividend,&
                            zero = 0.0e0, half = 0.5e0

        sigma = fcn_data % rdata(3)
        alpha = fcn_data % rdata(4)
        interest_rate = fcn_data % rdata(5)
        dividend = fcn_data % rdata(6)
        select case (iflag)
          case (1)
! The coefficient derivative d(sigma)/dx
            fkcoef = half*alpha*sigma*x**(alpha*half-1.0e0)
! The coefficient sigma(x)
          case (2)
            fkcoef = sigma*x**(alpha*half)
          case (3)
! The coefficient mu(x)
            fkcoef = (interest_rate - dividend) * x
          case (4)
```

```
 ! The coefficient kappa(x)
             fkcoef = interest_rate
           end select
 ! Note that there is no time dependence
         iflag = 0
         return
       end function fkcoef

       function fkinitcond(x, fcn_data)
         use mp_types
         implicit none
         real(kind(1e0)), intent(in) :: x
         type (s_fcn_data), optional :: fcn_data
         real(kind(1e0)) :: fkinitcond
         real(kind(1e0)) :: zero = 0.0e0
         real(kind(1e0)) :: strike_price

         strike_price = fcn_data % rdata(1)
 ! The payoff function
         fkinitcond = max(x - strike_price, zero)
         return
       end function fkinitcond

       subroutine fkbc (tx, iflag, bccoefs, fcn_data)
         use mp_types
         implicit none
         real(kind(1e0)), intent(in) :: tx
         integer, intent(inout) :: iflag
         real(kind(1e0)), dimension(:,:), intent(out) :: bccoefs
         type (s_fcn_data), optional :: fcn_data
         real(kind(1e0)) :: x_max, df, interest_rate, strike_price

         strike_price = fcn_data % rdata(1)
         x_max = fcn_data % rdata(2)
         interest_rate = fcn_data % rdata(5)
         select case (iflag)
           case (1)
             bccoefs(1,1:4) = (/1.0e0, 0.0e0, 0.0e0, 0.0e0/)
             bccoefs(2,1:4) = (/0.0e0, 1.0e0, 0.0e0, 0.0e0/)
             bccoefs(3,1:4) = (/0.0e0, 0.0e0, 1.0e0, 0.0e0/)
 ! Note no time dependence at left end
             iflag = 0
           case (2)
             df = exp(interest_rate * tx)
             bccoefs(1,1:4) = (/1.0e0, 0.0e0, 0.0e0,&
                                x_max - df*strike_price/)
             bccoefs(2,1:4) = (/0.0e0, 1.0e0, 0.0e0, 1.0e0/)
             bccoefs(3,1:4) = (/0.0e0, 0.0e0, 1.0e0, 0.0e0/)
         end select
       end subroutine fkbc
```

Output

```
      Constant Elasticity of Variance Model for Vanilla Call
           Interest Rate    0.050        Continuous Dividend    0.000
           Minimum and Maximum Prices of Underlying    0.00  60.00
           Number of equally spaced spline knots  120
           Number of unknowns  363

           Time in Years Prior to Expiration    0.0833 0.3333 0.5833
           Option valued at Underlying Prices    19.00  20.00  21.00

      Strike=15.00 Sigma= 0.20 Alpha= 2.00
                           Call Option Values   4.0624 4.2575 4.4730
                           Call Option Values   5.0624 5.2506 5.4490
                           Call Option Values   6.0624 6.2486 6.4385
```

```
Strike=20.00 Sigma= 0.20 Alpha= 2.00
                      Call Option Values   0.1310 0.5955 0.9699
                      Call Option Values   0.5018 1.0887 1.5101
                      Call Option Values   1.1977 1.7483 2.1752

Strike=25.00 Sigma= 0.20 Alpha= 2.00
                      Call Option Values   0.0000 0.0112 0.0745
                      Call Option Values   0.0000 0.0372 0.1621
                      Call Option Values   0.0007 0.1027 0.3141

Strike=15.00 Sigma= 0.30 Alpha= 2.00
                      Call Option Values   4.0637 4.3398 4.6622
                      Call Option Values   5.0626 5.2944 5.5786
                      Call Option Values   6.0624 6.2708 6.5240

Strike=20.00 Sigma= 0.30 Alpha= 2.00
                      Call Option Values   0.3109 1.0276 1.5494
                      Call Option Values   0.7326 1.5424 2.1017
                      Call Option Values   1.3765 2.1690 2.7379

Strike=25.00 Sigma= 0.30 Alpha= 2.00
                      Call Option Values   0.0006 0.1112 0.3543
                      Call Option Values   0.0038 0.2169 0.5548
                      Call Option Values   0.0184 0.3857 0.8222

Strike=15.00 Sigma= 0.40 Alpha= 2.00
                      Call Option Values   4.0755 4.5138 4.9675
                      Call Option Values   5.0662 5.4201 5.8326
                      Call Option Values   6.0634 6.3579 6.7301

Strike=20.00 Sigma= 0.40 Alpha= 2.00
                      Call Option Values   0.5115 1.4640 2.1273
                      Call Option Values   0.9621 1.9951 2.6929
                      Call Option Values   1.5814 2.6105 3.3216

Strike=25.00 Sigma= 0.40 Alpha= 2.00
                      Call Option Values   0.0083 0.3286 0.7790
                      Call Option Values   0.0285 0.5167 1.0657
                      Call Option Values   0.0813 0.7687 1.4103

Strike=15.00 Sigma= 0.20 Alpha= 1.00
                      Call Option Values   4.0624 4.2479 4.4311
                      Call Option Values   5.0624 5.2479 5.4311
                      Call Option Values   6.0624 6.2479 6.4311

Strike=20.00 Sigma= 0.20 Alpha= 1.00
                      Call Option Values   0.0000 0.0218 0.1045
                      Call Option Values   0.1498 0.4109 0.6485
                      Call Option Values   1.0832 1.3314 1.5773

Strike=25.00 Sigma= 0.20 Alpha= 1.00
                      Call Option Values   0.0000 0.0000 0.0000
                      Call Option Values   0.0000 0.0000 0.0000
                      Call Option Values   0.0000 0.0000 0.0000

Strike=15.00 Sigma= 0.30 Alpha= 1.00
                      Call Option Values   4.0624 4.2477 4.4309
                      Call Option Values   5.0624 5.2477 5.4309
                      Call Option Values   6.0624 6.2477 6.4309

Strike=20.00 Sigma= 0.30 Alpha= 1.00
                      Call Option Values   0.0011 0.0781 0.2201
                      Call Option Values   0.1994 0.5000 0.7543
                      Call Option Values   1.0835 1.3443 1.6023
```

```
    Strike=25.00 Sigma= 0.30 Alpha= 1.00
                         Call Option Values   0.0000 0.0000 0.0000
                         Call Option Values   0.0000 0.0000 0.0000
                         Call Option Values   0.0000 0.0000 0.0005

    Strike=15.00 Sigma= 0.40 Alpha= 1.00
                         Call Option Values   4.0624 4.2479 4.4312
                         Call Option Values   5.0624 5.2479 5.4312
                         Call Option Values   6.0624 6.2479 6.4312

    Strike=20.00 Sigma= 0.40 Alpha= 1.00
                         Call Option Values   0.0076 0.1563 0.3452
                         Call Option Values   0.2495 0.5907 0.8706
                         Call Option Values   1.0868 1.3779 1.6571

    Strike=25.00 Sigma= 0.40 Alpha= 1.00
                         Call Option Values   0.0000 0.0000 0.0001
                         Call Option Values   0.0000 0.0000 0.0008
                         Call Option Values   0.0000 0.0003 0.0063

    Strike=15.00 Sigma= 0.20 Alpha= 0.00
                         Call Option Values   4.0626 4.2479 4.4311
                         Call Option Values   5.0623 5.2480 5.4311
                         Call Option Values   6.0624 6.2480 6.4312

    Strike=20.00 Sigma= 0.20 Alpha= 0.00
                         Call Option Values   0.0001 0.0001 0.0002
                         Call Option Values   0.0816 0.3316 0.5748
                         Call Option Values   1.0818 1.3308 1.5748

    Strike=25.00 Sigma= 0.20 Alpha= 0.00
                         Call Option Values   0.0000 0.0000 0.0000
                         Call Option Values   0.0000 0.0000 0.0000
                         Call Option Values   0.0000 0.0000 0.0000

    Strike=15.00 Sigma= 0.30 Alpha= 0.00
                         Call Option Values   4.0625 4.2479 4.4312
                         Call Option Values   5.0623 5.2479 5.4312
                         Call Option Values   6.0624 6.2479 6.4312

    Strike=20.00 Sigma= 0.30 Alpha= 0.00
                         Call Option Values   0.0000 0.0000 0.0029
                         Call Option Values   0.0894 0.3326 0.5753
                         Call Option Values   1.0826 1.3306 1.5749

    Strike=25.00 Sigma= 0.30 Alpha= 0.00
                         Call Option Values   0.0000 0.0000 0.0000
                         Call Option Values   0.0000 0.0000 0.0000
                         Call Option Values   0.0000 0.0000 0.0000

    Strike=15.00 Sigma= 0.40 Alpha= 0.00
                         Call Option Values   4.0624 4.2479 4.4312
                         Call Option Values   5.0623 5.2479 5.4312
                         Call Option Values   6.0624 6.2479 6.4312

    Strike=20.00 Sigma= 0.40 Alpha= 0.00
                         Call Option Values   0.0000 0.0002 0.0113
                         Call Option Values   0.0985 0.3383 0.5781
                         Call Option Values   1.0830 1.3306 1.5749

    Strike=25.00 Sigma= 0.40 Alpha= 0.00
                         Call Option Values   0.0000 0.0000 0.0000
                         Call Option Values   0.0000 0.0000 0.0000
                         Call Option Values   0.0000 0.0000 0.0000
```

Example 2 – American Option vs. European Option On a Vanilla Put

The value of the American Option on a Vanilla Put can be no smaller than its European counterpart. That is due to the American Option providing the opportunity to exercise at any time prior to expiration. This example compares this difference – or premium value of the American Option – at two time values using the Black-Scholes model. The example is based on Wilmott et al. (1996, p. 176), and uses the non-linear forcing or weighting term described in Hanson, R. (2008), "*Integrating Feynman-Kac Equations Using Hermite Quintic Finite Elements*", for evaluating the price of the American Option. A call to the subroutine `fkinit_put` sets the initial conditions. One breakpoint is set exactly at the strike price.

The sets of parameters in the computation are:

1. Strike price K = {10.0}
2. Volatility σ = {0.4}
3. Times until expiration = {1/4,1/2}
4. Interest rate r = 0.1
5. $x_{\min}$ = 0.0, $x_{\max}$ = 30.0
6. nx = 121, $n = 3 \times nx$ = 363

The payoff function is the "vanilla option", $p(x) = \max(K - x, 0)$.

(Example feynman_kac_ex2.f90)

```
! Compute American Option Premium for Vanilla Put
      use feynman_kac_int
      use hqsval_int
      use mp_types
      use umach_int
      implicit none
! The strike price
      real(kind(1e0)) :: ks = 10.0e0
! The sigma value
      real(kind(1e0)) :: sigma = 0.4e0

! Time values for the options
      integer, parameter :: nt = 2
      real(kind(1e0)) :: time(nt)=(/0.25e0, 0.5e0/)
! Values of the underlying where evaluations are made
      integer, parameter :: nv = 9
      integer, parameter :: nlbc = 2, nrbc = 3, ndeg = 6

      integer :: i
      real(kind(1e0)) :: xs(nv) = (/((i-1)*2.0e0,i=1,nv)/)
! Value of the interest rate and continuous dividend
      real(kind(1e0)) :: r = 0.1e0, dividend = 0.0e0
! Values of the min and max underlying values modeled
      real(kind(1e0)) :: x_min = 0.0e0, x_max = 30.0e0
      real(kind(1e0)) :: atol(1), rtol(1)

! Define parameters for the integration step.
```

```
      integer, parameter :: nx = 121, nint = nx-1, n = 3*nx
      real(kind(1e0)) :: xgrid(nx), ye(n,0:nt), yeprime(n,0:nt),&
                         ya(n,0:nt), yaprime(n,0:nt),&
                         dx, fe(nv,nt), fa(nv,nt)
      type(s_fcn_data) fcn_data
      integer :: nout
      real(kind(1e0)), external :: fkcoef_put, fkinitcond_put
      external fkbc_put, fkinit_put, fkforce_put

      call umach(2, nout)
! Allocate space inside the derived type for holding
! data values. These are for the evaluation routines.
      allocate(fcn_data % rdata (6), fcn_data % idata (1))
! Define an equally-spaced grid of points for the underlying price
      dx = (x_max-x_min)/real(nint)
      xgrid(1) = x_min
      xgrid(nx) = x_max
      do i=2,nx-1
        xgrid(i) = xgrid(i-1) + dx
      end do

! Place a breakpoint at the strike price.
      do i = 1,nx
        if (xgrid(i) > ks) then
          xgrid(i-1) = ks
          exit
        end if
      end do
! Request less accuracy than the default values provide.
      atol(1) = 0.5e-2
      rtol(1) = 0.5e-2
      fcn_data % rdata = (/ks,x_max,sigma,r,dividend,atol(1)/)
      fcn_data % idata = (/ndeg/)

! Compute European then American Put Option Values.
      call feynman_kac (xgrid, time, nlbc, nrbc, fkcoef_put,&
                        fkinitcond_put, fkbc_put, ye, yeprime,&
                        FKINIT=fkinit_put, ATOL=atol,RTOL=rtol,&
                        FCN_DATA = fcn_data)
      call feynman_kac (xgrid, time, nlbc, nrbc, fkcoef_put,&
                        fkinitcond_put, fkbc_put, ya, yaprime,&
                        FKINIT=fkinit_put, ATOL=atol, RTOL=rtol,&
                        FKFORCE=fkforce_put, FCN_DATA = fcn_data)

! Evaluate solutions at vector of points XS(:), at each time value
! prior to expiration.
      do i=1,nt
        fe(:,i) = hqsval (xs, xgrid, ye(:,I))
        fa(:,I) = hqsval (xs, xgrid, ya(:,I))
      end do
      write(nout,'(T05,A,/,T05,A)')&
         "American Option Premium for Vanilla Put, 3 and 6 Months "//&
         "Prior to", "Expiry"
      write(nout,'(T08,"Number of equally spaced spline knots ",I4,'//&
               '/T08,"Number of unknowns ",I4)') nx,n
      write(nout,'(T08,"Strike= ",F5.2,", Sigma=", F5.2,", Interest'//&
             ' Rate=",F5.2,/T08,"Underlying", T26,"European",'//&
             'T42,"American",/(T10,5F8.4))') ks,sigma,r,&
             (xs(i), fe(i,1:nt), fa(i,1:nt),i=1,nv)
      end
! These routines define the coefficients, payoff, boundary
! conditions, forcing term and initial conditions for American and
! European Options.
      function fkcoef_put(x, tx, iflag, fcn_data)
        use mp_types
        implicit none
```

```
          integer, intent(inout) :: iflag
          real(kind(1e0)), intent(in) :: x, tx
          type(s_fcn_data), optional :: fcn_data
          real(kind(1e0)) :: fkcoef_put

          real(kind(1e0)) :: sigma, strike_price, interest_rate, &
                             dividend, zero=0.e0
          sigma = fcn_data % rdata(3)
          interest_rate = fcn_data % rdata(4)
          dividend = fcn_data % rdata(5)
          select case (iflag)
            case (1)
! The coefficient derivative d(sigma)/dx
              fkcoef_put = sigma
! The coefficient sigma(x)
            case (2)
              fkcoef_put = sigma*x
            case (3)
! The coefficient mu(x)
              fkcoef_put = (interest_rate - dividend)*x
            case (4)
! The coefficient kappa(x)
              fkcoef_put = interest_rate
          end select
! Note that there is no time dependence
          iflag = 0
          return
        end function fkcoef_put

        function fkinitcond_put(x, fcn_data)
          use mp_types
          implicit none
          real(kind(1e0)), intent(in) :: x
          type (s_fcn_data), optional :: fcn_data
          real(kind(1e0)) :: fkinitcond_put
          real(kind(1e0)) :: zero = 0.0e0
          real(kind(1e0)) :: strike_price

          strike_price = fcn_data % rdata(1)
! The payoff function
          fkinitcond_put = max(strike_price - x, zero)
          return
        end function fkinitcond_put

        subroutine fkbc_put (tx, iflag, bccoefs, fcn_data)
          use mp_types
          implicit none
          real(kind(1e0)), intent(in) :: tx
          integer, intent(inout) :: iflag
          real(kind(1e0)), dimension(:,:), intent(out) :: bccoefs
          type (s_fcn_data), optional :: fcn_data

          select case (iflag)
            case (1)
              bccoefs(1,1:4) = ((/0.0e0, 1.0e0, 0.0e0, -1.0e0/))
              bccoefs(2,1:4) = ((/0.0e0, 0.0e0, 1.0e0,  0.0e0/))
            case (2)
              bccoefs(1,1:4) = ((/1.0e0, 0.0e0, 0.0e0, 0.0e0/))
              bccoefs(2,1:4) = ((/0.0e0, 1.0e0, 0.0e0, 0.0e0/))
              bccoefs(3,1:4) = ((/0.0e0, 0.0e0, 1.0e0, 0.0e0/))
          end select
! Note no time dependence
          iflag = 0
        end subroutine fkbc_put

        subroutine fkforce_put (interval, t, hx, y, xlocal, qw, u,&
```

```
                                phi, dphi, fcn_data)
          use mp_types
          implicit none
          integer, parameter :: local = 6
          integer :: i, j, l, ndeg
          integer, intent(in) :: interval
          real(kind(1e0)), intent(in) :: y(:), t, hx, qw(:),&
                                         xlocal(:), u(:,:)
          real(kind(1e0)), intent(out) :: phi(:), dphi(:,:)
          type (s_fcn_data), optional :: fcn_data

          real(kind(1e0)) :: yl(local), bf(local)
          real(kind(1e0)) :: value, strike_price, interest_rate,&
                             zero=0.0e0, one=1.0e0, rt, mu

          yl = y(3*interval-2:3*interval+3)
          phi = zero

          value = fcn_data % rdata(6)
          strike_price = fcn_data % rdata(1)
          interest_rate = fcn_data % rdata(4)
          ndeg = fcn_data % idata(1)

          mu = 2
  ! This is the local definition of the forcing term
          do j=1,local
            do l=1,ndeg
              bf(1:3) = u(l,1:3)
              bf(4:6) = u(l,7:9)
              rt = dot_product(yl,bf)
              rt = value/(rt + value - (strike_price - xlocal(l)))
              phi(j) = phi(j) + qw(l) * bf(j) * rt**mu
            end do
          end do
          phi = -phi*hx*interest_rate*strike_price

  ! This is the local derivative matrix for the forcing term

          dphi = zero
          do j =1,local
            do i = 1,local
              do l=1,ndeg
                bf(1:3) = u(l,1:3)
                bf(4:6) = u(l,7:9)
                rt = dot_product(yl,bf)
                rt = one/(rt + value - (strike_price - xlocal(l)))
                dphi(i,j) = dphi(i,j) + qw(l) * bf(I) * bf(j) *&
                            rt**(mu+1)
              end do
            end do
          end do
          dphi = mu*dphi*hx*value**mu*interest_rate*strike_price
          return
        end subroutine fkforce_put

        subroutine fkinit_put(xgrid,tgrid,t,yprime,y,atol,rtol,&
                              fcn_data)
          use mp_types
          implicit none
          real(kind(1e0)), intent(in) :: xgrid(:), tgrid(:), t,&
                                         yprime(:)
          real(kind(1e0)), intent(inout) :: y(:), atol(:), rtol(:)
          type (s_fcn_data), optional :: fcn_data
          integer :: i

          if (t == 0.0e0) then
```

```
  ! Set initial data precisely.  The strike price is a breakpoint.
  ! Average the derivative limit values from either side.
            do i=1,size(xgrid)
              if (xgrid(i) < fcn_data % rdata(1)) then
                y(3*i-2) = fcn_data % rdata(1) - xgrid(i)
                y(3*i-1) = -1.0e0
                y(3*i)= 0.0e0
              else if (xgrid(i) ==  fcn_data % rdata(1)) then
                y(3*i-2) = 0.0e0
                y(3*i-1) = -0.5e0
                y(3*i) = 0.0e0
              else
                y(3*i-2) = 0.0e0
                y(3*i-1) = 0.0e0
                y(3*i) = 0.0e0
              end if
            end do
          end if
        end subroutine fkinit_put
```

Output

```
    American Option Premium for Vanilla Put, 3 and 6 Months Prior to
    Expiry
       Number of equally spaced spline knots  121
       Number of unknowns  363
       Strike= 10.00, Sigma= 0.40, Interest Rate= 0.10
       Underlying        European        American
           0.0000  9.7536  9.5137 10.0000 10.0000
           2.0000  7.7536  7.5138  8.0000  8.0000
           4.0000  5.7537  5.5156  6.0000  6.0000
           6.0000  3.7614  3.5680  4.0000  4.0000
           8.0000  1.9064  1.9162  2.0214  2.0909
          10.0000  0.6516  0.8540  0.6767  0.9034
          12.0000  0.1625  0.3365  0.1675  0.3515
          14.0000  0.0369  0.1266  0.0374  0.1322
          16.0000  0.0088  0.0481  0.0086  0.0504
```

Example 3 – European Option With Two Payoff Strategies

This example evaluates the price of a European Option using two payoff strategies: *Cash-or-Nothing* and *Vertical Spread*. In the first case the payoff function is

$$p(x) = \begin{cases} 0, & x \le K \\ B, & x > K \end{cases}$$

The value *B* is regarded as the bet on the asset price, see Wilmott et al. (1995, p. 39-40). The second case has the payoff function

$$p(x) = \max(x - K_1) - \max(x - K_2), \quad K_2 > K_1$$

Both problems use the same boundary conditions. Each case requires a separate integration of the Black-Scholes differential equation, but only the payoff function evaluation differs in each case. The sets of parameters in the computation are:

1. Strike and bet prices K_1={10.0}, K_2 = {15.0}, and B = {2.0}

2. Volatility σ = {0.4}.

3. Times until expiration = {1/4, 1/2}.

4. Interest rate r = 0.1.

5. x_{min} = 0, x_{max} = 30.

6. nx =121, n = 3 × nx = 363.

(Example feynman_kac_ex3.f90)

```
! Compute European Option Premium for a Cash-or-Nothing
! and a Vertical Spread Call.
      use feynman_kac_int
      use hqsval_int
      use mp_types
      use umach_int
      implicit none
! The strike price
      real(kind(1e0)) :: ks1 = 10.0e0
! The spread value
      real(kind(1e0)) :: ks2 = 15.0e0
! The Bet for the Cash-or-Nothing Call
      real(kind(1e0)) :: bet = 2.0e0
! The sigma value
      real(kind(1e0)) :: sigma = 0.4e0

! Time values for the options
      integer, parameter :: nt = 2
      real(kind(1e0)) :: time(nt)=(/0.25e0, 0.5e0/)
! Values of the underlying where evaluation are made
      integer, parameter :: nv = 12, nlbc = 3, nrbc = 3
      integer :: i
      real(kind(1e0)) :: xs(nv) = (/(2+(I-1)*2.0e0,I=1,NV)/)
! Value of the interest rate and continuous dividend -
      real(kind(1e0)) :: r = 0.1e0, dividend = 0.0e0
! Values of the min and max underlying values modeled -
      real(kind(1e0)) :: x_min = 0.0e0, x_max = 30.0e0

! Define parameters for the integration step.
      integer, parameter :: nx = 61, nint = nx-1, n=3*nx
      real(kind(1e0)) :: xgrid(nx), yb(n,0:nt), ybprime(n,0:nt),&
                         yv(n,0:nt), yvprime(n,0:nt),&
                         dx, fb(nv,nt), fv(nv,nt)
      type(s_fcn_data) fcn_data
      integer :: nout
      real(kind(1e0)), external :: fkcoef_call, fkinitcond_call
      external fkbc_call

      call umach(2, nout)
! Allocate space inside the derived type for holding
! data values. These are for the evaluation routines.
      allocate(fcn_data % rdata (7), fcn_data % idata (1))
! Define an equally-spaced grid of points for the underlying price
      dx = (x_max-x_min)/real(nint)
      xgrid(1) = x_min
      xgrid(nx) = x_max
      do i = 2,nx-1
        xgrid(i) = xgrid(i-1) + dx
      end do

      fcn_data % rdata = (/ks1,bet,ks2,x_max,sigma,r,dividend/)
```

```
! Flag the difference in payoff functions -
! 1 for the Bet, 2 for the Vertical Spread
      fcn_data % idata(1) = 1
      call feynman_kac (xgrid, time, nlbc, nrbc, fkcoef_call,&
                        fkinitcond_call, fkbc_call, yb, ybprime,&
                        FCN_DATA = fcn_data)

      fcn_data % idata(1) = 2
      call feynman_kac (Xgrid, time, nlbc, nrbc, fkcoef_call,&
                        fkinitcond_call, fkbc_call, yv, yvprime,&
                        FCN_DATA = fcn_data)

! Evaluate solutions at vector of points XS(:), at each time value
! prior to expiration.
      do i=1,nt
        fb(:,i) = hqsval (xs, xgrid, yb(:,I))
        fv(:,i) = hqsval (xs, xgrid, yv(:,I))
      end do
      write(nout,'(T05,A)') "European Option Value for A Bet",&
                           " and a Vertical Spread, 3 and 6 Months "//&
                           "Prior to Expiry"
      write(nout,'(T08,"Number of equally spaced spline knots "'//&
                     ',I4,/T08,"Number of unknowns ",I4)') NX,N
      write(nout,'(T08,"Strike = ",F5.2,", Sigma =", F5.2,'//&
            '", Interest Rate =",F5.2,'//&
            '/T08,"Bet = ",F5.2,", Spread Value = ", F5.2/'//&
            '/T10,"Underlying", T32,"A Bet", T40,"Vertical Spread",'//&
            '/(T10,5F9.4))') ks1, sigma, r, bet, ks2, &
              (xs(i), fb(i,1:nt), fv(i,1:nt),i=1,nv)
      end

! These routines define the coefficients, payoff, boundary
! conditions and forcing term for American and European Options.
      function fkcoef_call (x, tx, iflag, fcn_data) result(value)
      use mp_types
      implicit none

      integer, intent(inout) :: iflag
      real(kind(1e0)), intent(in) :: x, tx
      type(s_fcn_data), optional :: fcn_data
      real(kind(1e0)) :: value

      real(kind(1e0)) :: sigma, interest_rate, dividend
! Data passed through using allocated components
! of the derived type s_fcn_data
      sigma = fcn_data % rdata(5)
      interest_rate = fcn_data % rdata(6)
      dividend = fcn_data % rdata(7)
      select case (iflag)
        case (1)
! The coefficient derivative d(sigma)/dx
          value = sigma
! The coefficient sigma(x)
        case (2)
          value = sigma * x
        case (3)
! The coefficient mu(x)
          value = (interest_rate - dividend) * x
        case (4)
! The coefficient kappa(x)
          value = interest_rate
      end select
! Note that there is no time dependence
      iflag = 0
      return
```

```
      end function fkcoef_call

      function fkinitcond_call(x, fcn_data) result(value)
      use mp_types
      implicit none

      real(kind(1e0)), intent(in) :: x
      type(s_fcn_data), optional :: fcn_data
      real(kind(1e0)) :: value

      real(kind(1e0)) :: strike_price, spread, bet
      real(kind(1e0)), parameter :: zero = 0.0e0

      strike_price = fcn_data % rdata(1)
      bet = fcn_data % rdata(2)
      spread = fcn_data % rdata(3)
! The payoff function - Use flag passed to decide which
      select case (fcn_data % idata(1))
        case(1)
! After reaching the strike price the payoff jumps
! from zero to the bet value.
        value = zero
        if (x > strike_price) value = bet
        case(2)
! Function is zero up to strike price.
! Then linear between strike price and spread.
! Then has constant value Spread-Strike Price after
! the value Spread.
          value = max(x-strike_price, zero) - max(x-spread, zero)
      end select
      return
      end function fkinitcond_call

      subroutine fkbc_call (TX, iflag, bccoefs, fcn_data)
      use mp_types
      implicit none

      real(kind(1e0)), intent(in) :: tx
      integer, intent(inout) :: iflag
      real(kind(1e0)), dimension(:,:), intent(out) :: bccoefs
      type(s_fcn_data), optional :: fcn_data

      real(kind(1e0)) :: strike_price, spread, bet,&
                         interest_rate, df

      strike_price = fcn_data % rdata(1)
      bet = fcn_data % rdata(2)
      spread = fcn_data % rdata(3)
      interest_rate = fcn_data % rdata(6)
      select case (iflag)
        case (1)
          bccoefs(1,1:4) = ((/1.0e0, 0.0e0, 0.0e0, 0.0e0/))
          bccoefs(2,1:4) = ((/0.0e0, 1.0e0, 0.0e0, 0.0e0/))
          bccoefs(3,1:4) = ((/0.0e0, 0.0e0, 1.0e0, 0.0e0/))
        case (2)
! This is the discount factor using the risk-free
! interest rate
          df = exp(interest_rate * tx)
! Use flag passed to decide on boundary condition -
          select case (fcn_data % idata(1))
            case(1)
              bccoefs(1,1:4) = (/1.0e0, 0.0e0, 0.0e0, bet*df/)
            case(2)
              bccoefs(1,1:4) = (/1.0e0, 0.0e0, 0.0e0,&
                                 (spread-strike_price)*df/)
          end select
```

```
            bccoefs(2,1:4) = (/0.0e0, 1.0e0, 0.0e0, 0.0e0/)
            bccoefs(3,1:4) = (/0.0e0, 0.0e0, 1.0e0, 0.0e0/)
            return
        end select
! Note no time dependence in case (1) for iflag
        iflag = 0
        end subroutine fkbc_call
```

Output

```
      European Option Value for A Bet
       and a Vertical Spread, 3 and 6 Months Prior to Expiry
         Number of equally spaced spline knots    61
         Number of unknowns  183
         Strike= 10.00, Sigma= 0.40, Interest Rate= 0.10
         Bet =  2.00, Spread Value = 15.00

           Underlying              A Bet    Vertical Spread
              2.0000    0.0000    0.0000    0.0000    0.0000
              4.0000    0.0000    0.0014    0.0000    0.0006
              6.0000    0.0110    0.0723    0.0039    0.0447
              8.0000    0.2691    0.4302    0.1478    0.3832
             10.0000    0.9948    0.9781    0.8909    1.1926
             12.0000    1.6094    1.4290    2.1911    2.2273
             14.0000    1.8655    1.6922    3.4254    3.1553
             16.0000    1.9338    1.8175    4.2263    3.8264
             18.0000    1.9476    1.8700    4.6264    4.2492
             20.0000    1.9501    1.8904    4.7911    4.4921
             22.0000    1.9505    1.8979    4.8497    4.6231
             24.0000    1.9506    1.9007    4.8685    4.6909
```

Example 4– Convertible Bonds

This example evaluates the price of a convertible bond. Here, convertibility means that the bond may, at any time of the holder's choosing, be converted to a multiple of the specified asset. Thus a convertible bond with price x returns an amount K at time T *unless* the owner has converted the bond to νx, $\nu \geq 1$, units of the asset at some time prior to T. This definition, the differential equation and boundary conditions are given in Chapter 18 of Wilmott et al. (1996). Using a constant interest rate and volatility factor, the parameters and boundary conditions are:

1. Bond face value K = {1}, conversion factor $\nu = 1.125$
2. Volatility $\sigma = \{0.25\}$
3. Times until expiration = {1/2,1}
4. Interest rate $r = 0.1$, dividend D = 0.02
5. $x_{\text{min}} = 0$, $x_{\text{max}} = 4$
6. $nx = 61$, $n = 3 \times nx = 183$
7. Boundary conditions $f(0,t) = K\exp(-r(T-t)), f(x_{\max},t) = \nu x_{\max}$
8. Terminal data $f(x,T) = \max(K,\nu x)$

9. Constraint for bond holder $f(x,t) \geq \nu x$

Note that the error tolerance is set to a pure absolute error of value 10^{-3}. The free boundary constraint $f(x,t) = \nu x$ is achieved by use of a non-linear forcing term in the subroutine `fkforce_cbond`. The terminal conditions are provided with the user subroutine `fkinit_cbond`.

(Example feynman_kac_ex4.f90)

```
! Compute value of a Convertible Bond
      use feynman_kac_int
      use hqsval_int
      use mp_types
      use umach_int

      implicit none
! The face value
      real(kind(1e0)) :: ks = 1.0e0
! The sigma  or volatility value
      real(kind(1e0)) :: sigma = 0.25e0

! Time values for the options
      integer, parameter :: nt = 2
      real(kind(1e0)) :: time(nt)=(/0.5e0, 1.0e0/)
! Values of the underlying where evaluation are made
      integer, parameter :: nv = 13
      integer, parameter :: nlbc = 3, nrbc = 3, ndeg = 6
      integer :: i
      real(kind(1e0)) :: xs(nv) = (/((i-1)*0.25e0,i=1,nv)/)
! Value of the interest rate, continuous dividend and factor
      real(kind(1e0)) :: r = 0.1e0, dividend = 0.02e0,&
                         factor =1.125e0
! Values of the min and max underlying values modeled
      real(kind(1e0)) :: x_min = 0.0e0, x_max = 4.0e0
! Define parameters for the integration step.
      integer, parameter :: nx = 61, nint = nx-1, n = 3*nx
      real(kind(1e0)) :: xgrid(nx), y(n,0:nt), yprime(n,0:nt),&
                         dx, f(nv,0:nt)
! Relative and absolute error tolerances
      real(kind(1e0)) :: atol(1), rtol(1)
      type(s_fcn_data) fcn_data
      real(kind(1e0)), external :: fkcoef_cbond, fkinitcond_cbond
      external fkbc_cbond, fkforce_cbond, fkinit_cbond

      integer :: nout

      call umach(2,nout)
! Allocate space inside the derived type for holding
! data values. These are for the evaluation routines.
      allocate(fcn_data % rdata (7), fcn_data % idata (1))

! Define an equally-spaced grid of points for the underlying price
      dx = (x_max - x_min)/real(nint)
      xgrid(1) = x_min
      xgrid(nx) = x_max

      do i=2,nx-1
        xgrid(i) = xgrid(i-1) + dx
      end do

! Use a pure absolute error tolerance for the integration
! The default values require too much integation time.
      atol(1) = 1.0e-3
```

```
      rtol(1) = 0.0e0

! Pass the data for evaluation
      fcn_data % rdata = (/ks,x_max,sigma,r,dividend,factor,&
                          atol(1)/)
      fcn_data % idata = (/ndeg/)

! Compute value of convertible bond
      call feynman_kac (xgrid, time, nlbc, nrbc, fkcoef_cbond,&
                     fkinitcond_cbond, fkbc_cbond, y, yprime,&
                     ATOL=atol, RTOL=rtol, FKINIT = fkinit_cbond,&
                     FKFORCE = fkforce_cbond, FCN_DATA = fcn_data)

! Evaluate and display solutions at vector of points XS(:), at each
! time value prior to expiration.
      do i=0,nt
        f(:,i) = hqsval (xs, xgrid, y(:,i))
      end do

      write(nout,'(T05,A)')&
      "Convertible Bond Value, 0+, 6 and 12 Months Prior to Expiry"

      write(nout,'(T08,"Number of equally spaced spline knots ",I4,'//&
                '/T08,"Number of unknowns ",I4)') NX,N

      write(nout,'(T08,"Strike = ",F5.2,", Sigma =", F5.2,/'//&
         'T08,"Interest Rate =",F5.2,", Dividend =",F5.2,'//&
         '", Factor = ",F5.3,//T08,"Underlying", T26,"Bond Value",'//&
         '/(T10,4F8.4))') ks,sigma,r,dividend,factor,&
           (xs(i), f(i,0:nt),i=1,nv)
      end

! These routines define the coefficients, payoff, boundary
! conditions and forcing term.
      function fkcoef_cbond(x, tx, iflag, fcn_data) result(value)
      use mp_types
      implicit none
      integer, intent(inout) :: iflag
      real(kind(1e0)), intent(in) :: x, tx
      type(s_fcn_data), optional :: fcn_data
      real(kind(1e0)) :: value

      real(kind(1e0)) :: sigma, interest_rate, &
                         dividend, zero = 0.e0

      sigma = fcn_data % rdata(3)
      interest_rate = fcn_data % rdata(4)
      dividend = fcn_data % rdata(5)

      select case (iflag)
        case (1)
! The coefficient derivative d(sigma)/dx
          value = sigma
! The coefficient sigma(x)
        case (2)
          value = sigma * x
        case (3)
! The coefficient mu(x)
          value = (interest_rate - dividend) * x
        case (4)
! The coefficient kappa(x)
          value = interest_rate
      end select
! Note that there is no time dependence
      iflag = 0
      return
```

```
      end function fkcoef_cbond

      function fkinitcond_cbond(x, fcn_data) result(value)
      use mp_types
      implicit none
      real(kind(1e0)), intent(in) :: x
      type (s_fcn_data), optional :: fcn_data
      real(kind(1e0)) :: value

      real(kind(1e0)) :: strike_price, factor

      strike_price = fcn_data % rdata(1)
      factor = fcn_data % rdata(6)
      value = max(factor * x, strike_price)
      return
      end function fkinitcond_cbond

      subroutine fkbc_cbond (tx, iflag, bccoefs, fcn_data)
      use mp_types
      implicit none
      real(kind(1e0)), intent(in) :: tx
      integer, intent(inout) :: iflag
      real(kind(1e0)), dimension(:,:), intent(out) :: bccoefs
      type(s_fcn_data), optional :: fcn_data

      real(kind(1e0)) :: interest_rate, strike_price, dp,&
                         factor, x_max

      select case (iflag)
        case (1)
          strike_price = fcn_data % rdata(1)
          interest_rate = fcn_data % rdata(4)
          dp = strike_price * exp(tx*interest_rate)
          bccoefs(1,1:4) = (/1.0e0, 0.0e0, 0.0e0,    dp/)
          bccoefs(2,1:4) = (/0.0e0, 1.0e0, 0.0e0,  0.0e0/)
          bccoefs(3,1:4) = (/0.0e0, 0.0e0, 1.0e0,  0.0e0/)
          return
        case (2)
          x_max = fcn_data % rdata(2)
          factor = fcn_data % rdata(6)
          bccoefs(1,1:4) = (/1.0e0, 0.0e0, 0.0e0, factor * x_max/)
          bccoefs(2,1:4) = (/0.0e0, 1.0e0, 0.0e0, factor/)
          bccoefs(3,1:4) = (/0.0e0, 0.0e0, 1.0e0, 0.0e0/)
      end select
! Note no time dependence
      iflag = 0
      return
      end subroutine fkbc_cbond

      subroutine fkforce_cbond (interval, t, hx, y, xlocal, qw, u,&
                                phi, dphi, fcn_data)
      use mp_types
      implicit none
      integer :: i, j, l
      integer, parameter :: local = 6
      integer, intent(in) :: interval
      real(kind(1.e0)), intent(in) :: y(:), t, hx, qw(:),xlocal(:),&
                                      u(:,:)
      real(kind(1.e0)), intent(out) :: phi(:), dphi(:,:)

      integer :: ndeg
      real(kind(1.e0)) :: yl(local), bf(local)
      real(kind(1.e0)) :: value, strike_price, interest_rate,&
                          zero = 0.0e0, one = 1.0e0, rt, mu, factor
      type(s_fcn_data), optional :: fcn_data
```

```
      yl = y(3*interval-2:3*interval+3)
      phi = zero
      dphi = zero
      value = fcn_data % rdata(7)
      strike_price = fcn_data % rdata(1)
      interest_rate = fcn_data % rdata(4)
      factor = fcn_data % rdata(6)
      ndeg = fcn_data % idata(1)
      mu = 2
! This is the local definition of the forcing term
! It "forces" the constraint f >= factor*x.
      do j=1,local
        do l = 1,ndeg
          bf(1:3) = u(l,1:3)
          bf(4:6) = u(l,7:9)
          rt = dot_product(yl,bf)
          rt = value/(rt + value - factor * xlocal(l))
          phi(j) = phi(j) + qw(l) * bf(j) * rt**mu
        end do
      end do
      phi = -phi * hx * factor * strike_price
! This is the local derivative matrix for the forcing term -
      do j=1,local
        do i = 1,local
          do l=1,ndeg
            bf(1:3) = u(L,1:3)
            bf(4:6) = u(L,7:9)
            rt = dot_product(yl,bf)
            rt = one/(rt + value - factor * xlocal(l))
            dphi(i,j) = dphi(i,j) + qw(l) * bf(i) * bf(j)&
                 * (value * rt)**mu * rt
          end do
        end do
      end do
      dphi = -mu * dphi * hx * factor * strike_price
      return
      end subroutine fkforce_cbond

      subroutine fkinit_cbond(xgrid,tgrid,t,yprime,y,atol,rtol,&
                              fcn_data)
      use mp_types
      implicit none
      real(kind(1e0)), intent(inout) :: y(:), atol(:), rtol(:)
      real(kind(1e0)), intent(in) :: xgrid(:), tgrid(:), yprime(:),&
                                     t
      type(s_fcn_data), optional :: fcn_data

      integer :: i
      if (t == 0.0e0) then
! Set initial data precisely.
        do i=1,size(Xgrid)
          if (xgrid(i)*fcn_data % rdata(6) <&
              fcn_data % rdata(1)) then
            y(3*i-2) = fcn_data % rdata(1)
            y(3*i-1) = 0.0e0
            y(3*i  ) = 0.0e0
          else
            y(3*i-2) = xgrid(i) * fcn_data % rdata(6)
            y(3*i-1) = fcn_data % rdata(6)
            y(3*i  ) = 0.0e0
          end if
        end do
      end if
      end subroutine fkinit_cbond
```

Output

```
     Convertible Bond Value, 0+, 6 and 12 Months Prior to Expiry
        Number of equally spaced spline knots   61
        Number of unknowns  183
        Strike=  1.00, Sigma= 0.25
        Interest Rate= 0.10, Dividend= 0.02, Factor= 1.125

        Underlying        Bond Value
            0.0000  1.0000  0.9512  0.9048
            0.2500  1.0000  0.9512  0.9049
            0.5000  1.0000  0.9513  0.9065
            0.7500  1.0000  0.9737  0.9605
            1.0000  1.1250  1.1416  1.1464
            1.2500  1.4062  1.4117  1.4121
            1.5000  1.6875  1.6922  1.6922
            1.7500  1.9688  1.9731  1.9731
            2.0000  2.2500  2.2540  2.2540
            2.2500  2.5312  2.5349  2.5349
            2.5000  2.8125  2.8160  2.8160
            2.7500  3.0938  3.0970  3.0970
            3.0000  3.3750  3.3781  3.3781
```

Example 5– A Non-Standard American Option

This example illustrates a method for evaluating a certain “Bermudan Style” or non-standard American option. These options are American Style options restricted to certain dates where the option may be exercised. Since this agreement gives the holder more opportunity than a European option, it is worth more. But since the holder can only exercise at certain times it is worth no more than the American style option value that can be exercised at any time. Our solution method uses the same model and data as in Example 2, but allows exercise at weekly intervals. Thus we integrate, for half a year, over each weekly interval using a European style Black-Scholes model, but with initial data at each new week taken from the corresponding values of the American style option.

(Example feynman_kac_ex5.f90)

```
  ! Compute Bermudan-Style Option Premium for Vanilla Put
        use feynman_kac_int
        use hqsval_int
        use mp_types
        use umach_int

        implicit none
        integer :: nout
  ! The strike price
        real(kind(1e0)) :: ks = 10.0e0
  ! The sigma value
        real(kind(1e0)) :: sigma = 0.4e0
  ! Program working stores
        real(kind(1e0)) :: week
  ! Time values for the options
        integer, parameter :: nt = 26
        integer, parameter :: ndeg = 6
        real(kind(1e0)) :: time(nt), time_end = 0.5e0
  ! Values of the underlying where evaluation are made
        integer, parameter :: nv = 9, nlbc = 2, nrbc = 3
        integer :: i
        real(kind(1e0)) :: xs(nv) = (/((i-1)*2.0e0,i=1,nv)/)
  ! Value of the interest rate and continuous dividend
        real(kind(1e0)) :: r = 0.1e0, dividend = 0.0e0
  ! Values of the min and max underlying values modeled
```

```
      real(kind(1e0)) :: x_min = 0.0e0, x_max = 30.0e0

! Define parameters for the integration step.
      integer, parameter :: nx = 61, nint = nx-1, n = 3*nx
      real(kind(1e0)) :: xgrid(nx), yb(n,0:nt), ybprime(n,0:nt),&
                         ya(n,0:nt), yaprime(n,0:nt),&
                         ytemp(n,0:1), ytempprime(n,0:1),&
                         dx, fb(nv,nt), fa(nv,nt)
      real(kind(1e0)) :: atol
      type(s_fcn_data) fcn_data_amer, fcn_data_berm
      real(kind(1e0)), external :: fkcoef_put, fkinitcond_put
      external fkbc_put, fkforce_put, fkinit_amer_put, fkinit_berm_put

      call umach(2, nout)
! Allocate space inside the derived type for holding
! data values. These are for the evaluation routines.
      allocate(fcn_data_amer % rdata (6), fcn_data_amer % idata (1))
! Define an equally-spaced grid of points for the underlying price
      dx = (x_max-x_min)/real(nint)
      xgrid(1) = x_min
      xgrid(nx)= x_max
      do i=2,nx-1
        xgrid(i) = xgrid(i-1) + dx
      end do

! Place a breakpoint at the strike price.
      do i=1,nx
        if (xgrid(i) > ks) then
          xgrid(i-1) = ks
          exit
        end if
      end do

! Compute time values where American option is computed
      week = time_end/real(nt,kind(week))
      time(1) = week
      do i=2,nt-1
        time(i) = time(i-1) + week
      end do
      time(nt) = time_end

      atol = 1.0e-3
      fcn_data_amer % rdata = (/ks,x_max,sigma,r,dividend,atol/)
      fcn_data_amer % idata = (/ndeg/)

! Compute American Put Option Values at the weekly grid.
      call feynman_kac (xgrid, time, nlbc, nrbc, fkcoef_put,&
                        fkinitcond_put, fkbc_put, ya, yaprime,&
                        FKINIT = fkinit_amer_put,&
                        FKFORCE = fkforce_put,&
                        FCN_DATA = fcn_data_amer)
! Integrate once again over the weekly grid, using the American
! Option values as initial data for a piece-wise European option
!integration.

! Allocate space to hold coefficient data and initial values.
      allocate(fcn_data_berm % rdata(5+n))
      fcn_data_berm % rdata(1:5) = fcn_data_amer % rdata(1:5)
! Copy initial data so the payoff value is the same for
! American and Bermudan option values.
      yb(1:n,0) = ya(1:n,0)
      ybprime(1:n,0) = ya(1:n,0)

      do i=0,nt-1
! Move American Option values into place as initial conditions,
! but now integrating with European style over each period of
```

```
! the weekly grid.
        fcn_data_berm % rdata(6:) = ya(1:n,i)
        if (i .eq. 0) then
          call feynman_kac (xgrid, (/time(1)/), nlbc, nrbc,&
                            fkcoef_put, fkinitcond_put, fkbc_put,&
                            ytemp(:,0:1), ytempprime(:,0:1),&
                            FKINIT = fkinit_berm_put,&
                            FCN_DATA = fcn_data_berm)
        else
          call feynman_kac (xgrid, (/time(i+1)-time(i)/),&
                            nlbc, nrbc, fkcoef_put,&
                            fkinitcond_put, fkbc_put,&
                            ytemp(:,0:1), ytempprime(:,0:1),&
                            FKINIT = fkinit_berm_put,&
                            FCN_DATA = fcn_data_berm)
        end if
! Record values of the Bermudan option at the end of each integration.
        yb(1:n,i+1) = ytemp(1:n,1)
        ybprime(1:n,i+1) = ytempprime(1:n,1)
      end do
! Evaluate solutions at vector of points XS(:), at each time value
! prior to expiration.
      do i=1,nt
        fa(:,i) = hqsval (xs, xgrid, ya(:,i))
        fb(:,i) = hqsval (xs, xgrid, yb(:,i))
      end do

      write(nout,'(T05,A)')&
        "American Option Premium for Vanilla Put, 6 Months "//&
        "Prior to Expiry"
      write(nout,'(T05,A)')&
        "Exercise Opportunities At Weekly Intervals"
      write(nout,'(T08,"Number of equally spaced spline knots ",'//&
                 'I4,/T08,"Number of unknowns ",I4)') nx, n
      write(nout,'(T08,"Strike = ",F5.2,", Sigma =", F5.2,'//&
                 '", Interest Rate =",F5.2,//T08,"Underlying",'//&
                 'T20,"Bermudan Style", T42,"American",'//&
                 '/(T10,F8.4, T26, F8.4, T42, F8.4))')&
                 KS,SIGMA,R,&
                (xs(i), fb(i,nt:nt), fa(i,nt:nt),i=1,nv)
      end

! These subprograms set the coefficients, payoff, boundary
! conditions and forcing term for American and European Options.
      function fkcoef_put(x, tx, iflag, fcn_data_amer)&
                          result(value)
      use mp_types
      implicit none
      integer, intent(inout) :: iflag
      real(kind(1e0)), intent(in) :: x, tx
      type(s_fcn_data), optional :: fcn_data_amer
      real(kind(1e0)) :: value

      real(kind(1e0)) :: sigma, interest_rate, dividend, zero=0.0e0

      sigma = fcn_data_amer % rdata(3)
      interest_rate = fcn_data_amer % rdata(4)
      dividend = fcn_data_amer % rdata(5)
      select case (iflag)
        case (1)
! The coefficient derivative d(sigma)/dx
          value = sigma
! The coefficient sigma(x)
        case (2)
          value = sigma * x
        case (3)
```

```
! The coefficient mu(x)
          value = (interest_rate - dividend) * x
        case (4)
! The coefficient kappa(x)
          value = interest_rate
      end select
! Note that there is no time dependence
      iflag = 0
      return
      end function fkcoef_put

      function fkinitcond_put(x, fcn_data_amer) result(value)
      use mp_types
      implicit none

      real(kind(1e0)), intent(in) :: x
      type (s_fcn_data), optional :: fcn_data_amer

      real(kind(1e0)) :: value
      real(kind(1e0)) :: strike_price, zero = 0.0e0

      strike_price = fcn_data_amer % rdata(1)
! The payoff function
      value = max(strike_price - x, zero)
      return
      end function fkinitcond_put

      subroutine fkbc_put (tx, iflag, bccoefs, fcn_data)
      use mp_types
      implicit none
      real(kind(1e0)), intent(in) :: tx
      integer, intent(inout) :: iflag
      real(kind(1e0)), dimension(:,:), intent(out) :: bccoefs
      type (s_fcn_data), optional :: fcn_data

      select case (iflag)
        case (1)
          bccoefs(1,1:4) = ((/0.0e0, 1.0e0, 0.0e0, -1.0e0/))
          bccoefs(2,1:4) = ((/0.0e0, 0.0e0, 1.0e0,  0.0e0/))
        case (2)
          bccoefs(1,1:4) = ((/1.0e0, 0.0e0, 0.0e0, 0.0e0/))
          bccoefs(2,1:4) = ((/0.0e0, 1.0e0, 0.0e0, 0.0e0/))
          bccoefs(3,1:4) = ((/0.0e0, 0.0e0, 1.0e0, 0.0e0/))
      end select
! Note no time dependence
      iflag = 0
      end subroutine fkbc_put

      subroutine fkforce_put (interval, t, hx, y, xlocal, qw, u,&
                              phi, dphi, fcn_data_amer)
      use mp_types
      implicit none
      integer, parameter :: local = 6
      integer :: i, j, l, ndeg
      integer, intent(in) :: interval
      real(kind(1.e0)), intent(in) :: y(:), t, hx, qw(:),&
                                      xlocal(:), u(:,:)
      real(kind(1.e0)), intent(out) :: phi(:), dphi(:,:)
      type (s_fcn_data), optional :: fcn_data_amer

      real(kind(1.e0)) :: yl(local), bf(local)
      real(kind(1.e0)) :: value, strike_price, interest_rate,&
                          zero = 0.e0, one = 1.e0, rt, mu

      yl = y(3*interval-2:3*interval+3)
      phi = zero
```

```
      value = fcn_data_amer % rdata(6)
      strike_price = fcn_data_amer % rdata(1)
      interest_rate = fcn_data_amer % rdata(4)
      ndeg = fcn_data_amer % idata(1)

      mu = 2
! This is the local definition of the forcing term
      do j=1,local
        do l=1,ndeg
          bf(1:3) = U(L,1:3)
          bf(4:6) = U(L,7:9)
          rt = dot_product(YL,BF)
          rt = value/(rt + value-(strike_price-xlocal(l)))
          phi(j) = phi(j) + qw(l) * bf(j) * rt**mu
        end do
      end do
      phi = -phi * hx * interest_rate * strike_price
! This is the local derivative matrix for the forcing term
      dphi = zero
      do j=1,local
        do i = 1,local
          do l=1,ndeg
            bf(1:3) = u(L,1:3)
            bf(4:6) = u(L,7:9)
            rt = dot_product(yl,bf)
            rt = one/(rt + value - (strike_price - xlocal(l)))
            dphi(i,j) = dphi(i,j) + qw(l) * bf(i) * bf(j) *&
                        rt**(mu+1)
          end do
        end do
      end do
      dphi = mu * dphi * hx * value**mu * interest_rate *&
             strike_price
      end subroutine fkforce_put

      subroutine fkinit_amer_put(xgrid,tgrid,t,yprime,y,atol,rtol,&
                                 fcn_data_amer)
      use mp_types
      implicit none

      real(kind(1e0)), intent(in) :: xgrid(:), tgrid(:), t,&
                                     yprime(:)
      real(kind(1e0)), intent(inout) :: y(:), atol(:), rtol(:)
      type(s_fcn_data), optional :: fcn_data_amer
      integer :: i

      if (t == 0.0e0) then
! Set initial data precisely.  The strike price is a breakpoint.
! Average the derivative limit values from either side.
        do i=1,size(xgrid)
          if (xgrid(i) < fcn_data_amer % rdata(1)) then
            y(3*i-2) = fcn_data_amer % rdata(1) - xgrid(i)
            y(3*i-1) = -1.0e0
            y(3*i) = 0.0e0
          else if (xgrid(i) == fcn_data_amer % rdata(1)) then
            y(3*i-2) = 0.0e0
            y(3*i-1) = -0.5e0
            y(3*i) = 0.0e0
          else
            y(3*i-2) = 0.0e0
            y(3*i-1) = 0.0e0
            y(3*i) = 0.0e0
          end if
        end do
      end if
      end subroutine fkinit_amer_put
```

```
      subroutine fkinit_berm_put(xgrid,tgrid,t,yprime,y,atol,rtol,&
                                 fcn_data_berm)
      use mp_types
      implicit none

      real(kind(1e0)), intent(in) :: xgrid(:), tgrid(:), t,&
                                     yprime(:)
      real(kind(1e0)), intent(inout) :: y(:), atol(:), rtol(:)
      type(s_fcn_data), optional :: fcn_data_berm
      integer :: i

      if (t == 0.0e0) then
! Set initial data for each week at the previously computed
! American Option values.  These coefficients are passed
! in the derived type fcn_data_berm.
        do i=1,size(xgrid)
          y(3*i-2) = fcn_data_berm % rdata(3+3*i)
          y(3*i-1) = fcn_data_berm % rdata(4+3*i)
          y(3*i  ) = fcn_data_berm % rdata(5+3*i)
        end do
      end if
      end subroutine fkinit_berm_put
```

Output

```
American Option Premium for Vanilla Put, 6 Months Prior to Expiry
Exercise Opportunities At Weekly Intervals
   Number of equally spaced spline knots   61
   Number of unknowns  183
   Strike= 10.00, Sigma= 0.40, Interest Rate= 0.10

   Underlying  Bermudan Style        American
       0.0000          9.9808         10.0000
       2.0000          7.9808          8.0000
       4.0000          5.9808          6.0000
       6.0000          3.9808          4.0000
       8.0000          2.0924          2.0926
      10.0000          0.9139          0.9138
      12.0000          0.3570          0.3569
      14.0000          0.1309          0.1309
      16.0000          0.0468          0.0469
```

Example 6 – Oxygen Diffusion Problem

Our previous examples are from the field of financial engineering. A final example is a physical model. The Oxygen Diffusion Problem is summarized in Crank [4], p. 10-20, 261-262. We present the numerical treatment of the transformed one-dimensional system

$$f_t + f_{xx} = 1,\ 0 \le x \le s\left(t\right),\ f\left(0,x\right) = \tfrac{1}{2}\left(1-x\right)^2, \quad 0 \le x \le 1,$$
$$f(t,1) = f_x\left(t,0\right) = 0,\ t < 0.$$

A slight difference from the Crank development is that we have reflected the time variable $t \to -t$ to match our form of the Feynman-Kac equation. We have a free boundary problem because the interface $s(t)$ is implicit. This interface is implicitly defined by solving the variational relation $(f_t + f_{xx} - 1)f = 0$, $f \ge 0$. The first factor is zero for $0 \le x < s(t)$ and the second factor is zero for $s(t) \le x \le 1$. We list the Feynman-Kac equation coefficients, forcing term and boundary conditions, followed by comments.

$$\sigma(x,t) = \sqrt{2}; \quad \frac{\partial \sigma}{\partial x} = 0$$

$$\mu(x,t) = 0$$

$$\kappa(x,t) = 0$$

$$p(x) = \frac{1}{2}(1 - x)^2$$

$$\phi(f,x,t) \equiv 1 - \left(\frac{\varepsilon}{f + \varepsilon}\right)^{\mu}, \varepsilon = ATOL, \mu = 2$$

$$f_x(0,t) = \exp(t/\varepsilon^2)$$
$$f(1,t) = f_x(1,t) = 0, t < 0$$

The ϕ forcing term has the property of being almost the value 1 when the solution is larger than the factor ε. As the solution $f \downarrow 0$, the forcing term ϕ is almost the value zero. These properties combine to approximately achieve the variational relation that defines the free boundary. Note that the arc of the free boundary is not explicitly available with this numerical method. We have used $\varepsilon = ATOL$, the requested absolute error tolerance for the numerical integration.

The boundary condition $f_x(t,0) = 0$, $t < 0$ is discontinuous as $t \uparrow 0$, since the initial data yields $f_x(0,0) = 1$. For the numerical integration we have chosen a boundary value function that starts with the value 1 at $t = 0$ and rapidly blends to the value zero as the integration proceeds in the negative direction. It is necessary to give the integrator the opportunity to severely limit the step size near $t = 0$ to achieve continuity during the blending.

In the example code, values of $f(0,t)$ are checked against published values for certain values of t. Also checked are values of $f(0,s(t)) = 0$ at published values of the free boundary, for the same values of t.

(Example feynman_kac_ex6.f90)

```
! Integrate Oxygen Diffusion Model found in the book
! Crank, John. Free and Moving Boundary Problems,
! Oxford Univ. Press, (1984), p. 19-20 and p. 261-262.
      use feynman_kac_int
      use hqsval_int
      use mp_types
      use norm_int
      use umach_int
      implicit none

      integer :: nout
      real(kind(1e0)), allocatable :: xgrid(:), tgrid(:), y(:,:),&
                                      yprime(:,:), f(:,:), s(:)
      real(kind(1e0)) :: dx, x_min, x_max, zero=0.0e0, one=1.0e0
      real(kind(1e0)) :: atol(1), rtol(1)
      type(s_fcn_data) :: fk_ox2
      integer :: i, nint, n, nunit, ntimes = 8
      integer, parameter :: ndeg = 6, nlbc = 1, nrbc = 2
      real(kind(1e0)), external :: fkcoef_ox2, fkinitcond_ox2
      external fkbc_ox2, fkforce_ox2
```

```
      call umach(2,nout)

! Define number of equally spaced intervals for elements
      nint = 100
! Allocate the space needed for the integration process
      n = 3*(nint+1)
      allocate(xgrid(nint+1), y(n,0:ntimes), yprime(n,0:ntimes),&
               tgrid(ntimes), f(1,ntimes), s(ntimes))

! Allocate space inside the derived type for holding
! data values. These are for the evaluation routines.
      allocate(fk_ox2 % rdata (1), fk_ox2 % idata (1))

      atol(1) = 0.5e-2
      rtol(1) = 0.5e-2
      fk_ox2 % rdata(1) = atol(1)
      fk_ox2 % idata(1) = ndeg

! Define interval endpoints
      x_min = zero
      x_max = one
! Define interval widths
      dx = (x_max-x_min)/real(nint)
      xgrid(1) = x_min
      xgrid(nint+1) = x_max
! Define grid points of interval
      do i=2,nint
        xgrid(i) = xgrid(i-1) + dx
      end do
! Define time integration output points
! These correspond to published values in Crank's book, p. 261-262
      tgrid = (/0.04e0,0.06e0,0.10e0,0.12e0,0.14e0,&
               0.16e0,0.18e0,0.185e0/)
      call feynman_kac (xgrid, tgrid, nlbc, nrbc, fkcoef_ox2,&
                        fkinitcond_ox2, fkbc_ox2, y, yprime,&
                        ATOL = atol, RTOL = rtol,&
                        FKFORCE = fkforce_ox2, FCN_DATA = fk_ox2)
! Summarize output at the left end
      do i=1,ntimes
        f(:,i)= hqsval ((/zero/), xgrid, y(:,i))
      end do
! Check differences of evaluation and published left end values
      f(1,:) = f(1,:) - (/2.743e-01, 2.236e-01, 1.432e-01,&
           1.091e-01, 7.786e-02, 4.883e-02, 2.179e-02, 1.534e-02/)
      write(nout,*) "Oxygen Depletion Model, from Crank's "//&
                    "Book, p. 261-262,"
      write(nout,*) "'Free and Moving Boundary Value Problems'"
      if (norm(f(1,:)) < ntimes * atol(1)) then
        write(nout,*) "FEYNMAN_KAC Example 6 - Fixed Sealed "//&
                      "Surface Values are correct"
      else
        write(nout,*) "FEYNMAN_KAC Example 6 - does not agree with"//&
                      " published left end values"
      end if
! Define known position of free boundary at the time points
      s = (/0.9992e0,0.9918e0,0.9350e0,0.8792e0,&
            0.7989e0,0.6834e0,0.5011e0,0.4334e0/)

! Evaluate and verify solution is small near free boundary -
      do i=1,ntimes
        f(:,i) = hqsval ((/s(i)/), xgrid, y(:,i))
      end do

      if (norm(f(1,:)) < ntimes * atol(1)) then
        write(nout,*) "FEYNMAN_KAC Example 6 - Free Boundary "//&
```

```
                    "Position Values are correct"
      else
        write(nout,*) "FEYNMAN_KAC Example 6 - does not agree "//&
                    "with published free boundary values"
      end if
      end

      function fkcoef_ox2 (x, tx, iflag, fk_ox2) result(value)
      use mp_types
      implicit none
! Coefficient valuation routine for the Oxygen Diffusion
! Model found in Crank's book, p. 20
! Input/Ouput variables
      integer, intent(inout) :: iflag
      real(kind(1e0)), intent(in) :: x, tx
      type(s_fcn_data), optional :: fk_ox2
      real(kind(1e0)) :: value

! Local variables
      real(kind(1e0)) :: zero = 0.0e0, two = 2.0e0

      select case (iflag)
        case (1) ! Factor DSigma/Dx(x,t)
          value = zero
        case (2) !  Factor Sigma(x,t)
          value = sqrt(two)
        case (3) !  Factor Mu (x,t)
          value = zero
        case (4) !  Factor Kappa (x,t)
          value = zero
      end select
! Signal no dependence on tx=t=time for any coefficient.
      iflag = 0
      return
      end function fkcoef_ox2

      function fkinitcond_ox2(x, fk_ox2) result(value)
      use mp_types
      implicit none
      real(kind(1e0)), intent(in) :: x
      type (s_fcn_data), optional :: fk_ox2
      real(kind(1e0)) :: value

      real(kind(1e0)) :: half = 0.5e0, one = 1.0e0

      value = half * (one - x)**2
      return
      end function fkinitcond_ox2

      subroutine fkbc_ox2 (tx, iflag, bccoefs, fk_ox2)
      use mp_types
      implicit none
! Evaluation routine for Oxygen Diffusion Model
! boundary conditions.
! Input/Ouput variables
      real(kind(1e0)), intent(in) :: tx
      integer, intent(inout) :: iflag
      real(kind(1e0)), dimension(:,:), intent(out) :: bccoefs
      type (s_fcn_data), optional :: fk_ox2

! Local variables
      real(kind(1e0)) :: zero = 0.0e0, one = 1.0e0, atol

      atol = fk_ox2 % rdata(1)
      select case (iflag)
        case (1) ! Left Boundary Condition,  at X_min=0
```

```
  ! There is a rapid blending of the boundary condition to achieve
  ! a zero derivative value at the left end.
  ! The initial data has the derivative with value one.
  ! This boundary condition essentially abruptly changes that
  ! derivative value to zero.
  ! Returning iflag=1 signals time dependence.  This is important
  ! for this problem.
            bccoefs(1,1:4) = (/0.0e0, one, 0.0e0, exp(tx/atol**2)/)
            return
          case (2) ! Right Boundary Condition, at X_max=1
            bccoefs(1,1:4) = (/one, 0.0e0, 0.0e0, 0.0e0/)
            bccoefs(2,1:4) = (/0.0e0, one, 0.0e0, 0.0e0/)
        end select
        iflag = 0 ! Signal no dependence on tx=time.
        end subroutine fkbc_ox2

        subroutine fkforce_ox2 (interval, t, hx, y, xlocal, qw, u,&
                                phi, dphi, fk_ox2)
  ! Evaluation routine for Oxygen Diffusion model forcing function.
        use mp_types
        implicit none
        integer, parameter :: local = 6
        integer :: i, j, l, mu, ndeg
        integer, intent(in) :: interval

        real(kind(1e0)), intent(in) :: y(:), t, hx, qw(:),&
                                       xlocal(:), u(:,:)
        real(kind(1e0)), intent(out) :: phi(:), dphi(:,:)
        type (s_fcn_data), optional :: fk_ox2

        real(kind(1e0)) :: yl(local), bf(local)
        real(kind(1e0)) :: value, zero = 0.0e0, one = 1.0e0, rt

        yl = y(3*interval-2:3*interval+3)
        phi = zero

        value = fk_ox2 % rdata(1)
        ndeg = fk_ox2 % idata(1)

        mu = 2
        do j=1,local
          do l=1,ndeg
            bf(1:3) = u(l,1:3)
            bf(4:6) = u(l,7:9)
            rt = dot_product(yl,bf)
            rt = one - (value/(rt + value))**mu
            phi(j) = phi(j) + qw(l) * bf(j) * RT
          end do
        end do
        phi = phi * hx
  ! This is the local derivative matrix for the forcing term -
        dphi = zero
        do j=1,local
          do i = 1,local
            do l=1,ndeg
              bf(1:3) = u(l,1:3)
              bf(4:6) = u(l,7:9)
              rt = dot_product(yl,bf)
              rt = one/(rt + value)
              dphi(i,j) = dphi(i,j) + qw(l) * bf(i) * bf(j) *&
                          rt**(mu+1)
            end do
          end do
        end do
        dphi = mu * dphi * hx * value**mu
        return
```

```
        end subroutine fkforce_ox2
```

Output

```
 Oxygen Depletion Model, from Crank's Book, p. 261-262,
 'Free and Moving Boundary Value Problems'
 FEYNMAN_KAC Example 6 - Fixed Sealed Surface Values are correct
 FEYNMAN_KAC Example 6 - Free Boundary Position Values are correct
```

Example 7 – Calculating the Greeks

In this example, routine `FEYNMAN_KAC` is used to solve for the Greeks, i.e. various derivatives of Feynman-Kac (FK) solutions applicable to the pricing of options and related financial derivatives. In order to illustrate and verify these calculations, the Greeks are calculated by two methods. The first method involves the FK solution to the diffusion model for call options given in Example 1 for the Black-Scholes (BS) case, i.e. $\alpha = 2$. The second method calculates the Greeks using the closed-form BS evaluations which can be found at http://en.wikipedia.org/wiki/The_Greeks.

This example calculates FK and BS solutions *V*(*S*,*t*) to the BS problem and the following Greeks:

- *Delta* = $\frac{\partial V}{\partial S}$

  is the first derivative of the *Value*, *V*(*S*,*t*), of a portfolio of derivative security derived from underlying instrument with respect to the underlying instrument's price *S*.
- *Gamma* = $\frac{\partial^2 V}{\partial S^2}$
- *Theta* = $-\frac{\partial V}{\partial t}$ is the negative first derivative of *V* with respect to time *t*
- *Charm* = $\frac{\partial^2 V}{\partial S \partial t}$
- *Color* = $\frac{\partial^3 V}{\partial S^2 \partial t}$
- *Rho* = $-\frac{\partial V}{\partial r}$ is the first derivative of *V* with respect to the risk-free rate *r*
- *Vega* = $\frac{\partial V}{\partial \sigma}$ measures sensivity to volatility parameter α of the underlying *S*
- *Volga* = $\frac{\partial^2 V}{\partial \sigma^2}$
- *Vanna* = $\frac{\partial^2 V}{\partial S \partial \sigma}$
- *Speed* = $\frac{\partial^3 V}{\partial S^3}$

Intrinsic Greeks include derivatives involving only *S* and *t*, the intrinsic FK arguments. In the above list, *Value*, *Delta*, *Gamma*, *Theta*, *Charm*, *Color* and *Speed* are all intrinsic Greeks. As is discussed in Hanson, R. (2008) "*Integrating Feynman-Kac Equations Using Hermite Quintic Finite Elements*", the expansion of the FK solution function *V*(*S*,*t*) in terms of quintic polynomial functions defined on *S*-grid subintervals and subject to continuity constraints in derivatives 0, 1 and 2 across the boundaries of these subintervals allows *Value*, *Delta*, *Gamma*, *Theta*, *Charm* and *Color* to be calculated directly by routines `FEYNMAN_KAC` and `HQSVAL`.

Non-intrinsic Greeks are derivatives of V involving FK parameters other than the intrinsic arguments S and t, such as r and α. Non-intrinsic Greeks in the above list include *Rho*, *Vega*, *Volga* and *Vanna*. In order to calculate non-intrinsic Greek (parameter) derivatives or intrinsic Greek S-derivatives beyond the second (such as *Speed*) or t-derivatives beyond the first, the entire FK solution must be calculated 3 times (for a parabolic fit) or five times (for a quartic fit), at the point where the derivative is to be evaluated and at nearby points located symmetrically on either side.

Using a Taylor series expansion of $f(\sigma + \varepsilon)$ truncated to $m + 1$ terms (to allow an m-degree polynomial fit of $m+1$ data points),

$$f(\sigma+\varepsilon) = \sum_{n=0}^{m} \frac{f^{(n)}(\sigma)}{n!}\varepsilon^n$$

we are able to derive the following parabolic (3 point) estimation of first and second derivatives $f^{(1)}(\sigma)$ and $f^{(2)}(\sigma)$ in terms of the three values $f(\sigma - \varepsilon)$, $f(\sigma)$ and $f(\sigma + \varepsilon)$, where $\varepsilon = \varepsilon_{frac}\sigma$ and $0 < \varepsilon_{frac} << 1$:

$$f^{(1)}(\sigma) \equiv \frac{\partial f(\sigma)}{\partial \sigma} \approx f^{[1]}(\sigma,\varepsilon) \equiv \frac{f(\sigma+\varepsilon) - f(\sigma-\varepsilon)}{2\varepsilon}$$

$$f^{(2)}(\sigma) \equiv \frac{\partial^2 f(\sigma)}{\partial \sigma^2} \approx f^{[2]}(\sigma,\varepsilon) \equiv \frac{f(\sigma+\varepsilon) + f(\sigma-\varepsilon) - 2f(\sigma)}{\varepsilon^2}$$

Similarly, the quartic (5 point) estimation of $f^{(1)}(\sigma)$ and $f^{(2)}(\sigma)$ in terms of $f(\sigma - 2\varepsilon)$, $f(\sigma - \varepsilon)$, $f(\sigma)$, $f(\sigma + \varepsilon)$, and $f(\sigma + 2\varepsilon)$ is:

$$f^{(1)}(\sigma) \approx \tfrac{4}{3} f^{[1]}(\sigma,\varepsilon) - \tfrac{1}{3} f^{[1]}(\sigma,2\varepsilon)$$

$$f^{(2)}(\sigma) \approx \tfrac{4}{3} f^{[2]}(\sigma,\varepsilon) - \tfrac{1}{3} f^{[2]}(\sigma,2\varepsilon)$$

For our example, the quartic estimate does not appear to be significantly better than the parabolic estimate, so we have produced only parabolic estimates by setting variable `iquart` to 0. The user may try the example with the quartic estimate simply by setting `iquart` to 1.

As is pointed out in "*Integrating Feynman-Kac Equations Using Hermite Quintic Finite Elements*", the quintic polynomial expansion function used by `FEYNMAN_KAC` only allows for continuous derivatives through the second derivative. While up to fifth derivatives can be calculated from the quintic expansion (indeed function `HQSVAL` will allow the third derivative to be calculated by setting optional argument `IDERIV` to 3, as is done in this example), the accuracy is compromised by the inherent lack of continuity across grid points (i.e. subinterval boundaries).

The accurate second derivatives in S returned by function `HQSVAL` can be leveraged into a third derivative estimate by calculating three FK second derivative solutions, the first solution for grid and evaluation point set $\{S, f^{(2)}(S)\}$ and the second and third solutions for solution grid and evaluation point sets $\{S + \varepsilon, f^{(2)}(S + \varepsilon)\}$ and $\{S + \varepsilon, f^{(2)}(S - \varepsilon)\}$, where the solution grid and evaluation point sets are shifted up and down by ε. In this example, ε is set to $\varepsilon_{frac}\overline{S}$, where $\overline{S}$ is the average value of S over the range of grid values and $0 < \varepsilon_{frac} << 1$. The third derivative solution can then be obtained using the parabolic estimate

$$f^{(3)}(S) \equiv \frac{\partial f^{(2)}(\sigma)}{\partial S} \approx \frac{f^{(2)}(S+\varepsilon) + f^{(2)}(S-\varepsilon)}{2\varepsilon}$$

This procedure is implemented in the current example to calculate the Greek *Speed*. (For comparison purposes, *Speed* is also calculated directly by setting the optional argument `IDERIV` to 3 in the call to function `HQSVAL`. The output from this direct calculation is called "*Speed2*".)

To reach better accuracy results, all computations are done in double precision.

The average and maximum relative errors (defined as the absolute value of the difference between the BS and FK values divided by the BS value) for each of the Greeks is given at the end of the output. (These relative error statistics are given for nine combinations of Strike Price and volatility, but only one of the nine combinations is actually printed in the output.) Both intrinsic and non-intrinsic Greeks have good accuracy (average relative error is in the range 0.01 – 0.00001) except for *Volga*, which has an average relative error of about 0.05. This is probably a result of the fact that *Volga* involves differences of differences, which will more quickly erode accuracy than calculations using only one difference to approximate a derivative. Possible ways to improve upon the 2 to 4 significant digits of accuracy achieved in this example include increasing FK integration accuracy by reducing the initial stepsize (via optional argument `RINITSTEPSIZE`), by choosing more closely spaced S and t grid points (by adjusting `FEYNMAN_KAC`'s input arrays `XGRID` and `TGRID`) and by adjusting ε_{frac} so that the central differences used to calculate the derivatives are not too small to compromise accuracy.

(Example feynman_kac_ex7.f90)

```
! Greeks computation
      use feynman_kac_int
      use hqsval_int
      use mp_types
      use anordf_int
      use const_int
      use umach_int

      implicit none

      real(kind(1d0)), external :: fkcoef, fkinitcond
      external fkbc

! The set of strike prices
      real(kind(1d0)) :: ks(3) = (/15.0d0,20.0d0,25.0d0/)
! The set of sigma values
      real(kind(1d0)) :: sigma(3) = (/0.2d0, 0.3d0, 0.4d0/)
! The set of model diffusion powers: alpha = 2.0 <==> Black Scholes
```

```
      real(kind(1d0)) :: alpha(3) = (/2.0d0, 1.0d0, 0.0d0/)
! Time values for the options
      integer, parameter :: nt = 3
      real(kind(1d0)) :: time(nt)=(/1.d0/12., 4.d0/12., 7.d0/12./)
! Values of the min and max underlying values modeled
      real(kind(1d0)) :: x_min = 0.0d0, x_max = 60.0d0
! Value of the interest rate and continuous dividend
      real(kind(1d0)) :: r = 0.05d0, dividend = 0.0d0
! Values of the underlying where evaluations are made
      integer, parameter :: nv = 3
      real(kind(1d0)) :: eval_points(nv) = &
                            (/19.0d0, 20.0d0, 21.0d0/)
! Define parameters for the integration step.
      integer, parameter :: nx = 121, nint = nx-1, n = 3*nx
      real(kind(1d0)) :: xgrid(nx), y(n,0:nt), yprime(n,0:nt)
      type(d_fcn_data) fcn_data
! Number of left/right boundary conditions
      integer, parameter :: nlbc = 3, nrbc = 3
! Further parameters for the integration step
      real(kind(1d0)) :: dx, dx2, pi, sqrt2pi
! used to calc derivatives
      real(kind(1d0)) :: epsfrac = .001d0
      character(len=6) :: greek_name(12) = (/&
             " Value", " Delta", " Gamma", " Theta",&
             " Charm", " Color", "  Vega", " Volga",&
             " Vanna", "   Rho", " Speed", "Speed2"/)
! Time values for the options
      real(kind(1d0)) :: rex(12), reavg(12)
      integer :: irect(12)
      integer :: i, i2, i3, j, ig, iquart, nout

      real(kind(1d0)) ::&
                  spline_values(nv,nt,12), spline_values1(nv,nt),&
                  spline_valuesp(nv,nt), spline_valuesm(nv,nt),&
                  spline_valuespp(nv,nt), spline_valuesmm(nv,nt),&
                  xgridp(nx), xgridm(nx),xgridpp(nx), xgridmm(nx),&
                  eval_pointsp(nv), eval_pointspp(nv),&
                  eval_pointsm(nv), eval_pointsmm(nv),&
                  BS_values(nv,nt,12), sVo_array(nt)

      call umach(2, nout)
! Allocate space inside the derived type for holding
! data values. These are for the evaluation routines.
      allocate(fcn_data % rdata (6))

      pi = const('pi')
      sqrt2pi = sqrt(2.0 * pi)
      dx2 = epsfrac * 0.5d0 * (x_min + x_max)

! Compute Constant Elasticity of Variance Model for Vanilla Call
! Define equally-spaced grid of points for the underlying price

      dx = (x_max - x_min)/real(nint)
      xgrid(1) = x_min
      xgrid(nx) = x_max
      do i = 2,nx-1
        xgrid(i) = xgrid(i-1) + dx
      end do

      write(nout,'(T05,A)') "Constant Elasticity of Variance"//&
                            " Model for Vanilla Call Option"
      write(nout,'(T10,"Interest Rate: ", F7.3, T38,'//&
                  '"Continuous Dividend: ", F7.3  )') r, dividend
      write(nout,'(T10,"Minimum and Maximum Prices of '//&
                  ' Underlying: ", 2F7.2)') x_min, x_max
      write(nout,'(T10,"Number of equally spaced spline knots:",'//&
```

```
                     'I4)') nx - 1
        write(nout,'(T10,"Number of unknowns: ",I4)') n
        write(nout,*)
        write(nout,'(/T10,"Time in Years Prior to Expiration: ",'//&
                     '2X,3F7.4)') time
        write(nout,'(T10,"Option valued at Underlying Prices:  ",'//&
                     '3F7.2)') eval_points
        write(nout,*)

  !
  ! iquart = 0 : derivatives estimated with 3-point fitted parabola
  ! iquart = 1 : derivatives estimated with 5-point fitted quartic
  !              polynomial
  !

        iquart = 0
        if (iquart == 0) then
          write(nout,'(T10,"3 point (parabolic) estimate of '//&
                      'parameter derivatives")')
        else
          write(nout,'(T10,"5 point (quartic) estimate of parameter'//&
                    ' derivatives")')
        end if
        write(nout, '(T10,"epsfrac = ", F11.8)') epsfrac

        irect = 0
        reavg = 0.0d0
        rex = 0.0d0

  ! alpha:  Black-Scholes
        do i2 = 1, 3
  ! Loop over volatility
          do i3 = 1, 3
  ! Loop over strike price
            call calc_Greeks(i2, i3, iquart)
          end do
        end do

        write(nout,*)
        do ig = 1, 12
          reavg(ig) = reavg(ig)/irect(ig)
          write (nout, '(" Greek: ", A6, ";  avg rel err: ",'//&
                        'F15.12, ";  max rel err: ", F15.12)')&
                        greek_name(ig), reavg(ig), rex(ig)
        end do

        contains

        subroutine calc_Greeks(volatility, strike_price, iquart)
        implicit none
        integer, intent(in) :: volatility, strike_price, iquart
      ! Local variables
        integer :: i1 = 1, j, iSderiv, gNi, l, k
        integer :: nt = 3
        real(kind(1d0)) :: x_maxp, x_maxm, x_maxpp, x_maxmm
        real(kind(1d0)) :: eps, tau, sigsqtau, sqrt_sigsqtau, sigsq
        real(kind(1d0)) :: d1, d2, n01pdf_d1, nu, relerr, relerrmax
        real(kind(1d0)) :: sVo, BSVo, S

        if ((volatility == 1) .and. (strike_price == 1)) then
          write(nout,*)
          write(nout,'(/T10,"Strike = ",F5.2,", Sigma =", F5.2,'//&
                      '", Alpha =",F5.2,":")') ks(strike_price),&
                      sigma(volatility), alpha(i1)
          write(nout,*)
          write(nout,'(T10,"years to expiration: ", 3F7.4)')&
```

```
                    (time(j), j=1,3)
          write(nout,*)
        end if

        fcn_data % rdata = (/ks(strike_price), x_max,&
                sigma(volatility), alpha(i1), r, dividend/)

        call feynman_kac(xgrid, time, nlbc, nrbc, fkcoef,&
                         fkinitcond, fkbc, y, yprime,&
                         FCN_DATA = fcn_data)

! Compute Value, Delta, Gamma, Theta, Charm and Color
        do l = 0,2
          do i=1,NT
            spline_values(:,i,l+1) = hqsval(eval_points, xgrid,&
                                            y(:,i), IDERIV=l)
            spline_values(:,i,l+4) = hqsval(eval_points, xgrid,&
                                            yprime(:,i), IDERIV=l)
          end do
        end do
! Signs for Charm and Color must be inverted because FEYNMAN_KAC
! computes -d/dt instead of d/dt
        spline_values(:,:,5:6) = -spline_values(:,:,5:6)

! Speed2
        do i=1,nt
          spline_values(:,i,12) = hqsval(eval_points, xgrid, Y(:,i),&
                                         IDERIV=3)
        end do

! Compute Vega, Volga, Vanna, Rho, Speed
!       l =    7     8      9     10    11
        do l = 7,11
          xgridp = xgrid
          xgridm = xgrid
          eval_pointsp = eval_points
          eval_pointsm = eval_points
          x_maxp = x_max
          x_maxm = x_max
          fcn_data % rdata(3) = sigma(volatility)
          fcn_data % rdata(5) = r
          iSderiv = 0
          if (l == 9) iSderiv = 1 ! Vanna
          if (l == 11) iSderiv = 2 ! Speed
          if (l == 10) then
            fcn_data % rdata(5) = r * (1.0 + epsfrac) ! Rho
          else if (l < 10) then
            fcn_data % rdata(3) = sigma(volatility) * (1.0 + epsfrac)
          end if
            if (l == 11) then
               xgridp = xgrid + dx2
               xgridm = xgrid - dx2
               eval_pointsp = eval_points + dx2
               eval_pointsm = eval_points - dx2
               x_maxp = x_max + dx2
               x_maxm = x_max - dx2
            end if
            fcn_data % rdata(2) = x_maxp
            call feynman_kac(xgridp, time, nlbc, nrbc, fkcoef,&
                        fkinitcond, fkbc, y, yprime,&
                        FCN_DATA = fcn_data)
            do i=1,nt
              spline_valuesp(:,i) = hqsval(eval_pointsp, xgridp,&
                                           y(:,i), IDERIV=iSderiv)
            end do
```

```
          if (l == 10) then
             fcn_data % rdata(5) = r * (1.0 - epsfrac) ! Rho
          else if (l < 10) then
             fcn_data % rdata(3) = sigma(volatility) *&
                                   (1.0 - epsfrac)
          end if
          fcn_data % rdata(2) = x_maxm
! calculate spline values for sigmaM = sigmai2-1*(1. - epsfrac) or
! rM = r*(1. - epsfrac):
          call feynman_kac(xgridm, time, nlbc, nrbc, fkcoef,&
                           fkinitcond, fkbc, y, yprime,&
                           FCN_DATA = fcn_data)
          do i=1,NT
            spline_valuesm(:,i) = hqsval(eval_pointsm, xgridm,&
                                         y(:,i), IDERIV=iSderiv)
          end do

          if (iquart == 1) then
            xgridpp = xgrid
            xgridmm = xgrid
            eval_pointspp = eval_points
            eval_pointsmm = eval_points
            x_maxpp = x_max
            x_maxmm = x_max

            if (l == 11) then  ! Speed
              xgridpp = xgrid + 2.0 * dx2
              xgridmm = xgrid - 2.0 * dx2
              eval_pointspp = eval_points + 2.0 * dx2
              eval_pointsmm = eval_points - 2.0 * dx2
              x_maxpp = x_max + 2.0 * dx2
              x_maxmm = x_max - 2.0 * dx2
            end if

            fcn_data % rdata(2) = x_maxpp
            if (l == 10) then
! calculate spline values for rPP = r*(1. + 2.*epsfrac):
              fcn_data % rdata(5) = r * (1.0 + 2.0 * epsfrac)
            else if (l < 10) then
! calculate spline values for sigmaPP = sigma(i2)*(1. + 2.*epsfrac):
              fcn_data % rdata(3) = sigma(volatility) *&
                                    (1.0 + 2.0 * epsfrac)
            end if
            call feynman_kac (xgridpp, time, nlbc, nrbc, fkcoef,&
                              fkinitcond, fkbc, y, yprime,&
                              FCN_DATA = fcn_data)

            do i=1,nt
              spline_valuespp(:,i) = hqsval(eval_pointspp, xgridpp,&
                                            Y(:,i), IDERIV=iSderiv)
            end do

            fcn_data % rdata(2) = x_maxmm
! calculate spline values for sigmaMM = sigmai2-1*(1. - 2.*epsfrac)
! or rMM = r*(1. - 2.*epsfrac)
            if (l == 10) then
              fcn_data % rdata(5) = r * (1.0 - 2.0 * epsfrac)
            else if (l < 10) then
              fcn_data % rdata(3) = sigma(volatility) *&
                                   (1.0 - 2.0 * epsfrac)
            end if
            call feynman_kac (xgridmm, time, nlbc, nrbc, fkcoef,&
                              fkinitcond, fkbc, y, yprime,&
                              FCN_DATA = fcn_data)

            do i=1,nt
```

```
               spline_valuesmm(:,i) = hqsval(eval_pointsmm, xgridmm,&
                                              y(:,i), IDERIV=iSderiv)
             end do
           end if ! if (iquart == 1)

           if (l /= 8) then
             eps = sigma(volatility) * epsfrac
             if (l == 10) eps = r * epsfrac ! Rho
             if (l == 11) eps = dx2 ! Speed

             spline_values(:,:,l) = &
                (spline_valuesp - spline_valuesm) / (2.0 * eps)
             if (iquart /= 0)  then
               spline_values1 =&
                 (spline_valuespp - spline_valuesmm) /(4.0 * eps)
               spline_values(:,:,l)  =&
                 (4.0 * spline_values(:,:,l) - spline_values1) / 3.0
             end if
           end if

           if (l == 8) then ! Volga
             eps = sigma(volatility) * epsfrac
             spline_values(:,:,l) =&
                  (spline_valuesp + spline_valuesm - 2.0 * &
                   spline_values(:,:,l)) / (eps * eps)

              if (iquart /= 0) then
                spline_values1 =&
                  (spline_valuespp + spline_valuesmm - 2.0 * &
                    spline_values(:,:,l)) / (4.0 * eps * eps)
                spline_values(:,:,l) = &
                 (4.0 * spline_values(:,:,l) - spline_values1) / 3.0
           end if
         end if
       end do
! Evaluate BS solution at vector eval_points,
! at each time value prior to expiration.

       do i = 1,nt
!
!  Black-Scholes (BS) European call option
!  value = ValBSEC(S,t) = exp(-q*tau)*S*N01CDF(d1) -
!                         exp(-r*tau)*K*N01CDF(d2),
!  where:
!    tau = time to maturity = T - t;
!    q = annual dividend yield;
!    r = risk free rate;
!    K = strike price;
!    S = stock price;
!    N01CDF(x) = N(0,1)_CDF(x);
!    d1 = ( log( S/K ) +
!         ( r - q + 0.5*sigma**2 )*tau ) /
!         ( sigma*sqrt(tau) );
!    d2 = d1 - sigma*sqrt(tau)
!
! BS option values for tau = time(i):
         tau = time(i)
         sigsqtau = (sigma(volatility)**2) * tau
         sqrt_sigsqtau = sqrt(sigsqtau)
         sigsq = sigma(volatility) * sigma(volatility)
         do j = 1, nv
! Values of the underlying price where evaluations are made:
           S = eval_points(j)
           d1 = (log(S / ks(strike_price)) + (r - dividend)&
                 * tau + 0.5 * sigsqtau) / sqrt_sigsqtau
           n01pdf_d1 = exp((-0.5) * d1 * d1) / sqrt2pi
```

```
            nu = exp((-dividend) * tau) * S * n01pdf_d1 * sqrt(tau)

            d2 = d1 - sqrt_sigsqtau
            BS_values(j,i,1) = exp((-dividend) * tau) * S *&
                                anordf(d1) - exp((-r) * tau) *&
                                ks(strike_price) * anordf(d2)
 ! greek = Rho
            BS_values(j,i,10) = exp((-r) * tau) * ks(strike_price) *&
                                  tau * anordf(d2)
 ! greek = Vega
            BS_values(j,i,7) = nu
 ! greek = Volga
            BS_values(j,i,8) = nu * d1 * d2 / sigma(volatility)
 ! greek = delta
            BS_values(j,i,2) = exp((-dividend) * tau) * anordf(d1)
 ! greek = Vanna
            BS_values(j,i,9) = (nu / S) * (1.0 - d1 / sqrt_sigsqtau)
 ! greek = dgamma
            BS_values(j,i,3) = exp((-dividend) * tau) *&
                               n01pdf_d1 /(S * sqrt_sigsqtau)
 ! greek = speed
            BS_values(j,i,11) = (-exp((-dividend) * tau)) *&
                       n01pdf_d1 * (1.0 + d1 / sqrt_sigsqtau)&
                       / (S * S * sqrt_sigsqtau)
 ! greek = speed
            BS_values(j,i,12) = (-exp((-dividend) * tau)) * &
                     n01pdf_d1 * (1.0 + d1 / sqrt_sigsqtau) / &
                     (S * S * sqrt_sigsqtau)
            d2 = d1 - sqrt_sigsqtau
 ! greek = theta
            BS_values(j,i,4) = exp((-dividend) * tau) * S * &
                        (dividend * anordf(d1) - 0.5 * sigsq * &
                         n01pdf_d1 / sqrt_sigsqtau) - r * &
                         exp((-r) * tau) * ks(strike_price) * &
                         anordf(d2)
 ! greek = charm
            BS_values(j,i,5) = exp((-dividend) * tau) * ((-dividend)&
                         * anordf(d1) + n01pdf_d1 *&
                        ((r - dividend) * tau - 0.5 * d2 *&
                         sqrt_sigsqtau) / (tau * sqrt_sigsqtau))
 ! greek = color
            BS_values(j,i,6) = &
                        (-exp((-dividend) * tau)) * n01pdf_d1 *&
                        (2.0 * dividend * tau + 1.0 + d1 *&
                        (2.0 * (r - dividend) * tau - d2 *&
                         sqrt_sigsqtau) / sqrt_sigsqtau) / &
                        (2.0 * S * tau * sqrt_sigsqtau)
          end do
        end do

        do l=1,12
          relerrmax = 0.0
          do i = 1,nv
            do j = 1,nt
              sVo = spline_values(i,j,l)
              BSVo = BS_values(i,j,l)
              relerr = abs((sVo - BSVo) / BSVo)
              if (relerr > relerrmax) relerrmax = relerr
              reavg(l) = reavg(l) + relerr
              irect(l) = irect(l) + 1
            end do
          end do
          if (relerrmax > rex(l)) rex(l) = relerrmax

          if ((volatility == 1) .and. (strike_price == 1)) then
            do i=1,nv
```

```
              sVo_array(1:nt) = spline_values(i,1:nt,l)
              write(nout,'("underlying price: ", F4.1,"; FK ",'//&
                    'A6,": ", 3(F13.10,TR1))') eval_points(i),&
                    greek_name(l),&
                    (sVo_array(k), k=1,nt)
              write(nout, '(T25, "BS ", A6,": ", 3(F13.10,TR1))')&
                    greek_name(l), (BS_values(i,k,l), k=1,nt)
             end do
          end if
        end do
        end subroutine calc_Greeks
        end

  ! These functions and routines  define the coefficients, payoff and boundary conditions.
        function fkcoef (x, tx, iflag, fcn_data)
        use mp_types
        implicit none
        real(kind(1d0)), intent(in) :: x, tx
        integer, intent(inout) :: iflag
        type(d_fcn_data), optional :: fcn_data
        real(kind(1d0)) :: fkcoef

        real(kind(1d0)) :: sigma, interest_rate, alpha, dividend,&
                           half = 0.5d0
        sigma = fcn_data % rdata(3)
        alpha = fcn_data % rdata(4)
        interest_rate = fcn_data % rdata(5)
        dividend = fcn_data % rdata(6)
        select case (iflag)
          case (1)
  ! The coefficient derivative d(sigma)/dx
            fkcoef = half*alpha*sigma*x**(alpha*half-1.0d0)
  ! The coefficient sigma(x)
          case (2)
            fkcoef = sigma*x**(alpha*half)
          case (3)
  ! The coefficient mu(x)
            fkcoef = (interest_rate - dividend) * x
          case (4)
  ! The coefficient kappa(x)
            fkcoef = interest_rate
        end select
  ! Note that there is no time dependence
        iflag = 0
        return
        end function fkcoef

        function fkinitcond(x, fcn_data)
        use mp_types
        implicit none
        real(kind(1d0)), intent(in) :: x
        type (d_fcn_data), optional :: fcn_data
        real(kind(1d0)) :: fkinitcond
        real(kind(1d0)) :: zero = 0.0d0
        real(kind(1d0)) :: strike_price

        strike_price = fcn_data % rdata(1)
  ! The payoff function
        fkinitcond = max(x - strike_price, zero)
        return
        end function fkinitcond

        subroutine fkbc (tx, iflag, bccoefs, fcn_data)
        use mp_types
        implicit none
        real(kind(1d0)), intent(in) :: tx
```

```
      integer, intent(inout) :: iflag
      real(kind(1d0)), dimension(:,:), intent(out) :: bccoefs
      type (d_fcn_data), optional :: fcn_data
      real(kind(1d0)) :: x_max, df, interest_rate, strike_price

      strike_price = fcn_data % rdata(1)
      x_max = fcn_data % rdata(2)
      interest_rate = fcn_data % rdata(5)
      select case (iflag)
        case (1)
          bccoefs(1,1:4) = (/1.0d0, 0.0d0, 0.0d0, 0.0d0/)
          bccoefs(2,1:4) = (/0.0d0, 1.0d0, 0.0d0, 0.0d0/)
          bccoefs(3,1:4) = (/0.0d0, 0.0d0, 1.0d0, 0.0d0/)
! Note no time dependence at left end
          iflag = 0
        case (2)
          df = exp(interest_rate * tx)
          bccoefs(1,1:4) = (/1.0d0, 0.0d0, 0.0d0, x_max -&
                              df*strike_price/)
          bccoefs(2,1:4) = (/0.0d0, 1.0d0, 0.0d0, 1.0d0/)
          bccoefs(3,1:4) = (/0.0d0, 0.0d0, 1.0d0, 0.0d0/)
      end select
      end subroutine fkbc
```

Output

```
     Constant Elasticity of Variance Model for Vanilla Call Option
          Interest Rate:   0.050      Continuous Dividend:   0.000
          Minimum and Maximum Prices of Underlying:    0.00  60.00
          Number of equally spaced spline knots:  120
          Number of unknowns:  363


          Time in Years Prior to Expiration:    0.0833 0.3333 0.5833
          Option valued at Underlying Prices:    19.00  20.00  21.00

          3 point (parabolic) estimate of parameter derivatives
          epsfrac =  0.00100000


          Strike =15.00 Sigma = 0.20 Alpha = 2.00:

          years to expiration:  0.0833 0.3333 0.5833

 underlying price: 19.0; FK  Value:  4.0623732450  4.2575924184  4.4733805278
                         BS  Value:  4.0623732509  4.2575929678  4.4733814062
 underlying price: 20.0; FK  Value:  5.0623700127  5.2505145764  5.4492418798
                         BS  Value:  5.0623700120  5.2505143129  5.4492428547
 underlying price: 21.0; FK  Value:  6.0623699727  6.2485587059  6.4385718831
                         BS  Value:  6.0623699726  6.2485585270  6.4385720688
 underlying price: 19.0; FK  Delta:  0.9999864098  0.9877532309  0.9652249945
                         BS  Delta:  0.9999863811  0.9877520034  0.9652261127
 underlying price: 20.0; FK  Delta:  0.9999998142  0.9964646548  0.9842482622
                         BS  Delta:  0.9999998151  0.9964644003  0.9842476147
 underlying price: 21.0; FK  Delta:  0.9999999983  0.9990831687  0.9932459040
                         BS  Delta:  0.9999999985  0.9990834124  0.9932451927
 underlying price: 19.0; FK  Gamma:  0.0000543456  0.0144908955  0.0264849216
                         BS  Gamma:  0.0000547782  0.0144911447  0.0264824761
 underlying price: 20.0; FK  Gamma:  0.0000008315  0.0045912854  0.0129288434
                         BS  Gamma:  0.0000008437  0.0045925328  0.0129280372
 underlying price: 21.0; FK  Gamma:  0.0000000080  0.0012817012  0.0058860348
                         BS  Gamma:  0.0000000077  0.0012818272  0.0058865489
 underlying price: 19.0; FK  Theta: -0.7472631891 -0.8301000450 -0.8845209253
                         BS  Theta: -0.7472638978 -0.8301108199 -0.8844992143
 underlying price: 20.0; FK  Theta: -0.7468881086 -0.7706770630 -0.8152217385
                         BS  Theta: -0.7468880640 -0.7706789470 -0.8152097697
```

```
underlying price: 21.0; FK  Theta: -0.7468815742 -0.7479185416 -0.7728950748
                        BS  Theta: -0.7468815673 -0.7479153725 -0.7728982104
underlying price: 19.0; FK  Charm: -0.0014382828 -0.0879903285 -0.0843323992
                        BS  Charm: -0.0014397520 -0.0879913927 -0.0843403333
underlying price: 20.0; FK  Charm: -0.0000284881 -0.0364107814 -0.0547260337
                        BS  Charm: -0.0000285354 -0.0364209077 -0.0547074804
underlying price: 21.0; FK  Charm: -0.0000003396 -0.0126436426 -0.0313343015
                        BS  Charm: -0.0000003190 -0.0126437838 -0.0313252716
underlying price: 19.0; FK  Color:  0.0051622176  0.0685064195  0.0299871130
                        BS  Color:  0.0051777484  0.0684737183  0.0300398444
underlying price: 20.0; FK  Color:  0.0001188761  0.0355826975  0.0274292189
                        BS  Color:  0.0001205713  0.0355891884  0.0274307898
underlying price: 21.0; FK  Color:  0.0000015432  0.0143174420  0.0190897159
                        BS  Color:  0.0000015141  0.0143247729  0.0190752019
underlying price: 19.0; FK   Vega:  0.0003289870  0.3487168323  1.1153520921
                        BS   Vega:  0.0003295819  0.3487535501  1.1153536190
underlying price: 20.0; FK   Vega:  0.0000056652  0.1224632724  0.6032458218
                        BS   Vega:  0.0000056246  0.1224675413  0.6033084039
underlying price: 21.0; FK   Vega:  0.0000000623  0.0376974472  0.3028275297
                        BS   Vega:  0.0000000563  0.0376857196  0.3028629419
underlying price: 19.0; FK  Volga:  0.0286254576  8.3705173459 16.7944554708
                        BS  Volga:  0.0286064650  8.3691191978 16.8219823169
underlying price: 20.0; FK  Volga:  0.0007137402  4.2505025277 12.9315441466
                        BS  Volga:  0.0007186004  4.2519372748 12.9612638820
underlying price: 21.0; FK  Volga:  0.0000100364  1.7613083436  8.6626161799
                        BS  Volga:  0.0000097963  1.7617504949  8.6676581034
underlying price: 19.0; FK  Vanna: -0.0012418872 -0.3391850563 -0.6388552010
                        BS  Vanna: -0.0012431594 -0.3391932673 -0.6387423326
underlying price: 20.0; FK  Vanna: -0.0000244490 -0.1366771953 -0.3945466661
                        BS  Vanna: -0.0000244825 -0.1367114682 -0.3945405194
underlying price: 21.0; FK  Vanna: -0.0000002904 -0.0466333335 -0.2187406645
                        BS  Vanna: -0.0000002726 -0.0466323413 -0.2187858632
underlying price: 19.0; FK    Rho:  1.2447807022  4.8365676561  8.0884594648
                        BS    Rho:  1.2447806658  4.8365650322  8.0884502627
underlying price: 20.0; FK    Rho:  1.2448021850  4.8929216544  8.3041708173
                        BS    Rho:  1.2448021908  4.8929245641  8.3041638392
underlying price: 21.0; FK    Rho:  1.2448024992  4.9107294560  8.4114197621
                        BS    Rho:  1.2448024996  4.9107310444  8.4114199038
underlying price: 19.0; FK  Speed: -0.0002124684 -0.0156265453 -0.0179534748
                        BS  Speed: -0.0002123854 -0.0156192867 -0.0179536520
underlying price: 20.0; FK  Speed: -0.0000037247 -0.0055877024 -0.0097502607
                        BS  Speed: -0.0000037568 -0.0055859333 -0.0097472434
underlying price: 21.0; FK  Speed: -0.0000000385 -0.0017085830 -0.0048143174
                        BS  Speed: -0.0000000378 -0.0017082128 -0.0048130214
underlying price: 19.0; FK Speed2: -0.0002310655 -0.0156276977 -0.0179516855
                        BS Speed2: -0.0002123854 -0.0156192867 -0.0179536520
underlying price: 20.0; FK Speed2: -0.0000043215 -0.0055923924 -0.0097502997
                        BS Speed2: -0.0000037568 -0.0055859333 -0.0097472434
underlying price: 21.0; FK Speed2: -0.0000000475 -0.0017117661 -0.0048153107
                        BS Speed2: -0.0000000378 -0.0017082128 -0.0048130214

  Greek:  Value;  avg rel err:  0.000146171196;  max rel err:  0.009030737566
  Greek:  Delta;  avg rel err:  0.000035817272;  max rel err:  0.001158483076
  Greek:  Gamma;  avg rel err:  0.001088392379;  max rel err:  0.044845800289
  Greek:  Theta;  avg rel err:  0.000054196359;  max rel err:  0.001412847300
  Greek:  Charm;  avg rel err:  0.001213347059;  max rel err:  0.064576457415
  Greek:  Color;  avg rel err:  0.003323954467;  max rel err:  0.136355681544
  Greek:   Vega;  avg rel err:  0.001514753397;  max rel err:  0.106255126885
  Greek:  Volga;  avg rel err:  0.058531380389;  max rel err:  1.639564208085
  Greek:  Vanna;  avg rel err:  0.001061525805;  max rel err:  0.065629483069
  Greek:    Rho;  avg rel err:  0.000146868262;  max rel err:  0.009438788128
  Greek:  Speed;  avg rel err:  0.002065441607;  max rel err:  0.073086615101
  Greek: Speed2;  avg rel err:  0.008429883935;  max rel err:  0.255746328973
```

HQSVAL

This rank-1 array function evaluates a Hermite quintic spline or one of its derivatives for an array of input points. In particular, it computes solution values for the Feynman-Kac PDE handled by routine FEYNMAN_KAC.

Function Return Value

HQSVAL — Rank-1 array containing the values or derivatives of the Hermite quintic spline at the points given in array XVAL. (Output)
size = size(*XVAL*).

Required Arguments

XVAL — Rank-1 array containing the points at which the Hermite quintic spline is to be evaluated. (Input)
Let *NXVAL* = size(XVAL). The points in XVAL must lie within the range of array BREAK, i.e.
BREAK(1) ≤ XVAL(I) ≤ BREAK(*NXVAL*), I=1, …, *NXVAL*.

BREAK — Rank-1 array containing the breakpoints for the Hermite quintic spline representation. (Input)
When applied to the output from routine FEYNMAN_KAC, array BREAK is identical to array XGRID.
Let *NBREAK* = size(BREAK). *NBREAK* must be at least 2 and the values in BREAK must be in strictly increasing order.

COEFFS — Rank-1 array of size 3 * *NBREAK* containing the coefficients of the Hermite quintic spline representation. (Input)
When applied to the output arrays Y or YPRIME from routine FEYNMAN_KAC, array COEFFS is identical to one of the columns of arrays Y or YPRIME, respectively.

Optional Argument

IDERIV — Order of the derivative to be evaluated. (Input)
It is required that IDERIV = 0, 1, 2 or 3. Use 0 for the function itself, 1 for the first derivative, etc.
Default: IDERIV = 0.

FORTRAN 90 Interface

Generic: HQSVAL (XVAL, BREAK, COEFFS [, …])

Specific: The specific interface names are S_HQSVAL and D_HQSVAL.

Description

The Hermite quintic spline interpolation is done over the composite interval $[x_{min}, x_{max}]$, where `BREAK(I)` $= x_i$ are given by $(x_{min} =)\ x_1 < x_2 < \ldots < x_m\ (= x_{max})$.

The Hermite quintic spline function is constructed using three primary functions, defined by

$$
\begin{aligned}
b_0(z) &= -6z^5 + 15z^4 - 10z^3 + 1 = (1-z)^3(6z^2 + 3z + 1),\\
b_1(z) &= -3z^5 + 8z^4 - 6z^3 + z = (1-z)^3 z(3z+1),\\
b_2(z) &= \tfrac{1}{2}(-z^5 + 3z^4 - 3z^3 + z^2) = \tfrac{1}{2}(1-z)^3 z^2.
\end{aligned}
$$

For each

$$x \in [x_i, x_{i+1}],\ h_i = x_{i+1} - x_i,\ z_i = (x - x_i)/h_i,\ i = 1, \ldots, m-1,$$

the spline is locally defined by

$$
\begin{aligned}
H(x) &= y_{3i-2} b_0(z) + y_{3i+1} b_0(1-z) + h_i y_{3i-1} b_1(z)\\
&- h_i y_{3i+2} b_1(1-z) + h_i^2 y_{3i} b_2(z) + h_i^2 y_{3i+3} b_2(1-z),
\end{aligned}
$$

where

$$
\begin{aligned}
y_{3i-2} &= f(x_i),\\
y_{3i-1} &= (\partial f/\partial x)(x_i) = f_x(x_i),\\
y_{3i} &= (\partial^2 f/\partial x^2)(x_i) = f_{xx}(x_i),\quad i = 1, \ldots, m.
\end{aligned}
$$

are the values of a given twice continuously differentiable function f and its first two derivatives at the breakpoints. The approximating function $H(x)$ is twice continuously differentiable on $[x_{min}, x_{max}]$, whereas the third derivative is in general only continuous within the interior of the intervals $[x_i, x_{i+1}]$. From the local representation of $H(x)$ it follows that

$$
\begin{aligned}
H(x_i) &= f(x_i) = y_{3i-2},\\
H'(x_i) &= f'(x_i) = y_{3i-1},\\
H''(x_i) &= y_{3i},\ i = 1, \ldots, m
\end{aligned}
$$

The spline coefficients y_i, $i = 1, \ldots, 3m$ are stored as successive triplets in array `COEFFS`. For a given $w \in [x_{min}, x_{max}]$, `function HQSVAL` uses the information in `COEFFS` together with the values of b_0, b_1, b_2 and its derivatives at w to compute $H^{(d)}(w)$, $d = 0, \ldots 3$ using the local representation on the particular subinterval containing w.

When using arrays XGRID and Y(:,I) from routine FEYNMAN_KAC as input arrays BREAK and COEFFS, function HQSVAL allows for computation of approximate solutions f, f_x, f_{xx}, f_{xxx} to the Feynman-Kac PDE for IDERIV=0, 1, 2, 3, respectively. The solution values are evaluated at the array of points (XVAL(:),TGRID(I)) for I=1, ...,size(TGRID) and (XVAL(:),0) for I=0 . Similarly, using arrays XGRID and YPRIME(:,I) allows for computation of approximate solutions $f_t, f_{tx}, f_{txx}, f_{txxx}$ to the Feynman-Kac PDE.

Example: Exact Interpolation with Hermite Quintic

Consider function $f(x) = x^5$, a polynomial of degree 5, on the interval [−1,1] with breakpoints ±1. Then, the end derivative values are

$$y_1 = f\left(-1\right) = -1,\ y_2 = f'\left(-1\right) = 5,\ y_3 = f''\left(-1\right) = -20$$

and

$$y_4 = f\left(1\right) = 1,\ y_5 = f'\left(1\right) = 5,\ y_6 = f''\left(1\right) = 20$$

Since the Hermite quintic interpolates all polynomials up to degree 5 exactly, the spline interpolation on [−1,1] must agree with the exact function values up to rounding errors.

```
      use hqsval_int
      use umach_int

      implicit none

      integer :: i, nout
      real(kind(1e0)) :: break(2), xval(7), coeffs(6), interpolant(7)

! Define arrays
      break = (/ -1.0, 1.0 /)
      xval = (/ -0.75, -0.5, -0.25, 0.0, 0.25, 0.5, 0.75 /)
      coeffs = (/ -1.0, 5.0, -20.0, 1.0, 5.0, 20.0 /)

! Compute interpolant
      interpolant = hqsval(xval, break, coeffs)

      call umach(2, nout)
! Compare interpolant with exact function.
      write(nout,'(A6,A10,A15,A10)')'x', 'F(x)', 'Interpolant', 'Error'
      write(nout,'(f8.3,f9.3,f11.3,f15.7)') (xval(i), F(xval(i)), &
              interpolant(i), abs(F(xval(i))-interpolant(i)), &
              i=1,7)

      contains
      function F(x)
        implicit none
        real(kind(1e0)) :: F, x

        F = x**5
        return
      end function F
      end
```

Output

```
     x       F(x)    Interpolant     Error
  -0.750   -0.237      -0.237      0.0000000
  -0.500   -0.031      -0.031      0.0000000
  -0.250   -0.001      -0.001      0.0000000
   0.000    0.000       0.000      0.0000000
   0.250    0.001       0.001      0.0000000
   0.500    0.031       0.031      0.0000000
   0.750    0.237       0.237      0.0000000
```

FPS2H

more...

Solves Poisson's or Helmholtz's equation on a two-dimensional rectangle using a fast Poisson solver based on the HODIE finite-difference scheme on a uniform mesh.

Required Arguments

PRHS — User-supplied FUNCTION to evaluate the right side of the partial differential equation. The form is PRHS(X, Y), where

X – X-coordinate value. (Input)

Y – Y-coordinate value. (Input)

PRHS – Value of the right side at (X, Y). (Output)

PRHS must be declared EXTERNAL in the calling program.

BRHS — User-supplied FUNCTION to evaluate the right side of the boundary conditions. The form is BRHS(ISIDE, X, Y), where

ISIDE – Side number. (Input)

See IBCTY below for the definition of the side numbers.

X – X-coordinate value. (Input)

Y – Y-coordinate value. (Input)

BRHS – Value of the right side of the boundary condition at (X, Y). (Output)

BRHS must be declared EXTERNAL in the calling program.

COEFU — Value of the coefficient of U in the differential equation. (Input)

NX — Number of grid lines in the X-direction. (Input)
NX must be at least 4. See Comment 2 for further restrictions on NX.

NY — Number of grid lines in the Y-direction. (Input)
NY must be at least 4. See Comment 2 for further restrictions on NY.

AX — The value of X along the left side of the domain. (Input)

BX — The value of X along the right side of the domain. (Input)

AY — The value of Y along the bottom of the domain. (Input)

BY — The value of Y along the top of the domain. (Input)

IBCTY — Array of size 4 indicating the type of boundary condition on each side of the domain or that the solution is periodic. (Input)
The sides are numbered 1 to 4 as follows:

Side	Location
1 – Right	(X = BX)
2 – Bottom	(Y = AY)
3 – Left	(X = AX)
4 – Top	(Y = BY)

There are three boundary condition types.

IBCTY	Boundary Condition
1	Value of U is given. (Dirichlet)
2	Value of dU/dX is given (sides 1 and/or 3). (Neumann) Value of dU/dY is given (sides 2 and/or 4).
3	Periodic.

U — Array of size NX by NY containing the solution at the grid points. (Output)

Optional Arguments

IORDER — Order of accuracy of the finite-difference approximation. (Input)
It can be either 2 or 4. Usually, IORDER = 4 is used.
Default: IORDER = 4.

LDU — Leading dimension of U exactly as specified in the dimension statement of the calling program. (Input)
Default: LDU = size (U,1).

FORTRAN 90 Interface

Generic: CALL FPS2H (PRHS, BRHS, COEFU, NX, NY, AX, BX, AY, BY, IBCTY, U [, …])

Specific: The specific interface names are `S_FPS2H` and `D_FPS2H`.

FORTRAN 77 Interface

Single: CALL FPS2H (PRHS, BRHS, COEFU, NX, NY, AX, BX, AY, BY, IBCTY, IORDER, U, LDU)

Double: The double precision name is DFPS2H.

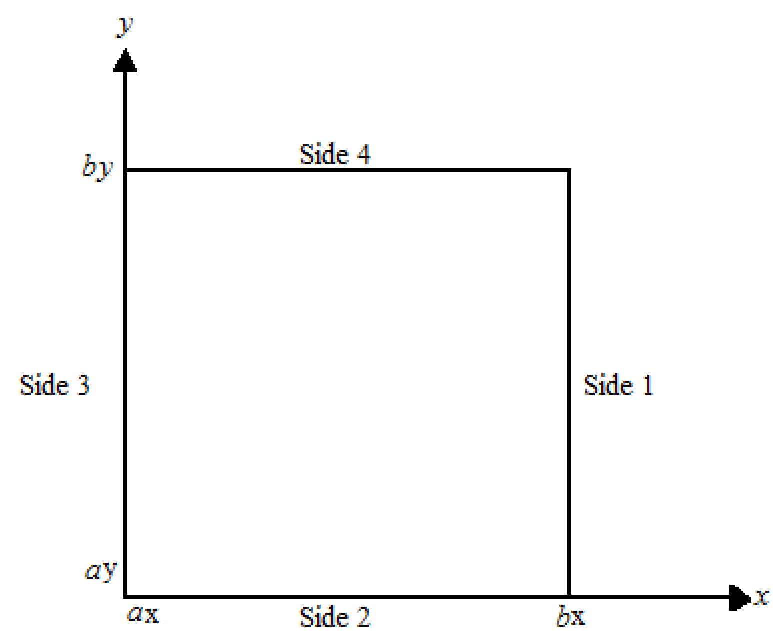
Description

Let c = COEFU, a_x = AX, b_x = BX, a_y = AY, b_y = BY, n_x = NX and n_y = NY.

FPS2H is based on the code HFFT2D by Boisvert (1984). It solves the equation

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + cu = p$$

on the rectangular domain $(a_x, b_x) \times (a_y, b_y)$ with a user-specified combination of Dirichlet (solution prescribed), Neumann (first-derivative prescribed), or periodic boundary conditions. The sides are numbered clockwise, starting with the right side.



When $c = 0$ and only Neumann or periodic boundary conditions are prescribed, then any constant may be added to the solution to obtain another solution to the problem. In this case, the solution of minimum ∞-norm is returned.

The solution is computed using either a second-or fourth-order accurate finite-difference approximation of the continuous equation. The resulting system of linear algebraic equations is solved using fast Fourier transform techniques. The algorithm relies upon the fact that $n_x - 1$ is highly composite (the product of small primes). For details of the algorithm, see Boisvert (1984). If $n_x - 1$ is highly composite then the execution time of FPS2H is proportional to $n_x n_y \log_2 n_x$. If evaluations of $p(x, y)$ are inexpensive, then the difference in running time between IORDER = 2 and IORDER = 4 is small.

Comments

1. Workspace may be explicitly provided, if desired, by use of F2S2H/DF2S2H. The reference is:

   CALL F2S2H (PRHS, BRHS, COEFU, NX, NY, AX, BX, AY, BY, IBCTY, IORDER, U, LDU, UWORK, WORK)

   The additional arguments are as follows:

   UWORK — Work array of size NX + 2 by NY + 2. If the actual dimensions of U are large enough, then U and UWORK can be the same array.

   WORK — Work array of length
   (NX + 1)(NY + 1)(IORDER − 2)/2 + 6(NX + NY) + NX/2 + 16.

2. The grid spacing is the distance between the (uniformly spaced) grid lines. It is given by the formulas HX = (BX − AX)/(NX − 1) and HY = (BY − AY)/(NY − 1). The grid spacings in the X and Y directions must be the same, i.e., NX and NY must be such that HX equals HY. Also, as noted above, NX and NY must both be at least 4. To increase the speed of the fast Fourier transform, NX − 1 should be the product of small primes. Good choices are 17, 33, and 65.

3. If −COEFU is nearly equal to an eigenvalue of the Laplacian with homogeneous boundary conditions, then the computed solution might have large errors.

Example

In this example, the equation

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + 3u = -2\sin(x + 2y) + 16e^{2x+3y}$$

with the boundary conditions $\partial u/\partial y = 2\cos(x + 2y) + 3\exp(2x + 3y)$ on the bottom side and $u = \sin(x + 2y) + \exp(2x + 3y)$ on the other three sides. The domain is the rectangle $[0, 1/4] \times [0, 1/2]$. The output of FPS2H is a 17 $\times$ 33 table of U values. The quadratic interpolation routine QD2VL is used to print a table of values.

```
      USE FPS2H_INT
      USE QD2VL_INT
```

```
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    NCVAL, NX, NXTABL, NY, NYTABL
      PARAMETER  (NCVAL=11, NX=17, NXTABL=5, NY=33, NYTABL=5)
!
      INTEGER    I, IBCTY(4), IORDER, J, NOUT
      REAL       AX, AY, BRHS, BX, BY, COEFU, ERROR, FLOAT, PRHS, &
                TRUE, U(NX,NY), UTABL, X, XDATA(NX), Y, YDATA(NY)
      INTRINSIC  FLOAT
      EXTERNAL   BRHS, PRHS
!                                  Set rectangle size
      AX = 0.0
      BX = 0.25
      AY = 0.0
      BY = 0.50
!                                  Set boundary condition types
      IBCTY(1) = 1
      IBCTY(2) = 2
      IBCTY(3) = 1
      IBCTY(4) = 1
!                                  Coefficient of U
      COEFU = 3.0
!                                  Order of the method
      IORDER = 4
!                                  Solve the PDE
      CALL FPS2H (PRHS, BRHS, COEFU, NX, NY, AX, BX, AY, BY, IBCTY, U)
!                                  Setup for quadratic interpolation
      DO 10  I=1, NX
         XDATA(I) = AX + (BX-AX)*FLOAT(I-1)/FLOAT(NX-1)
   10 CONTINUE
      DO 20  J=1, NY
         YDATA(J) = AY + (BY-AY)*FLOAT(J-1)/FLOAT(NY-1)
   20 CONTINUE
!                                  Print the solution
      CALL UMACH (2, NOUT)
      WRITE (NOUT,'(8X,A,11X,A,11X,A,8X,A)') 'X', 'Y', 'U', 'Error'
      DO 40  J=1, NYTABL
         DO 30  I=1, NXTABL
            X     = AX + (BX-AX)*FLOAT(I-1)/FLOAT(NXTABL-1)
            Y     = AY + (BY-AY)*FLOAT(J-1)/FLOAT(NYTABL-1)
            UTABL = QD2VL(X,Y,XDATA,YDATA,U)
            TRUE  = SIN(X+2.*Y) + EXP(2.*X+3.*Y)
            ERROR = TRUE - UTABL
            WRITE (NOUT,'(4F12.4)') X, Y, UTABL, ERROR
   30 CONTINUE
   40 CONTINUE
      END
!
      REAL FUNCTION PRHS (X, Y)
      REAL       X, Y
!
      REAL       EXP, SIN
      INTRINSIC  EXP, SIN
!                                  Define right side of the PDE
      PRHS = -2.*SIN(X+2.*Y) + 16.*EXP(2.*X+3.*Y)
      RETURN
      END
!
      REAL FUNCTION BRHS (ISIDE, X, Y)
      INTEGER    ISIDE
      REAL       X, Y
!
      REAL       COS, EXP, SIN
      INTRINSIC  COS, EXP, SIN
!                                  Define the boundary conditions
```

```
      IF (ISIDE .EQ. 2) THEN
         BRHS = 2.*COS(X+2.*Y) + 3.*EXP(2.*X+3.*Y)
      ELSE
         BRHS = SIN(X+2.*Y) + EXP(2.*X+3.*Y)
      END IF
      RETURN
      END
```

Output

```
    X            Y            U         Error
 0.0000       0.0000       1.0000       0.0000
 0.0625       0.0000       1.1956       0.0000
 0.1250       0.0000       1.4087       0.0000
 0.1875       0.0000       1.6414       0.0000
 0.2500       0.0000       1.8961       0.0000
 0.0000       0.1250       1.7024       0.0000
 0.0625       0.1250       1.9562       0.0000
 0.1250       0.1250       2.2345       0.0000
 0.1875       0.1250       2.5407       0.0000
 0.2500       0.1250       2.8783       0.0000
 0.0000       0.2500       2.5964       0.0000
 0.0625       0.2500       2.9322       0.0000
 0.1250       0.2500       3.3034       0.0000
 0.1875       0.2500       3.7148       0.0000
 0.2500       0.2500       4.1720       0.0000
 0.0000       0.3750       3.7619       0.0000
 0.0625       0.3750       4.2163       0.0000
 0.1250       0.3750       4.7226       0.0000
 0.1875       0.3750       5.2878       0.0000
 0.2500       0.3750       5.9199       0.0000
 0.0000       0.5000       5.3232       0.0000
 0.0625       0.5000       5.9520       0.0000
 0.1250       0.5000       6.6569       0.0000
 0.1875       0.5000       7.4483       0.0000
 0.2500       0.5000       8.3380       0.0000
```

FPS3H

more...

Solves Poisson's or Helmholtz's equation on a three-dimensional box using a fast Poisson solver based on the HODIE finite-difference scheme on a uniform mesh.

Required Arguments

PRHS — User-supplied FUNCTION to evaluate the right side of the partial differential equation. The form is PRHS (X, Y, Z), where

X – The *x*-coordinate value. (Input)

Y – The *y*-coordinate value. (Input)

Z – The *z*-coordinate value. (Input)

PRHS – Value of the right side at (X, Y, Z). (Output)

PRHS must be declared EXTERNAL in the calling program.

BRHS — User-supplied FUNCTION to evaluate the right side of the boundary conditions. The form is BRHS (ISIDE, X, Y, Z), where

ISIDE – Side number. (Input)

See IBCTY for the definition of the side numbers.

X – The *x*-coordinate value. (Input)

Y – The *y*-coordinate value. (Input)

Z – The *z*-coordinate value. (Input)

BRHS – Value of the right side of the boundary condition at (X, Y, Z). (Output)

BRHS must be declared EXTERNAL in the calling program.

COEFU — Value of the coefficient of U in the differential equation. (Input)

NX — Number of grid lines in the *x*-direction. (Input)
NX must be at least 4. See Comment 2 for further restrictions on NX.

NY — Number of grid lines in the *y*-direction. (Input)
NY must be at least 4. See Comment 2 for further restrictions on NY.

NZ — Number of grid lines in the *z*-direction. (Input)
NZ must be at least 4. See Comment 2 for further restrictions on NZ.

AX — Value of X along the left side of the domain. (Input)

BX — Value of X along the right side of the domain. (Input)

AY — Value of Y along the bottom of the domain. (Input)

BY — Value of Y along the top of the domain. (Input)

AZ — Value of Z along the front of the domain. (Input)

BZ — Value of Z along the back of the domain. (Input)

IBCTY — Array of size 6 indicating the type of boundary condition on each face of the domain or that the solution is periodic. (Input)
The sides are numbers 1 to 6 as follows:

Side	Location
1 − Right	(X = BX)
2 − Bottom	(Y = AY)
3 − Left	(X = AX)
4 − Top	(Y = BY)
5 − Front	(Z = BZ)
6 − Back	(Z = AZ)

There are three boundary condition types.

IBCTY	Boundary Condition
1	Value of U is given. (Dirichlet)
2	Value of dU/dX is given (sides 1 and/or 3). (Neumann) Value of dU/dY is given (sides 2 and/or 4). Value of dU/dZ is given (sides 5 and/or 6).
3	Periodic.

U — Array of size NX by NY by NZ containing the solution at the grid points. (Output)

Optional Arguments

IORDER — Order of accuracy of the finite-difference approximation. (Input)
It can be either 2 or 4. Usually, IORDER = 4 is used.
Default: IORDER = 4.

LDU — Leading dimension of U exactly as specified in the dimension statement of the calling program. (Input)
Default: LDU = size (U,1).

MDU — Middle dimension of U exactly as specified in the dimension statement of the calling program. (Input)
Default: MDU = size (U,2).

FORTRAN 90 Interface

Generic: CALL FPS3H (PRHS, BRHS, COEFU, NX, NY, NZ, AX, BX, AY, BY, AZ, BZ, IBCTY, U [, …])

Specific: The specific interface names are S_FPS3H and D_FPS3H.

FORTRAN 77 Interface

Single: CALL FPS3H (PRHS, BRHS, COEFU, NX, NY, NZ, AX, BX, AY, BY, AZ, BZ, IBCTY, IORDER, U, LDU, MDU)

Double: The double precision name is DFPS3H.

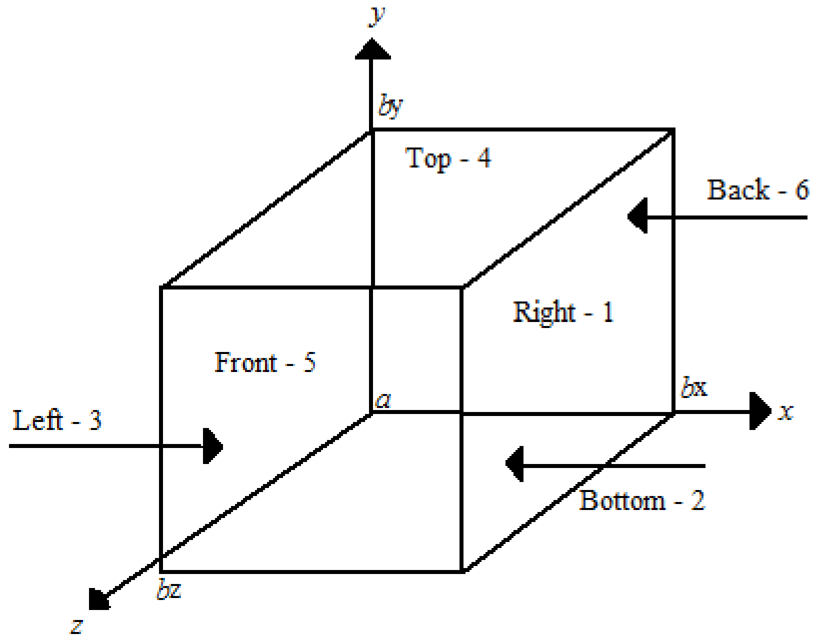
Description

Let c = COEFU, a_x = AX, b_x = BX, n_x = NX, a_y = AY, b_y = BY, n_y = NY, a_z = AZ, b_z = BZ, and n_z = NZ.

FPS3H is based on the code HFFT3D by Boisvert (1984). It solves the equation

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} + cu = p$$

on the domain $(a_x, b_x) \times (a_y, b_y) \times (a_z, b_z)$ (a box) with a user-specified combination of Dirichlet (solution prescribed), Neumann (first derivative prescribed), or periodic boundary conditions. The six sides are numbered as shown in the following diagram.



When c = 0 and only Neumann or periodic boundary conditions are prescribed, then any constant may be added to the solution to obtain another solution to the problem. In this case, the solution of minimum∞-norm is returned.

The solution is computed using either a second-or fourth-order accurate finite-difference approximation of the continuous equation. The resulting system of linear algebraic equations is solved using fast Fourier transform techniques. The algorithm relies upon the fact that $n_x - 1$ and $n_z - 1$ are highly composite (the product of small primes). For details of the algorithm, see Boisvert (1984). If $n_x - 1$ and $n_z - 1$ are highly composite, then the execution time of `FPS3H` is proportional to

$$n_x n_y n_z \left(\log_2^2 n_x + \log_2^2 n_z \right)$$

If evaluations of $p(x, y, z)$ are inexpensive, then the difference in running time between `IORDER` = 2 and `IORDER` = 4 is small.

Comments

1. Workspace may be explicitly provided, if desired, by use of `F2S3H/DF2S3H`. The reference is:

   `CALL F2S3H (PRHS, BRHS, COEFU, NX, NY, NZ, AX, BX, AY, BY, AZ, BZ, IBCTY, IORDER, U, LDU, MDU, UWORK, WORK)`

   The additional arguments are as follows:

UWORK — Work array of size NX + 2 by NY + 2 by NZ + 2. If the actual dimensions of U are large enough, then U and UWORK can be the same array.

WORK — Work array of length
(NX + 1)(NY + 1)(NZ + 1)(IORDER − 2)/2 + 2(NX * NY + NX * NZ + NY * NZ) + 2(NX + NY + 1) + MAX(2 * NX * NY, 2 * NX + NY + 4 * NZ + (NX + NZ)/2 + 29)

2. The grid spacing is the distance between the (uniformly spaced) grid lines. It is given by the formulas

   HX = (BX − AX)/(NX − 1),

   HY = (BY − AY)/(NY − 1), and

   HZ = (BZ − AZ)/(NZ − 1).

   The grid spacings in the X, Y and Z directions must be the same, i.e., NX, NY and NZ must be such that HX = HY = HZ. Also, as noted above, NX, NY and NZ must all be at least 4. To increase the speed of the Fast Fourier transform, NX − 1 and NZ − 1 should be the product of small primes. Good choices for NX and NZ are 17, 33 and 65.

3. If −COEFU is nearly equal to an eigenvalue of the Laplacian with homogeneous boundary conditions, then the computed solution might have large errors.

Example

This example solves the equation

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} + 10u = -4\cos\left(3x + y - 2z\right) + 12e^{x-z} + 10$$

with the boundary conditions $\partial u/\partial z = -2\sin(3x + y - 2z) - \exp(x - z)$ on the front side and $u = \cos(3x + y - 2z) + \exp(x - z) + 1$ on the other five sides. The domain is the box $[0, 1/4] \times [0, 1/2] \times [0, 1/2]$. The output of FPS3H is a $9 \times 17 \times 17$ table of U values. The quadratic interpolation routine QD3VL is used to print a table of values.

```
      USE FPS3H_INT
      USE UMACH_INT
      USE QD3VL_INT

      IMPLICIT   NONE
!                                 SPECIFICATIONS FOR PARAMETERS
      INTEGER    LDU, MDU, NX, NXTABL, NY, NYTABL, NZ, NZTABL
      PARAMETER  (NX=5, NXTABL=4, NY=9, NYTABL=3, NZ=9, &
                 NZTABL=3, LDU=NX, MDU=NY)
!
      INTEGER    I, IBCTY(6), IORDER, J, K, NOUT
      REAL       AX, AY, AZ, BRHS, BX, BY, BZ, COEFU, FLOAT, PRHS, &
                 U(LDU,MDU,NZ), UTABL, X, ERROR, TRUE, &
                 XDATA(NX), Y, YDATA(NY), Z, ZDATA(NZ)
      INTRINSIC  COS, EXP, FLOAT
      EXTERNAL   BRHS, PRHS
!                                 Define domain
```

```
      AX = 0.0
      BX = 0.125
      AY = 0.0
      BY = 0.25
      AZ = 0.0
      BZ = 0.25
!                                  Set boundary condition types
      IBCTY(1) = 1
      IBCTY(2) = 1
      IBCTY(3) = 1
      IBCTY(4) = 1
      IBCTY(5) = 2
      IBCTY(6) = 1
!                                  Coefficient of U
      COEFU = 10.0
!                                  Order of the method
      IORDER = 4
!                                  Solve the PDE
      CALL FPS3H (PRHS, BRHS, COEFU, NX, NY, NZ, AX, BX, AY, BY, AZ, &
                 BZ, IBCTY, U)
!                                  Set up for quadratic interpolation
      DO 10  I=1, NX
         XDATA(I) = AX + (BX-AX)*FLOAT(I-1)/FLOAT(NX-1)
   10 CONTINUE
      DO 20  J=1, NY
         YDATA(J) = AY + (BY-AY)*FLOAT(J-1)/FLOAT(NY-1)
   20 CONTINUE
      DO 30  K=1, NZ
         ZDATA(K) = AZ + (BZ-AZ)*FLOAT(K-1)/FLOAT(NZ-1)
   30 CONTINUE
!                                  Print the solution
      CALL UMACH (2, NOUT)
      WRITE (NOUT,'(8X,5(A,11X))') 'X', 'Y', 'Z', 'U', 'Error'
      DO 60  K=1, NZTABL
         DO 50  J=1, NYTABL
            DO 40  I=1, NXTABL
               X     = AX + (BX-AX)*FLOAT(I-1)/FLOAT(NXTABL-1)
               Y     = AY + (BY-AY)*FLOAT(J-1)/FLOAT(NYTABL-1)
               Z     = AZ + (BZ-AZ)*FLOAT(K-1)/FLOAT(NZTABL-1)
               UTABL = QD3VL(X,Y,Z,XDATA,YDATA,ZDATA,U, CHECK=.false.)
               TRUE = COS(3.0*X+Y-2.0*Z) + EXP(X-Z) + 1.0
               ERROR = UTABL - TRUE
               WRITE (NOUT,'(5F12.4)') X, Y, Z, UTABL, ERROR
   40       CONTINUE
   50    CONTINUE
   60 CONTINUE
      END
!
      REAL FUNCTION PRHS (X, Y, Z)
      REAL       X, Y, Z
!
      REAL       COS, EXP
      INTRINSIC  COS, EXP
!                                  Right side of the PDE
      PRHS = -4.0*COS(3.0*X+Y-2.0*Z) + 12*EXP(X-Z) + 10.0
      RETURN
      END
!
      REAL FUNCTION BRHS (ISIDE, X, Y, Z)
      INTEGER    ISIDE
      REAL       X, Y, Z
!
      REAL       COS, EXP, SIN
      INTRINSIC  COS, EXP, SIN
!                                  Boundary conditions
      IF (ISIDE .EQ. 5) THEN
```

```
         BRHS = -2.0*SIN(3.0*X+Y-2.0*Z) - EXP(X-Z)
      ELSE
         BRHS = COS(3.0*X+Y-2.0*Z) + EXP(X-Z) + 1.0
      END IF
      RETURN
      END
```

Output

```
   X            Y            Z            U            Error
   0.0000       0.0000       0.0000       3.0000       0.0000
   0.0417       0.0000       0.0000       3.0348       0.0000
   0.0833       0.0000       0.0000       3.0558       0.0001
   0.1250       0.0000       0.0000       3.0637       0.0001
   0.0000       0.1250       0.0000       2.9922       0.0000
   0.0417       0.1250       0.0000       3.0115       0.0000
   0.0833       0.1250       0.0000       3.0175       0.0000
   0.1250       0.1250       0.0000       3.0107       0.0000
   0.0000       0.2500       0.0000       2.9690       0.0001
   0.0417       0.2500       0.0000       2.9731       0.0000
   0.0833       0.2500       0.0000       2.9645       0.0000
   0.1250       0.2500       0.0000       2.9440      -0.0001
   0.0000       0.0000       0.1250       2.8514       0.0000
   0.0417       0.0000       0.1250       2.9123       0.0000
   0.0833       0.0000       0.1250       2.9592       0.0000
   0.1250       0.0000       0.1250       2.9922       0.0000
   0.0000       0.1250       0.1250       2.8747       0.0000
   0.0417       0.1250       0.1250       2.9211       0.0010
   0.0833       0.1250       0.1250       2.9524       0.0010
   0.1250       0.1250       0.1250       2.9689       0.0000
   0.0000       0.2500       0.1250       2.8825       0.0000
   0.0417       0.2500       0.1250       2.9123       0.0000
   0.0833       0.2500       0.1250       2.9281       0.0000
   0.1250       0.2500       0.1250       2.9305       0.0000
   0.0000       0.0000       0.2500       2.6314      -0.0249
   0.0417       0.0000       0.2500       2.7420      -0.0004
   0.0833       0.0000       0.2500       2.8112      -0.0042
   0.1250       0.0000       0.2500       2.8609      -0.0138
   0.0000       0.1250       0.2500       2.7093       0.0000
   0.0417       0.1250       0.2500       2.8153       0.0344
   0.0833       0.1250       0.2500       2.8628       0.0237
   0.1250       0.1250       0.2500       2.8825       0.0000
   0.0000       0.2500       0.2500       2.7351      -0.0127
   0.0417       0.2500       0.2500       2.8030      -0.0011
   0.0833       0.2500       0.2500       2.8424      -0.0040
   0.1250       0.2500       0.2500       2.8735      -0.0012
```

SLEIG

Determines eigenvalues, eigenfunctions and/or spectral density functions for Sturm-Liouville problems in the form

$$-\frac{d}{dx}\left(p(x)\frac{du}{dx}\right)+q(x)u=\lambda r(x)u \quad \text{for } x \text{ in } (a,b)$$

with boundary conditions (at regular points)

$$\begin{aligned} a_1u-a_2(pu') &= \lambda\left(a'_1u-a'_2(pu')\right) \quad \text{at } a \\ b_1u+b_2(pu') &= 0 \quad \text{at } b \end{aligned}$$

Required Arguments

CONS — Array of size eight containing

$$a_1,\ a_1',\ a_2,\ a_2',\ b_1,\ b_2,\ a, \text{ and } b$$

in locations CONS(1) through CONS(8), respectively. (Input)

COEFFN — User-supplied `subroutine` to evaluate the coefficient functions. The usage is `CALL COEFFN (X, PX, QX, RX)`

X — Independent variable. (Input)

PX — The value of *p*(*x*) at X. (Output)

QX — The value of *q*(*x*) at X. (Output)

RX — The value of *r*(*x*) at X. (Output)

COEFFN must be declared EXTERNAL in the calling program.

ENDFIN — Logical array of size two. `ENDFIN(1) = .true.` if the endpoint *a* is finite, `ENDFIN(2) = .true.` if endpoint *b* is finite. (Input)

INDEX — Vector of size NUMEIG containing the indices of the desired eigenvalues. (Input)

EVAL — Array of length NUMEIG containing the computed approximations to the eigenvalues whose indices are specified in INDEX. (Output)

Optional Arguments

NUMEIG — The number of eigenvalues desired. (Input)
Default: NUMEIG = size (INDEX,1).

TEVLAB — Absolute error tolerance for eigenvalues. (Input)
Default: TEVLAB = 10 * machine precision.

TEVLRL — Relative error tolerance for eigenvalues. (Input)
Default: TEVLRL = SQRT(machine precision).

FORTRAN 90 Interface

Generic: CALL SLEIG (CONS, COEFFN, ENDFIN, INDEX, EVAL [, …])

Specific: The specific interface names are S_SLEIG and D_SLEIG.

FORTRAN 77 Interface

Single: CALL SLEIG (CONS, COEFFN, ENDFIN, NUMEIG, INDEX, TEVLAB, TEVLRL, EVAL)

Double: The double precision name is DSLEIG.

Description

This subroutine is designed for the calculation of eigenvalues, eigenfunctions and/or spectral density functions for Sturm-Liouville problems in the form

$$-\frac{d}{dx}\left(p(x)\frac{du}{dx}\right)+q(x)u=\lambda r(x)u \quad \text{for } x \text{ in } (a,b) \qquad (1)$$

with boundary conditions (at regular points)

$$a_1u-a_2(pu')=\lambda\left(a'_1u-a'_2(pu')\right) \quad \text{at } a$$
$$b_1u+b_2(pu')=0 \quad \text{at } b$$

We assume that

$$a'_1a_2-a_1a'_2>0$$

when $a'_1 \ne 0$ and $a'_2 \ne 0$. The problem is considered regular if and only if

- *a* and *b* are finite,
- *p*(*x*) and *r*(*x*) are positive in (*a*, *b*),

- $1/p(x)$, $q(x)$ and $r(x)$ are locally integrable near the endpoints.

Otherwise the problem is called singular. The theory assumes that p, p', q, and r are at least continuous on (a, b), though a finite number of jump discontinuities can be handled by suitably defining an input mesh.

For regular problems, there are an infinite number of eigenvalues

$$\lambda_0 < \lambda_1 < \ldots < \lambda_k,\ k \to \infty$$

Each eigenvalue has an associated eigenfunction which is unique up to a constant. For singular problems, there is a wide range in the behavior of the eigenvalues.

As presented in Pruess and Fulton (1993) the approach is to replace (1) by a new problem

$$-\left(\hat{p}\hat{u}'\right)' + \hat{q}\hat{u} = \hat{\lambda}\hat{r}\hat{u} \quad (2)$$

with analogous boundary conditions

$$a_1\hat{u}(a) - a_2\left(\hat{p}\hat{u}'\right)(a) = \hat{\lambda}\left[a'_1\hat{u}(a) - a_2{}'\left(\hat{p}\hat{u}'\right)(a)\right]$$
$$b_1\hat{u}(b) + b_2\left(\hat{p}\hat{u}'\right)(b) = 0$$

where

$$\hat{p},\ \hat{q} \text{ and } \hat{r}$$

are step function approximations to p, q, and r, respectively. Given the mesh $a = x_1 < x_2 < \ldots < x_{N+1} = b$, the usual choice for the step functions uses midpoint interpolation, i. e.,

$$\hat{p}(x) = p_n \equiv p\left(\frac{x_n + x_{n+1}}{2}\right)$$

for x in (x_n, x_{n+1}) and similarly for the other coefficient functions. This choice works well for regular problems. Some singular problems require a more sophisticated technique to capture the asymptotic behavior. For the midpoint interpolants, the differential equation (2) has the known closed form solution in (x_n, x_{n+1})

$$\hat{u}(x) = \hat{u}(x_n)\phi'_n(x - x_n) + \left(\hat{p}\hat{u}'\right)(x_n)\phi_n(x - x_n) / p_n$$

with

$$\phi_n(t) = \begin{cases} \sin\ \omega_n t\ /\ \omega_n,\ \tau_n > 0 \\ \sinh\ \omega_n t\ /\ \omega_n,\ \tau_n < 0 \\ t,\ \tau = 0 \end{cases}$$

where

$$\tau_n = \left(\hat{\lambda} r_n - q_n\right) / p_n$$

and

$$\omega_n = \sqrt{|\tau_n|}$$

Starting with,

$$\hat{u}(a) \text{ and } \left(\hat{p}\hat{u}'\right)(a)$$

consistent with the boundary condition,

$$\begin{aligned} \hat{u}(a) &= a_2 - a_2{}' \hat{\lambda} \\ \left(\hat{p}\hat{u}'\right)(a) &= a_1 - a_1{}' \hat{\lambda} \end{aligned}$$

an algorithm is to compute for n = 1, 2, …, N,

$$\begin{aligned} \hat{u}(x_{n+1}) &= \hat{u}(x_n)\phi_n{}'(h_n) + \left(\hat{p}\hat{u}'\right)(x_n)\phi_n(h_n) / p_n \\ \left(\hat{p}\hat{u}'\right)(x_{n+1}) &= -\tau_n p_n \hat{u}(x_n)\phi_n{}'(h_n) + \left(\hat{p}\hat{u}'\right)(x_n)\phi_n(h_n) \end{aligned}$$

which is a shooting method. For a fixed mesh we can iterate on the approximate eigenvalue until the boundary condition at b is satisfied. This will yield an $O(h^2)$ approximation

$$\hat{\lambda}_k$$

to some $\boldsymbol{\lambda_k}$.

The problem (2) has a step spectral function given by

$$\hat{\rho}(t) = \sum \frac{1}{\int \hat{r}(x)\hat{u}_k^2(x)dx + \alpha}$$

where the sum is taken over k such that

$$\hat{\lambda}_k \le t$$

and

$$\alpha = a'_1 a_2 - a_1 a'_2$$

Comments

1. Workspace may be explicitly provided, if desired, by use of S2EIG/DS2EIG. The reference is:

   CALL S2EIG (CONS, COEFFN, ENDFIN, NUMEIG, INDEX, TEVLAB, TEVLRL, EVAL, JOB, IPRINT, TOLS, NUMX, XEF, NRHO, T, TYPE, EF, PDEF, RHO, IFLAG, WORK, IWORK)

   The additional arguments are as follows:

   JOB — Logical array of length five. (Input)

   JOB(1) = .true. if a set of eigenvalues are to be computed but not their eigenfunctions.

   JOB(2) = .true. if a set of eigenvalue and eigenfunction pairs are to be computed.

   JOB(3) = .true. if the spectral function is to be computed over some subinterval of the essential spectrum.

   JOB(4) = .true. if the normal automatic classification is overridden. If JOB(4) = .true. then TYPE(*,*) must be entered correctly. Most users will not want to override the classification process, but it might be appropriate for users experimenting with problems for which the coefficient functions do not have power-like behavior near the singular endpoints. The classification is considered sufficiently important for spectral density function calculations that JOB(4) is ignored with JOB(3) = .true..

   JOB(5) = .true. if mesh distribution is chosen by SLEIG. If JOB(5) = .true. and NUMX is zero, the number of mesh points are also chosen by SLEIG. If NUMX > 0 then NUMX mesh points will be used. If JOB(5) = .false., the number NUMX and distribution XEF(*) must be input by the user.

   IPRINT — Control levels of internal printing. (Input)
   No printing is performed if IPRINT = 0. If either JOB(1) or JOB(2) is true:

IPRINT	Printed Output
1	Initial mesh (the first 51 or fewer points), eigenvalue estimate at each level.
4	The above and at each level matching point for eigenfunction shooting, X(*), EF(*) and PDEF(*) values.
5	The above and at each level the brackets for the eigenvalue search, intermediate shooting information for the eigenfunction and eigenfunction norm.

   If JOB(3) = .true.

IPRINT	Printed Output
1	The actual (a, b) used at each iteration and the total number of eigenvalues computed.
2	The above and switchover points to the asymptotic formulas, and some intermediate (*t*) approximations.
3	The above and initial meshes for each iteration, the index of the largest eigenvalue which may be computed, and various eigenvalue and R_N values.
4	The above and $\hat{\rho}$ values at each level.
5	The above and R_N add eigenvalues below the switchover point

If JOB(4) = .false.

IPRINT	Printed Output
2	Output a description of the spectrum.
3	The above and the constants for the Friedrichs' boundary condition(s).
5	The above and and intermediate details of the classification calculation.

TOLS — Array of length 4 containing tolerances. (Input)

TOLS(1) — absolute error tolerance for eigenfunctions

TOLS(2) — relative error tolerance for eigenfunctions

TOLS(3) — absolute error tolerance for eigenfunction derivatives

TOLS(4) — relative error tolerance for eigenfunction derivatives

The absolute tolerances must be positive.The relative tolerances must be at least 100 * amach(4)

NUMX — Integer whose value is the number of output points where each eigenfunction is to be evaluated (the number of entries in XEF(*)) when JOB(2) = .true.. If JOB(5)= .false. and NUMX is greater than zero, then NUMX is the number of points in the initial mesh used. If JOB(5) = .false., the points in XEF(*) should be chosen with a reasonable distribution. Since the endpoints *a* and *b* must be part of any mesh, NUMX cannot be one in this case. If JOB(5) = .false. and JOB(3) = .true., then NUMX must be positive. On output, NUMX is set to the number of points for eigenfunctions when input NUMX = 0, and JOB(2) or JOB(5) = .true.. (Input/Output)

XEF — Array of points on input where eigenfunction estimates are desired, if JOB(2) = .true.. Otherwise, if JOB(5) = .false. and NUMX is greater than zero, the user's initial mesh is entered. The entries must be ordered so that *a* = XEF(1) < XEF(2) < < XEF(NUMX) = *b*. If either endpoint is infinite, the corresponding XEF(1) or XEF(NUMX) is ignored. However, it is required that XEF(2) be negative when ENDFIN(1) = .false., and that XEF(NUMX−1) be positive when ENDFIN(2) = .false.. On output, XEF(*) is changed only if JOB(2) and JOB(5) are true. If JOB(2) = .false., this vector is not referenced. If JOB(2) = .true. and NUMX is greater than zero on input, XEF(*) should be dimensioned at least NUMX + 16. If JOB(2) is true and NUMX is zero on input, XEF(*) should be dimensioned at least 31.

NRHO — The number of output values desired for the array RHO(*). NRHO is not used if JOB(3) = .false.. (Input)

T — Real vector of size NRHO containing values where the spectral function RHO(*) is desired. The entries must be sorted in increasing order. The existence and location of a continuous spectrum can be determined by calling SLEIG with the first four entries of JOB set to false and IPRINT set to 1. T(*) is not used if JOB(3) = .false.. (Input)

TYPE — 4 by 2 logical matrix. Column 1 contains information about endpoint *a* and column 2 refers to endpoint *b*.
TYPE(1,*) = .true. if and only if the endpoint is regular
TYPE(2,*) = .true. if and only if the endpoint is limit circle
TYPE(3,*) = .true. if and only if the endpoint is nonoscillatory for all eigenvalues
TYPE(4,*) = .true. if and only if the endpoint is oscillatory for all eigenvalues
Note: all of these values must be correctly input if JOB(4) = .true..
Otherwise, TYPE(*,*) is output. (Input/Output)

EF — Array of eigenfunction values. EF((k−1)*NUMX + i) is the estimate of u(XEF(i)) corresponding to the eigenvalue in EV(k). If JOB(2) = .false. then this vector is not referenced. If JOB(2) = .true. and NUMX is greater than zero on entry, then EF(*) should be dimensioned at least NUMX * NUMEIG. If JOB(2) = .true. and NUMX is zero on input, then EF(*) should be dimensioned 31 * NUMEIG. (Output)

PDEF — Array of eigenfunction derivative values. PDEF((k−1)*NUMX + i) is the estimate of (*pu'*)(XEF(i)) corresponding to the eigenvalue in EV(k). If JOB(2) = .false. this vector is not referenced. If JOB(2) = .true., it must be dimensioned the same as EF(*). (Output)

RHO — Array of size NRHO containing values for the spectral density function $\rho(t)$, RHO(I) = ρ(T(I)). This vector is not referenced if JOB(3) is false. (Output)

IFLAG — Array of size max(1, numeig) containing information about the output. IFLAG(K) refers to the K-th eigenvalue, when JOB(1) or JOB(2) = .true.. Otherwise, only IFLAG(1) is used. Negative values are associated with fatal errors, and the calculations are ceased. Positive values indicate a warning. (Output)
These are the possible values for IFLAG(K)

IFLAG(K)	Description
−1	Too many levels needed for the eigenvalue calculation; problem seems too difficult at this tolerance. Are the coefficient functions nonsmooth?
−2	Too many levels needed for the eigenfunction calculation; problem seems too difficult at this tolerance. Are the eigenfunctions ill-conditioned?
−3	Too many levels needed for the spectral density calculation; problem seems too difficult at this tolerance.

IFLAG(K)	Description
−4	The user has requested the spectral density function for a problem which has no continuous spectrum.
−5	The user has requested the spectral density function for a problem with both endpoints generating essential spectrum, i.e. both endpoints either OSC or O-NO.
−6	The user has requested the spectral density function for a problem in spectral category 2 for which a proper normalization of the solution at the NONOSC endpoint is not known; for example, problems with an irregular singular point or infinite endpoint at one end and continuous spectrum generated at the other.
−7	Problems were encountered in obtaining a bracket.
−8	Too small a step was used in the integration. The `TOLS(*)` values may be too small for this problem.
−9	Too small a step was used in the spectral density function calculation for which the continuous spectrum is generated by a finite endpoint.
−10	An argument to the circular trig functions is too large. Try running the problem again with a finer initial mesh or, for singular problems, use interval truncation.
−15	p(x) and r(x) are not positive in the interval (a, b).
−20	Eigenvalues and/or eigenfunctions were requested for a problem with an OSC singular endpoint. Interval truncation must be used on such problems.
1	Failure in the bracketing procedure probably due to a cluster of eigenvalues which the code cannot separate. Calculations have continued but any eigenfunction results are suspect. Try running the problem again with tighter input tolerances to separate the cluster.
2	There is uncertainty in the classification for this problem. Because of the limitations of floating point arithmetic, and the nature of the finite sampling, the routine cannot be certain about the classification information at the requested tolerance.
3	There may be some eigenvalues embedded in the essential spectrum. Use of `IPRINT` greater than zero will provide additional output giving the location of the approximating eigenvalues for the step function problem. These could be extrapolated to estimate the actual eigenvalue embedded in the essential spectrum.
4	A change of variables was made to avoid potentially slow convergence. However, the global error estimates may not be as reliable. Some experimentation using different tolerances is recommended.
6	There were problems with eigenfunction convergence in a spectral density calculation. The output $\rho(t)$ may not be accurate.

WORK — Array of size MAX(1000, NUMEIG + 22) used for workspace.

IWORK — Integer array of size NUMEIG + 3 used for workspace.

Examples

Example 1

This example computes the first ten eigenvalues of the problem from Titchmarsh (1962) given by

$p(x) = r(x) = 1$

$q(x) = x$

$[a, b] = [0, \infty]$

$u(a) = u(b) = 0$

The eigenvalues are known to be the zeros of

$$f(\lambda) = J_{1/3}\left(\frac{2}{3}\lambda^{3/2}\right) + J_{-1/3}\left(\frac{2}{3}\lambda^{3/2}\right)$$

For each eigenvalue λ_k, the program prints k, λ_k and $f(\lambda_k)$.

```
      USE SLEIG_INT
      USE CBJS_INT

      IMPLICIT   NONE
!                                  SPECIFICATIONS FOR LOCAL VARIABLES
      INTEGER    I, INDEX(10), NUMEIG, NOUT
      REAL       CONS(8), EVAL(10), LAMBDA, TEVLAB,&
                 TEVLRL, XNU
      COMPLEX    CBS1(1), CBS2(1), Z
      LOGICAL    ENDFIN(2)
!                                  SPECIFICATIONS FOR INTRINSICS
      INTRINSIC  CMPLX, SQRT
      REAL       SQRT
      COMPLEX    CMPLX
!                                  SPECIFICATIONS FOR SUBROUTINES
!                                  SPECIFICATIONS FOR FUNCTIONS
      EXTERNAL   COEFF
!
      CALL UMACH (2, NOUT)
!                                  Define boundary conditions
      CONS(1) = 1.0
      CONS(2) = 0.0
      CONS(3) = 0.0
      CONS(4) = 0.0
      CONS(5) = 1.0
      CONS(6) = 0.0
      CONS(7) = 0.0
      CONS(8) = 0.0
!
      ENDFIN(1) = .TRUE.
      ENDFIN(2) = .FALSE.
```

```
!                                  Compute the first 10 eigenvalues
      NUMEIG = 10
      DO 10  I=1, NUMEIG
         INDEX(I) = I - 1
   10 CONTINUE
!                                  Set absolute and relative tolerance
!
      CALL SLEIG (CONS, COEFF, ENDFIN, INDEX, EVAL)
!
      XNU = -1.0/3.0
      WRITE(NOUT,99998)
      DO 20  I=1, NUMEIG
         LAMBDA = EVAL(I)
         Z      = CMPLX(2.0/3.0*LAMBDA*SQRT(LAMBDA),0.0)
         CALL CBJS (XNU, Z, 1, CBS1)
         CALL CBJS (-XNU, Z, 1, CBS2)
         WRITE (NOUT,99999) I-1, LAMBDA, REAL(CBS1(1) + CBS2(1))
   20 CONTINUE
!
99998 FORMAT(/, 2X, 'index', 5X, 'lambda', 5X, 'f(lambda)',/)
99999 FORMAT(I5, F13.4, E15.4)
      END
!
      SUBROUTINE COEFF (X, PX, QX, RX)
!                                  SPECIFICATIONS FOR ARGUMENTS
      REAL       X, PX, QX, RX
!
      PX = 1.0
      QX = X
      RX = 1.0
      RETURN
      END
```

Output

```
  index     lambda     f(lambda)

    0       2.3381    -0.8285E-05
    1       4.0879    -0.1651E-04
    2       5.5205     0.6843E-04
    3       6.7867    -0.4523E-05
    4       7.9440     0.8952E-04
    5       9.0227     0.1123E-04
    6      10.0401     0.1031E-03
    7      11.0084    -0.7913E-04
    8      11.9361    -0.5095E-04
    9      12.8293     0.4645E-03
```

Example 2

In this problem from Scott, Shampine and Wing (1969),

$$p(x) = r(x) = 1$$

$$q(x) = x^2 + x^4$$

$$[a, b] = [-\infty, \infty]$$

$$u(a) = u(b) = 0$$

the first eigenvalue and associated eigenfunction, evaluated at selected points, are computed. As a rough check of the correctness of the results, the magnitude of the residual

$$-\frac{d}{dx}\left(p(x)\frac{du}{dx}\right)+q(x)u-\lambda r(x)u$$

is printed. We compute a spline interpolant to u' and use the function CSDER to estimate the quantity $-(p(x)u')'$.

```
      USE S2EIG_INT
      USE CSDER_INT
      USE UMACH_INT
      USE CSAKM_INT

      IMPLICIT   NONE
!                                  SPECIFICATIONS FOR LOCAL VARIABLES

      INTEGER    I, IFLAG(1), INDEX(1), IWORK(100), NINTV, NOUT, NRHO, &
                 NUMEIG, NUMX
      REAL       BRKUP(61), CONS(8), CSCFUP(4,61), EF(61), EVAL(1), &
                 LAMBDA, PDEF(61), PX, QX, RESIDUAL, RHO(1), RX, T(1), &
                 TEVLAB, TEVLRL, TOLS(4), WORK(3000), X, XEF(61)
      LOGICAL    ENDFIN(2), JOB(5), TYPE(4,2)
!                                  SPECIFICATIONS FOR INTRINSICS
      INTRINSIC  ABS, REAL
      REAL       ABS, REAL
!                                  SPECIFICATIONS FOR SUBROUTINES
      EXTERNAL   COEFF
!                                  Define boundary conditions
      CONS(1) = 1.0
      CONS(2) = 0.0
      CONS(3) = 0.0
      CONS(4) = 0.0
      CONS(5) = 1.0
      CONS(6) = 0.0
      CONS(7) = 0.0
      CONS(8) = 0.0
!                                  Compute eigenvalue and eigenfunctions
      JOB(1) = .FALSE.
      JOB(2) = .TRUE.
      JOB(3) = .FALSE.
      JOB(4) = .FALSE.
      JOB(5) = .FALSE.
!
      ENDFIN(1) = .FALSE.
      ENDFIN(2) = .FALSE.
!                                  Compute eigenvalue with index 0
      NUMEIG   = 1
      INDEX(1) = 0
!
      TEVLAB  = 1.0E-3
      TEVLRL  = 1.0E-3
      TOLS(1) = TEVLAB
      TOLS(2) = TEVLRL
      TOLS(3) = TEVLAB
      TOLS(4) = TEVLRL
      NRHO    = 0
!                                  Set up mesh, points at which u and
!                                  u' will be computed
      NUMX = 61
      DO 10  I=1, NUMX
         XEF(I) = 0.05*REAL(I-31)
   10 CONTINUE
!
```

```
      CALL S2EIG (CONS, COEFF, ENDFIN, NUMEIG, INDEX, TEVLAB, TEVLRL, &
                  EVAL, JOB, 0, TOLS, NUMX, XEF, NRHO, T, TYPE, EF, &
                  PDEF, RHO, IFLAG, WORK, IWORK)
!
      LAMBDA = EVAL(1)
   20 CONTINUE
!                                   Compute spline interpolant to u'
!
      CALL CSAKM (XEF, PDEF, BRKUP, CSCFUP)
      NINTV = NUMX - 1
!
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99997) '     lambda = ', LAMBDA
      WRITE (NOUT,99999)
!                                   At a subset of points from the
!                                   input mesh, compute residual =
!                                   abs( -(u')' + q(x)u - lambda*u ).
!                                   We know p(x) = 1 and r(x) = 1.
      DO 30  I=1, 41, 2
         X = XEF(I+10)
         CALL COEFF (X, PX, QX, RX)
!
!                                   Use the spline fit to u' to
!                                   estimate u'' with CSDER
!
         RESIDUAL = ABS(-CSDER(1,X,BRKUP,CSCFUP)+QX*EF(I+10)- &
                    LAMBDA*EF(I+10))
         WRITE (NOUT,99998) X, EF(I+10), PDEF(I+10), RESIDUAL
   30 CONTINUE
!
99997 FORMAT (/, A14, F10.5, /)
99998 FORMAT (5X, F4.1, 3F15.5)
99999 FORMAT (7X, 'x', 11X, 'u(x)', 10X, 'u''(x)', 9X, 'residual', /)
      END
!
      SUBROUTINE COEFF (X, PX, QX, RX)
!                                   SPECIFICATIONS FOR ARGUMENTS
      REAL       X, PX, QX, RX
!
      PX = 1.0
      QX = X*X + X*X*X*X
      RX = 1.0
      RETURN
      END
```

Output

```
     lambda =    1.39247
        x          u(x)          u'(x)        residual
      -1.0        0.38632        0.65019        0.00189
      -0.9        0.45218        0.66372        0.00081
      -0.8        0.51837        0.65653        0.00023
      -0.7        0.58278        0.62827        0.00113
      -0.6        0.64334        0.57977        0.00183
      -0.5        0.69812        0.51283        0.00230
      -0.4        0.74537        0.42990        0.00273
      -0.3        0.78366        0.33393        0.00265
      -0.2        0.81183        0.22811        0.00273
      -0.1        0.82906        0.11570        0.00278
       0.0        0.83473        0.00000        0.00136
       0.1        0.82893       -0.11568        0.00273
       0.2        0.81170       -0.22807        0.00273
       0.3        0.78353       -0.33388        0.00267
       0.4        0.74525       -0.42983        0.00265
       0.5        0.69800       -0.51274        0.00230
```

```
           0.6         0.64324       -0.57967         0.00182
           0.7         0.58269       -0.62816         0.00113
           0.8         0.51828       -0.65641         0.00023
           0.9         0.45211       -0.66361         0.00081
           1.0         0.38626       -0.65008         0.00189
```

SLCNT

Calculates the indices of eigenvalues of a Sturm-Liouville problem of the form for

$$-\frac{d}{dx}\left(p(x)\frac{du}{dx}\right)+q(x)u=\lambda r(x)u \quad \text{for } x \text{ in } [a,b]$$

with boundary conditions (at regular points)

$$a_1u-a_2(pu')=\lambda\left(a_1{}'u-a_2{}'(pu')\right) \quad \text{at } a$$
$$b_1u+b_2(pu')=0 \quad \text{at } b$$

in a specified subinterval of the real line, [α, β].

Required Arguments

ALPHA — Value of the left end point of the search interval. (Input)

BETAR — Value of the right end point of the search interval. (Input)

CONS — Array of size eight containing

$$a_1,\ a_1{}',\ a_2,\ a_2{}',\ b_1,\ b_2,\ a \text{ and } b$$

in locations `CONS(1)` `CONS(8)`, respectively. (Input)

COEFFN — User-supplied `subroutine` to evaluate the coefficient functions. The usage is `CALL COEFFN (X, PX, QX, RX)`

`X` — Independent variable. (Input)

`PX` — The value of *p*(*x*) at `X`. (Output)

`QX` — The value of *q*(*x*) at `X`. (Output)

`RX` — The value of *r*(*x*) at `X`. (Output)

`COEFFN` must be declared `EXTERNAL` in the calling program.

ENDFIN — Logical array of size two. `ENDFIN = .true.` if and only if the endpoint *a* is finite. `ENDFIN(2) = .true.` if and only if endpoint *b* is finite. (Input)

IFIRST — The index of the first eigenvalue greater than α. (Output)

NTOTAL — Total number of eigenvalues in the interval [α, β]. (Output)

FORTRAN 90 Interface

Generic: `CALL SLCNT (ALPHA, BETAR, CONS, COEFFN, ENDFIN, IFIRST, NTOTAL)`

Specific: The specific interface names are `S_SLCNT` and `D_SLCNT`.

FORTRAN 77 Interface

Single: `CALL SLCNT (ALPHA, BETAR, CONS, COEFFN, ENDFIN, IFIRST, NTOTAL)`

Double: The double precision name is `DSLCNT`.

Description

This subroutine computes the indices of eigenvalues, if any, in a subinterval of the real line for Sturm-Liouville problems in the form

$$-\frac{d}{dx}\left(p(x)\frac{du}{dx}\right)+q(x)u=\lambda r(x)u \quad \text{for } x \text{ in } (a,b)$$

with boundary conditions (at regular points)

$$a_1u-a_2(pu')=\lambda\left(a'_1u-a'_2(pu')\right) \quad \text{at } a$$
$$b_1u+b_2(pu')=0 \quad \text{at } b$$

It is intended to be used in conjunction with `SLEIG`. `SLCNT` is based on the routine `INTERV` from the package `SLEDGE`.

Example

Consider the harmonic oscillator (Titchmarsh) defined by

p(x) = 1

q(x) = x^2

r(x) = 1

[a, b] = [−∞,∞]

u(a) = 0

u(b) = 0

The eigenvalues of this problem are known to be

$\lambda_k = 2k + 1, k = 0, 1, \ldots$

Therefore in the interval [10, 16] we expect `SLCNT` to note three eigenvalues, with the first of these having index five.

```
      USE SLCNT_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                  SPECIFICATIONS FOR LOCAL VARIABLES
      INTEGER    IFIRST, NOUT, NTOTAL
      REAL       ALPHA, BETAR, CONS(8)
      LOGICAL    ENDFIN(2)
!                                  SPECIFICATIONS FOR SUBROUTINES
!                                  SPECIFICATIONS FOR FUNCTIONS
      EXTERNAL   COEFFN
!
      CALL UMACH (2, NOUT)
!                                  set u(a) = 0, u(b) = 0
      CONS(1) = 1.0E0
      CONS(2) = 0.0E0
      CONS(3) = 0.0E0
      CONS(4) = 0.0E0
      CONS(5) = 1.0E0
      CONS(6) = 0.0E0
      CONS(7) = 0.0E0
      CONS(8) = 0.0E0
!
      ENDFIN(1) = .FALSE.
      ENDFIN(2) = .FALSE.
!
      ALPHA = 10.0
      BETAR  = 16.0
!
      CALL SLCNT (ALPHA, BETAR, CONS, COEFFN, ENDFIN, IFIRST, NTOTAL)
!
      WRITE (NOUT,99998) ALPHA, BETAR, IFIRST
      WRITE (NOUT,99999) NTOTAL
!
99998 FORMAT (/, 'Index of first eigenvalue in [', F5.2, ',', F5.2, &
            '] IS ', I2)
99999 FORMAT ('Total number of eigenvalues in this interval: ', I2)
!
      END
!
      SUBROUTINE COEFFN (X, PX, QX, RX)
!                                  SPECIFICATIONS FOR ARGUMENTS
      REAL       X, PX, QX, RX
!
      PX = 1.0E0
      QX = X*X
      RX = 1.0E0
      RETURN
      END
```

Output

```
Index of first eigenvalue in [10.00,16.00] is 5
Total number of eigenvalues in this interval: 3
```

Transforms

Routines

6.6. Convolutions and Correlations

6.7. Laplace Transform

Usage Notes

Fast Fourier Transforms

A Fast Fourier Transform (FFT) is simply a discrete Fourier transform that can be computed efficiently. Basically, the straightforward method for computing the Fourier transform takes approximately N^2 operations where N is the number of points in the transform, while the FFT (which computes the same values) takes approximately $N \log N$ operations. The algorithms in this chapter are modeled on the Cooley-Tukey (1965) algorithm; hence, the computational savings occur, not for all integers N, but for N which are highly composite. That is, N (or in certain cases $N + 1$ or $N - 1$) should be a product of small primes.

All of the FFT routines compute a *discrete* Fourier transform. The routines accept a vector x of length N and return a vector

$$\hat{x}$$

defined by

$$\hat{x}_m := \sum_{n=1}^{N} x_n \omega_{nm}$$

The various transforms are determined by the selection of ω. In the following table, we indicate the selection of ω for the various transforms. This table should not be mistaken for a definition since the precise transform definitions (at times) depend on whether N or m is even or odd.

Routine	ω_{nm}
FFTRF	$\cos \text{ or } \sin \dfrac{(m-1)(n-1)2\pi}{N}$
FFTRB	$\cos \text{ or } \sin \dfrac{(m-1)(n-1)2\pi}{N}$
FFTCF	$\exp^{-2\pi i(n-1)(m-1)/N}$
FFTCB	$\exp^{2\pi i(n-1)(m-1)/N}$
FSINT	$\sin \dfrac{nm\pi}{N+1}$

Routine	ω_{nm}
FCOST	$\cos \frac{(n-1)(m-1)\pi}{N-1}$
QSINF	$2 \sin \frac{(2m-1)n\pi}{2N}$
QSINB	$4 \sin \frac{(2n-1)m\pi}{2N}$
QCOSF	$2 \cos \frac{(2m-1)(n-1)\pi}{2N}$
QCOSB	$4 \cos \frac{(2n-1)(m-1)\pi}{2N}$

For many of the routines listed above, there is a corresponding "`I`" (for initialization) routine. Use these routines *only* when repeatedly transforming sequences of the same length. In this situation, the "`I`" routine will compute the initial setup once, and then the user will call the corresponding "2" routine. This can result in substantial computational savings. For more information on the usage of these routines, the user should consult the documentation under the appropriate routine name.

In addition to the one-dimensional transformations described above, we also provide complex two and three-dimensional FFTs and their inverses based on calls to either `FFTCF` or `FFTCB`. If you need a higher dimensional transform, then you should consult the example program for `FFTCI`, which suggests a basic strategy one could employ.

Continuous versus Discrete Fourier Transform

There is, of course, a close connection between the discrete Fourier transform and the continuous Fourier transform. Recall that the continuous Fourier transform is defined (Brigham, 1974) as

$$\hat{f}(\omega) = (Ff)(\omega) = \int_{-\infty}^{\infty} f(t) e^{-2\pi i \omega t} dt$$

We begin by making the following approximation:

$$\begin{aligned}\hat{f}(\omega) &\approx \int_{-T/2}^{T/2} f(t)e^{-2\pi i\omega t}dt \\ &= \int_0^T f(t-T/2)e^{-2\pi i\omega(t-T/2)}dt \\ &= e^{\pi i\omega T}\int_0^T f(t-T/2)e^{-2\pi i\omega}dt\end{aligned}$$

If we approximate the last integral using the rectangle rule with spacing $h = T/N$, we have

$$\hat{f}(\omega) \approx e^{\pi i\omega T} h \sum_{k=0}^{N-1} e^{-2\pi i\omega kh} f(kh - T/2)$$

Finally, setting $\omega = j/T$ for $j = 0, \ldots, N - 1$ yields

$$\hat{f}(j/T) \approx e^{\pi ij} h \sum_{k=0}^{N-1} e^{-2\pi ijk/N} f(kh - T/2) = (-1)^j h \sum_{k=0}^{N-1} e^{-2\pi ijk/N} f_k^h$$

where the vector $f^h = (f(-T/2),\ldots, f((N-1)h - T/2))$. Thus, after scaling the components by $(-1)^j h$, the discrete Fourier transform as computed in FFTCF (with input f^h) is related to an approximation of the continuous Fourier transform by the above formula. This is seen more clearly by making a change of variables in the last sum. Set

$$n = k + 1, m = j + 1, \text{and } f_k^h = x_n$$

then, for $m = 1, \ldots, N$ we have

$$\hat{f}((m-1)/T) \approx -(-1)^m h\hat{x}_m = -(-1)^m h \sum_{n=1}^{N} e^{-2\pi i(m-1)(n-1)/N} x_n$$

If the function f is expressed as a FORTRAN function routine, then the continuous Fourier transform

$$\hat{f}$$

can be approximated using the IMSL routine QDAWF (see *Chapter 4, "Integration and Differentiation"*).

Laplace

The last two routines described in this chapter, INLAP and SINLP, compute the inverse Laplace transforms.

FAST_DFT

more...

Computes the Discrete Fourier Transform (DFT) of a rank-1 complex array, *x*.

Required Arguments

No required arguments; pairs of optional arguments are required. These pairs are `forward_in` and `forward_out` or `inverse_in` and `inverse_out`.

Optional Arguments

forward_in = `x` (Input)
Stores the input complex array of rank-1 to be transformed.

forward_out = `y` (Output)
Stores the output complex array of rank-1 resulting from the transform.

inverse_in = `y` (Input)
Stores the input complex array of rank-1 to be inverted.

inverse_out = `x` (Output)
Stores the output complex array of rank-1 resulting from the inverse transform.

ndata = `n` (Input)
Uses the sub-array of size `n` for the numbers.
Default value: `n` = size(`x`).

ido = `ido` (Input/Output)
Integer flag that directs user action. Normally, this argument is used only when the working variables required for the transform and its inverse are saved in the calling program unit. Computing the working variables and saving them in internal arrays within `fast_dft` is the default. This initialization step is expensive.

There is a two-step process to compute the working variables just once. Example 3 illustrates this usage. The general algorithm for this usage is to enter fast_dft with ido = 0. A return occurs thereafter with ido < 0. The optional rank-1 complex array w(:) with size(w) >= –ido must be re-allocated. Then, re-enter `fast_dft`. The next return from `fast_dft` has the output value ido = 1. The variables required for the transform and its inverse are saved in w(:). Thereafter, when the routine is entered with ido = 1 and for the same value of n, the contents of w(:) will be used for the working variables. The expensive initialization step is avoided. The optional arguments "ido=" and "work_array=" must be used together.

work_array = `w(:)` (Output/Input)
Complex array of rank-1 used to store working variables and values between calls to `fast_dft`. The value for size(`w`) must be at least as large as the value – `ido` for the value of `ido` < 0.

iopt = `iopt(:)` (Input/Output)
Derived type array with the same precision as the input array; used for passing optional data to `fast_dft`. The options are as follows:

Packaged Options for FAST_DFT		
Option Prefix = ?	Option Name	Option Value
`c_, z_`	`fast_dft_scan_for_NaN`	1
`c_, z_`	`fast_dft_near_power_of_2`	2
`c_, z_`	`fast_dft_scale_forward`	3
`c_, z_`	`Fast_dft_scale_inverse`	4

iopt(IO) = `?_options(?_fast_dft_scan_for_NaN, ?_dummy)`
Examines each input array entry to find the first value such that `isNaN(x(i)) ==.true.`.
See the `isNaN()` function, *Chapter 10*.
Default: Does not scan for NaNs.

iopt(IO) = `?_options(?_fast_dft_near_power_of_2, ?_dummy)`
Nearest power of 2 ≥ *n* is returned as an output in `iopt(IO + 1)%idummy`.

iopt(IO) = `?_options(?_fast_dft_scale_forward, real_part_of_scale)`

iopt(IO+1) = `?_options(?_dummy, imaginary_part_of_scale)`
Complex number defined by the factor
cmplx(`real_part_of_scale, imaginary_part_of_scale`) is multiplied by the forward transformed array.
Default value is 1.

iopt(IO) = `?_options(?_fast_dft_scale_inverse, real_part_of_scale)`

iopt(IO+1) = `?_options(?_dummy, imaginary_part_of_scale)`

Complex number defined by the factor

cmplx(`real_part_of_scale, imaginary_part_of_scale`) is multiplied by the inverse transformed array.

Default value is 1.

FORTRAN 90 Interface

Generic: None

Specific: The specific interface names are `S_FAST_DFT`, `D_FAST_DFT`, `C_FAST_DFT`, and `Z_FAST_DFT`.

Description

The `fast_dft` routine is a Fortran 90 version of the FFT suite of IMSL (1994, pp. 772-776). The maximum computing efficiency occurs when the size of the array can be factored in the form

$$n = 2^{i_1} 3^{i_2} 4^{i_3} 5^{i_4}$$

using non-negative integer values $\{i_1, i_2, i_3, i_4\}$. There is no further restriction on $n \geq 1$.

Fatal and Terminal Messages

See the *messages.gls* file for error messages for `FAST_DFT`. These error messages are numbered 651–661; 701–711.

Examples

Example 1: Transforming an Array of Random Complex Numbers

An array of random complex numbers is obtained. The transform of the numbers is inverted and the final results are compared with the input array.

```
      use fast_dft_int
      use rand_gen_int

      implicit none

! This is Example 1 for FAST_DFT.

      integer, parameter :: n=1024
      real(kind(1e0)), parameter :: one=1e0
      real(kind(1e0)) err, y(2*n)
```

```
      complex(kind(1e0)), dimension(n) :: a, b, c


! Generate a random complex sequence.
      call rand_gen(y)
      a = cmplx(y(1:n),y(n+1:2*n),kind(one))
      c = a

! Transform and then invert the sequence back.
      call c_fast_dft(forward_in=a, &
           forward_out=b)
      call c_fast_dft(inverse_in=b, &
           inverse_out=a)

! Check that inverse(transform(sequence)) = sequence.
      err = maxval(abs(c-a))/maxval(abs(c))
      if (err <= sqrt(epsilon(one))) then
         write (*,*) 'Example 1 for FAST_DFT is correct.'
      end if

      end
```

Output

```
Example 1 for FAST_DFT is correct.
```

Example 2: Cyclical Data with a Linear Trend

This set of data is sampled from a function $x(t) = at + b + y(t)$, where $y(t)$ is a harmonic series. The independent variable is normalized as $-1 \le t \le 1$. Thus, the data is said to have cyclical components plus a linear trend. As a first step, the linear terms are effectively removed from the data using the least-squares system solver LIN_SOL_LSQ, *Chapter 1*. Then, the residuals are transformed and the resulting frequencies are analyzed.

```
      use fast_dft_int
      use lin_sol_lsq_int
      use rand_gen_int
      use sort_real_int

      implicit none

! This is Example 2 for FAST_DFT.

      integer i
      integer, parameter :: n=64, k=4
      integer ip(n)
      real(kind(1e0)), parameter :: one=1e0, two=2e0, zero=0e0
      real(kind(1e0)) delta_t, pi
      real(kind(1e0)) y(k), z(2), indx(k), t(n), temp(n)
      complex(kind(1e0)) a_trend(n,2), a, b_trend(n,1), b, c(k), f(n),&
               r(n), x(n), x_trend(2,1)

! Generate random data for linear trend and harmonic series.
      call rand_gen(z)
      a = z(1); b = z(2)
      call rand_gen(y)
! This emphasizes harmonics 2 through k+1.
      c = y + one

! Determine sampling interval.
      delta_t = two/n
```

```
      t=(/(-one+i*delta_t, i=0,n-1)/)

! Compute pi.
      pi = atan(one)*4E0
      indx=(/(i*pi,i=1,k)/)

! Make up data set as a linear trend plus harmonics.
      x = a + b*t + &
         matmul(exp(cmplx(zero,spread(t,2,k)*spread(indx,1,n),kind(one))),c)

! Define least-squares matrix data for a linear trend.
      a_trend(1:,1) = one
      a_trend(1:,2) = t
      b_trend(1:,1) = x

! Solve for a linear trend.
      call lin_sol_lsq(a_trend, b_trend, x_trend)

! Compute harmonic residuals.
      r = x -  reshape(matmul(a_trend,x_trend),(/n/))

! Transform harmonic residuals.
      call c_fast_dft(forward_in=r, forward_out=f)
      ip=(/(i,i=1,n)/)

! The dominant frequencies should be 2 through k+1.
! Sort the magnitude of the transform first.
      call s_sort_real(-(abs(f)), temp, iperm=ip)

! The dominant frequencies are output in ip(1:k).
! Sort these values to compare with 2 through k+1.
      call s_sort_real(real(ip(1:k)), temp)
      ip(1:k)=(/(i,i=2,k+1)/)

! Check the results.
      if (count(int(temp(1:k)) /= ip(1:k)) == 0) then
         write (*,*) 'Example 2 for FAST_DFT is correct.'
      end if

      end
```

Output

```
Example 2 for FAST_DFT is correct.
```

Example 3: Several Transforms with Initialization

In this example, the optional arguments `ido` and `work_array` are used to save working variables in the calling program unit. This results in maximum efficiency of the transform and its inverse since the working variables do not have to be precomputed following each entry to routine `fast_dft`.

```
      use fast_dft_int
      use rand_gen_int

      implicit none

! This is Example 3 for FAST_DFT.

! The value of the array size for work(:) is computed in the
! routine fast_dft as a first step.
```

```
      integer, parameter :: n=64
      integer ido_value
      real(kind(1e0)) :: one=1e0
      real(kind(1e0)) err, y(2*n)
      complex(kind(1e0)), dimension(n) :: a, b, save_a
      complex(kind(1e0)), allocatable :: work(:)


! Generate a random complex array.
      call rand_gen(y)
      a = cmplx(y(1:n),y(n+1:2*n),kind(one))
      save_a = a

! Transform and then invert the sequence using the pre-computed
! working values.
      ido_value = 0
      do
         if(allocated(work)) deallocate(work)

! Allocate the space required for work(:).
         if (ido_value <= 0) allocate(work(-ido_value))

         call c_fast_dft(forward_in=a, forward_out=b, &
          ido=ido_value, work_array=work)

         if (ido_value == 1) exit
      end do

! Re-enter routine with working values available in work(:).
      call c_fast_dft(inverse_in=b, inverse_out=a, &
            ido=ido_value, work_array=work)

! Deallocate the space used for work(:).
      if (allocated(work)) deallocate(work)

! Check the results.
      err = maxval(abs(save_a-a))/maxval(abs(save_a))
      if (err <= sqrt(epsilon(one))) then
         write (*,*) 'Example 3 for FAST_DFT is correct.'
      end if

      end
```

Output

```
Example 3 for FAST_DFT is correct.
```

Example 4: Convolutions using Fourier Transforms

In this example we compute sums

$$c_k = \sum_{j=0}^{n-1} a_j b_{k-j}, k = 0, \ldots, n-1$$

The definition implies a matrix-vector product. A direct approach requires about n^2 operations consisisting of an add and multiply. An efficient method consisting of computing the products of the transforms of the

$$\{a_j\} \text{ and } \{b_j\}$$

then inverting this product, is preferable to the matrix-vector approach for large problems. The example is also illustrated in `operator_ex37`, *Chapter 10* using the generic function interface FFT and IFFT.

```
      use fast_dft_int
      use rand_gen_int

      implicit none

! This is Example 4 for FAST_DFT.

      integer j
      integer, parameter :: n=40
      real(kind(1e0)) :: one=1e0
      real(kind(1e0)) err
      real(kind(1e0)), dimension(n) :: x, y, yy(n,n)
      complex(kind(1e0)), dimension(n) :: a, b, c, d, e, f

! Generate two random complex sequence 'a' and 'b'.

      call rand_gen(x)
      call rand_gen(y)
      a=x; b=y

! Compute the convolution 'c' of 'a' and 'b'.
! Use matrix times vector for test results.
      yy(1:,1)=y
      do j=2,n
        yy(2:,j)=yy(1:n-1,j-1)
        yy(1,j)=yy(n,j-1)
      end do

      c=matmul(yy,x)

! Transform the 'a' and 'b' sequences into 'd' and 'e'.

      call c_fast_dft(forward_in=a, &
           forward_out=d)
      call c_fast_dft(forward_in=b, &
           forward_out=e)

! Invert the product d*e.

      call c_fast_dft(inverse_in=d*e, &
           inverse_out=f)

! Check the Convolution Theorem:
! inverse(transform(a)*transform(b)) = convolution(a,b).

      err = maxval(abs(c-f))/maxval(abs(c))
      if (err <= sqrt(epsilon(one))) then
         write (*,*) 'Example 4 for FAST_DFT is correct.'
      end if

      end
```

Output

```
Example 4 for FAST_DFT is correct.
```

FAST_2DFT

more...

Computes the Discrete Fourier Transform (2DFT) of a rank-2 complex array, *x*.

Required Arguments

No required arguments; pairs of optional arguments are required. These pairs are `forward_in` and `forward_out` or `inverse_in` and `inverse_out`.

Optional Arguments

forward_in = `x` (Input)
Stores the input complex array of rank-2 to be transformed.

forward_out = `y` (Output)
Stores the output complex array of rank-2 resulting from the transform.

inverse_in = `y` (Input)
Stores the input complex array of rank-2 to be inverted.

inverse_out = `x` (Output)
Stores the output complex array of rank-2 resulting from the inverse transform.

mdata = `m` (Input)
Uses the sub-array in first dimension of size m for the numbers.
Default value: m = size(`x`, `1`).

ndata = `n` (Input)
Uses the sub-array in the second dimension of size `n` for the numbers.
Default value: `n` = size(`x`, `2`).

ido = `ido` (Input/Output)

Integer flag that directs user action. Normally, this argument is used only when the working variables required for the transform and its inverse are saved in the calling program unit. Computing the working variables and saving them in internal arrays within `fast_2dft` is the default. This initialization step is expensive.

There is a two-step process to compute the working variables just once. Example 3 illustrates this usage. The general algorithm for this usage is to enter fast_2dft with ido = 0. A return occurs thereafter with ido < 0. The optional rank-1 complex array w(:) with size(w) >= –ido must be re-allocated. Then, re-enter fast_2dft. The next return from fast_2dft has the output value ido = 1. The variables required for the transform and its inverse are saved in w(:). Thereafter, when the routine is entered with ido = 1 and for the same values of m and n, the contents of w(:) will be used for the working variables. The expensive initialization step is avoided. The optional arguments "ido=" and "work_array=" must be used together.

work_array = `w(:)` (Output/Input)Complex array of rank-1 used to store working variables and values between calls to `fast_2dft`. The value for size(`w`) must be at least as large as the value `-ido` for the value of `ido` < 0.

iopt = `iopt(:)` (Input/Output)

Derived type array with the same precision as the input array; used for passing optional data to `fast_2dft`. The options are as follows:

Packaged Options for FAST_2DFT		
Option Prefix = ?	Option Name	Option Value
`c_, z_`	`fast_2dft_scan_for_NaN`	1
`c_, z_`	`fast_2dft_near_power_of_2`	2
`c_, z_`	`fast_2dft_scale_forward`	3
`c_, z_`	`fast_2dft_scale_inverse`	4

iopt(IO) = `?_options(?_fast_2dft_scan_for_NaN, ?_dummy)`

Examines each input array entry to find the first value such that `isNaN(x(i,j)) ==.true.` See the `isNaN()` function, *Chapter 10*.

Default: Does not scan for NaNs.

iopt(IO) = `?_options(?_fast_2dft_near_power_of_2, ?_dummy)`

Nearest powers of 2≥*m* and ≥*n* are returned as outputs in `iopt(IO + 1)%idummy` and `iopt(IO + 2)%idummy`.

iopt(IO) = `?_options(?_fast_2dft_scale_forward, real_part_of_scale)`

iopt(IO+1) = `?_options(?_dummy, imaginary_part_of_scale)`

Complex number defined by the factor

cmplx(`real_part_of_scale, imaginary_part_of_scale`) is multiplied by the forward transformed array.

Default value is 1.

iopt(IO) = `?_options(?_fast_2dft_scale_inverse, real_part_of_scale)`

iopt(IO+1) = `?_options(?_dummy, imaginary_part_of_scale)`

Complex number defined by the factor cmplx(`real_part_of_scale, imaginary_part_of_scale`) is multiplied by the inverse transformed array.

Default value is 1.

FORTRAN 90 Interface

Generic: None

Specific: The specific interface names are `S_FAST_2DFT`, `D_FAST_2DFT`, `C_FAST_2DFT`, and `Z_FAST_2DFT`.

Description

The `fast_2dft` routine is a Fortran 90 version of the FFT suite of IMSL (1994, pp. 772-776).

Fatal and Terminal Messages

See the *messages.gls* file for error messages for `FAST_2DFT`. These error messages are numbered 670–680; 720–730.

Examples

Example 1: Transforming an Array of Random Complex Numbers

An array of random complex numbers is obtained. The transform of the numbers is inverted and the final results are compared with the input array.

```
      use fast_2dft_int
      use rand_int

      implicit none

! This is Example 1 for FAST_2DFT.

      integer, parameter :: n=24
```

```
      integer, parameter :: m=40
      real(kind(1e0)) :: err, one=1e0
      complex(kind(1e0)), dimension(n,m) :: a, b, c


! Generate a random complex sequence.
      a=rand(a); c=a

! Transform and then invert the transform.
      call c_fast_2dft(forward_in=a, &
           forward_out=b)
      call c_fast_2dft(inverse_in=b, &
           inverse_out=a)

! Check that inverse(transform(sequence)) = sequence.
      err = maxval(abs(c-a))/maxval(abs(c))
      if (err <= sqrt(epsilon(one))) then
         write (*,*) 'Example 1 for FAST_2DFT is correct.'
      end if

     end
```

Output

```
Example 1 for FAST_2DFT is correct.
```

Example 2: Cyclical 2D Data with a Linear Trend

This set of data is sampled from a function $x(s, t) = a + bs + ct + y(s, t)$, where $y(s, t)$ is an harmonic series. The independent variables are normalized as $-1 \le s \le 1$ and $-1 \le t \le 1$. Thus, the data is said *to have cyclical components plus a linear trend*. As a first step, the linear terms are effectively removed from the data using the least-squares system solver. Then, the residuals are transformed and the resulting frequencies are analyzed.

```
      use fast_2dft_int
      use lin_sol_lsq_int
      use sort_real_int
      use rand_int
      implicit none

! This is Example 2 for FAST_2DFT.

      integer i
      integer, parameter :: n=8, k=15
      integer ip(n*n), order(k)
      real(kind(1e0)), parameter :: one=1e0, two=2e0, zero=0e0
      real(kind(1e0)) delta_t
      real(kind(1e0)) rn(3), s(n), t(n), temp(n*n), new_order(k)
      complex(kind(1e0)) a, b, c, a_trend(n*n,3), b_trend(n*n,1),  &
               f(n,n), r(n,n), x(n,n), x_trend(3,1)
      complex(kind(1e0)), dimension(n,n) :: g=zero, h=zero

! Generate random data for planar trend.
      rn = rand(rn)
      a = rn(1)
      b = rn(2)
      c = rn(3)

! Generate the frequency components of the harmonic series.
! Non-zero random amplitudes given on two edges of the square domain.
      g(1:,1)=rand(g(1:,1))
      g(1,1:)=rand(g(1,1:))
```

```
! Invert 'g' into the harmonic series 'h' in time domain.
      call c_fast_2dft(inverse_in=g, inverse_out=h)


! Compute sampling interval.
      delta_t = two/n
      s = (/(-one + (i-1)*delta_t, i=1,n)/)
      t = (/(-one + (i-1)*delta_t, i=1,n)/)

! Make up data set as a linear trend plus harmonics.
      x = a + b*spread(s,dim=2,ncopies=n) +   &
              c*spread(t,dim=1,ncopies=n) + h

! Define least-squares matrix data for a planar trend.
      a_trend(1:,1) = one
      a_trend(1:,2) = reshape(spread(s,dim=2,ncopies=n),(/n*n/))
      a_trend(1:,3) = reshape(spread(t,dim=1,ncopies=n),(/n*n/))
      b_trend(1:,1) = reshape(x,(/n*n/))

! Solve for a linear trend.
      call lin_sol_lsq(a_trend, b_trend, x_trend)

! Compute harmonic residuals.
      r = x -  reshape(matmul(a_trend,x_trend),(/n,n/))

! Transform harmonic residuals.
      call c_fast_2dft(forward_in=r, forward_out=f)

      ip = (/(i,i=1,n**2)/)

! Sort the magnitude of the transform.
      call s_sort_real(-(abs(reshape(f,(/n*n/)))), &
                                      temp, iperm=ip)

! The dominant frequencies are output in ip(1:k).
! Sort these values to compare with the original frequency order.
      call s_sort_real(real(ip(1:k)), new_order)

      order(1:n) = (/(i,i=1,n)/)
      order(n+1:k) = (/((i-n)*n+1,i=n+1,k)/)

! Check the results.
      if (count(order /= int(new_order)) == 0) then
         write (*,*) 'Example 2 for FAST_2DFT is correct.'
      end if

      end
```

Output

```
Example 2 for FAST_2DFT is correct.
```

Example 3: Several 2D Transforms with Initialization

In this example, the optional arguments `ido` and `work_array` are used to save working variables in the calling program unit. This results in maximum efficiency of the transform and its inverse since the working variables do not have to be precomputed following each entry to routine `fast_2dft`.

```
      use fast_2dft_int

      implicit none
```

```
! This is Example 3 for FAST_2DFT.

      integer i, j
      integer, parameter :: n=256
      real(kind(1e0)), parameter :: one=1e0, zero=0e0
      real(kind(1e0)) r(n,n), err
      complex(kind(1e0)) a(n,n), b(n,n), c(n,n)

! The value of the array size for work(:) is computed in the
! routine fast_dft as a first step.

      integer ido_value
      complex(kind(1e0)), allocatable :: work(:)


! Fill in value one for points inside the circle with r=64.
      a = zero
      r = reshape((/(((i-n/2)**2 + (j-n/2)**2, i=1,n), &
                  j=1,n)/),(/n,n/))
      where (r <= (n/4)**2) a = one
      c = a

! Transform and then invert the sequence using the pre-computed
! working values.
      ido_value = 0
      do
         if(allocated(work)) deallocate(work)

! Allocate the space required for work(:).
         if (ido_value <= 0) allocate(work(-ido_value))

! Transform the image and then invert it back.
      call c_fast_2dft(forward_in=a, &
           forward_out=b, IDO=ido_value, work_array=work)
         if (ido_value == 1) exit
      end do
      call c_fast_2dft(inverse_in=b, &
           inverse_out=a, IDO=ido_value, work_array=work)

! Deallocate the space used for work(:).
      if (allocated(work)) deallocate(work)

! Check that inverse(transform(image)) = image.
      err = maxval(abs(c-a))/maxval(abs(c))
      if (err <= sqrt(epsilon(one))) then
         write (*,*) 'Example 3 for FAST_2DFT is correct.'
      end if

      end
```

Output

```
Example 3 for FAST_2DFT is correct.
```

FAST_3DFT

more...

Computes the Discrete Fourier Transform (3DFT) of a rank-3 complex array.

Required Arguments

No required arguments; pairs of optional arguments are required. These pairs are `forward_in` and `forward_out` or `inverse_in` and `inverse_out`.

Optional Arguments

forward_in = `x` (Input)
Stores the input complex array of rank-3 to be transformed.

forward_out = `y` (Output)
Stores the output complex array of rank-3 resulting from the transform.

inverse_in = `y` (Input)
Stores the input complex array of rank-3 to be inverted.

inverse_out = x (Output)Stores the output complex array of rank-3 resulting from the inverse transform.

mdata = `m` (Input)
Uses the sub-array in first dimension of size `m` for the numbers.
Default value: m = size(`x`, `1`).

ndata = n (Input)
Uses the sub-array in the second dimension of size `n` for the numbers.
Default value: `n` = size(`x`, `2`).

kdata = `k` (Input)
Uses the sub-array in the third dimension of size `k` for the numbers.
Default value: `k` = size(`x`, `3`).

ido = `ido` (Input/Output)

Integer flag that directs user action. Normally, this argument is used only when the working variables required for the transform and its inverse are saved in the calling program unit. Computing the working variables and saving them in internal arrays within `fast_3dft` is the default. This initialization step is expensive.

There is a two-step process to compute the working variables just once. The general algorithm for this usage is to enter fast_3dft with ido = 0. A return occurs thereafter with ido < 0. The optional rank-1 complex array w(:) with size(w) >= –ido must be re-allocated. Then, re-enter fast_3dft. The next return from fast_3dft has the output value ido = 1. The variables required for the transform and its inverse are saved in w(:). Thereafter, when the routine is entered with ido = 1 and for the same values of m and n, the contents of w(:) will be used for the working variables. The expensive initialization step is avoided. The optional arguments "ido=" and "work_array=" must be used together.

work_array = `w(:)` (Output/Input)

Complex array of rank-1 used to store working variables and values between calls to `fast_3dft`. The value for size(`w`) must be at least as large as the value `-ido` for the value of `ido` < 0.

iopt = iopt(:) (Input/Output)Derived type array with the same precision as the input array; used for passing optional data to ***fast_3dft***. The options are as follows:

Packaged Options for FAST_3DFT		
Option Prefix = ?	Option Name	Option Value
`C_, z_`	`fast_3dft_scan_for_NaN`	1
`C_, z_`	`fast_3dft_near_power_of_2`	2
`C_, z_`	`fast_3dft_scale_forward`	3
`C_, z_`	`fast_3dft_scale_inverse`	4

iopt(IO) = `?_options(?_fast_3dft_scan_for_NaN, ?_dummy)`

Examines each input array entry to find the first value such that `isNaN(x(i,j,k)) ==.true.` See the `isNaN()` function, *Chapter 10*.

Default: Does not scan for NaNs.

iopt(IO) = `?_options(?_fast_3dft_near_power_of_2, ?_dummy)`

Nearest powers of 2 ≥ m, ≥ n, and ≥ k are returned as an outputs in `iopt(IO+1)%idummy`, `iopt(IO+2)%idummy` and `iopt(IO+3)%idummy`

iopt(IO) = `?_options(?_fast_3dft_scale_forward, real_part_of_scale)`

iopt(IO+1) = `?_options(?_dummy, imaginary_part_of_scale)`

Complex number defined by the factor
cmplx(`real_part_of_scale, imaginary_part_of_scale`) is multiplied by the forward transformed array.
Default value is 1.

iopt(IO) = `?_options(?_fast_3dft_scale_inverse, real_part_of_scale)`

iopt(IO+1) = `?_options(?_dummy, imaginary_part_of_scale)`

Complex number defined by the factor
cmplx(`real_part_of_scale, imaginary_part_of_scale`) is multiplied by the inverse transformed array.
Default value is 1.

FORTRAN 90 Interface

Generic: None

Specific: The specific interface names are `S_FAST_3DFT`, `D_FAST_3DFT`, `C_FAST_3DFT`, and `Z_FAST_3DFT`.

Description

The `fast_3dft` routine is a Fortran 90 version of the FFT suite of IMSL (1994, pp. 772-776).

Fatal and Terminal Messages

See the *messages.gls* file for error messages for `FAST_3DFT`. These error messages are numbered 685–695; 740–750.

Example

An array of random complex numbers is obtained. The transform of the numbers is inverted and the final results are compared with the input array.

```
      use fast_3dft_int
      implicit none
! This is Example 1 for FAST_3DFT.
      integer i, j, k
```

```
       integer, parameter :: n=64
       real(kind(1e0)), parameter :: one=1e0, zero=0e0
       real(kind(1e0)) r(n,n,n), err
       complex(kind(1e0)) a(n,n,n), b(n,n,n), c(n,n,n)

 ! Fill in value one for points inside the sphere
 ! with radius=16.
       a = zero
       do i=1,n
         do j=1,n
           do k=1,n
             r(i,j,k) = (i-n/2)**2+(j-n/2)**2+(k-n/2)**2
           end do
         end do
       end do
       where (r <= (n/4)**2) a = one
       c = a

 ! Transform the image and then invert it back.
        call c_fast_3dft(forward_in=a, &
            forward_out=b)
        call c_fast_3dft(inverse_in=b, &
            inverse_out=a)

 ! Check that inverse(transform(image)) = image.
       err = maxval(abs(c-a))/maxval(abs(c))
       if (err <= sqrt(epsilon(one))) then
          write (*,*) 'Example 1 for FAST_3DFT is correct.'
       end if

       end
```

Output

```
Example 1 for FAST_3DFT is correct.
```

FFTRF

more...

Computes the Fourier coefficients of a real periodic sequence.

Required Arguments

N — Length of the sequence to be transformed. (Input)

SEQ — Array of length `N` containing the periodic sequence. (Input)

COEF — Array of length `N` containing the Fourier coefficients. (Output)

FORTRAN 90 Interface

Generic: `CALL FFTRF (N, SEQ, COEF)`

Specific: The specific interface names are `S_FFTRF` and `D_FFTRF`.

FORTRAN 77 Interface

Single: `CALL FFTRF (N, SEQ, COEF)`

Double: The double precision name is `DFFTRF`.

Description

The routine `FFTRF` computes the discrete Fourier transform of a real vector of size *N*. It uses the Intel® Math Kernel Library or IBM Engineering and Scientific Subroutine Library for the computation, if available. Otherwise, the method used is a variant of the Cooley-Tukey algorithm that is most efficient when *N* is a product of small prime factors. If *N* satisfies this condition, then the computational effort is proportional to $N \log N$.

Specifically, given an *N*-vector s = `SEQ`, `FFTRF` returns in c = `COEF`, if *N* is even:

$$c_{2m-2} = \sum_{n=1}^{N} s_n \cos\left[\frac{(m-1)(n-1)2\pi}{N}\right] m = 2, \ldots, N/2+1$$

$$c_{2m-1} = -\sum_{n=1}^{N} s_n \sin\left[\frac{(m-1)(n-1)2\pi}{N}\right] m = 2, \ldots, N/2$$

$$c_1 = \sum_{n=1}^{N} s_n$$

If N is odd, c_m is defined as above for m from 2 to $(N + 1)/2$.

We now describe a fairly common usage of this routine. Let f be a real valued function of time. Suppose we sample f at N equally spaced time intervals of length Δ seconds starting at time t_0. That is, we have

$$\text{SEQ}_i := f(t_0 + (i-1)\Delta) \quad i = 1, 2, \ldots, N$$

The routine `FFTRF` treats this sequence as if it were periodic of period N. In particular, it assumes that $f(t_0) = f(t_0 + N\Delta)$. Hence, the period of the function is assumed to be $T = N\Delta$.

Now, `FFTRF` accepts as input `SEQ` and returns as output coefficients c = `COEF` that satisfy the following relation when N is odd (N even is similar):

$$\text{SEQ}_i = \frac{1}{N}\left[c_1 + 2\sum_{n=2}^{(N+1)/2} c_{2n-2}\cos\left[\frac{2\pi(n-1)(i-1)}{N}\right] - 2\sum_{n=2}^{(N+1)/2} c_{2n-1}\sin\left[\frac{2\pi(n-1)(i-1)}{N}\right]\right]$$

This formula is very revealing. It can be interpreted in the following manner. The coefficients produced by `FFTRF` produce an interpolating trigonometric polynomial to the data. That is, if we define

$$\begin{aligned} g(t) &:= \frac{1}{N}\left[c_1 + 2\sum_{n=2}^{(N+1)/2} c_{2n-2}\cos\left[\frac{2\pi(n-1)(t-t_0)}{N\Delta}\right] - 2\sum_{n=2}^{(N+1)/2} c_{2n-1}\sin\left[\frac{2\pi(n-1)(t-t_0)}{N\Delta}\right]\right] \\ &= \frac{1}{N}\left[c_1 + 2\sum_{n=2}^{(N+1)/2} c_{2n-2}\cos\left[\frac{2\pi(n-1)(t-t_0)}{T}\right] - 2\sum_{n=2}^{(N+1)/2} c_{2n-1}\sin\left[\frac{2\pi(n-1)(t-t_0)}{T}\right]\right] \end{aligned}$$

then, we have

$$f(t_0 + (i-1)\Delta) = g(t_0 + (i-1)\Delta)$$

Now, suppose we want to discover the dominant frequencies. One forms the vector P of length $N/2$ as follows:

$$P_1 := |c_1|$$
$$P_k := \sqrt{c_{2k-2}^2 + c_{2k-1}^2} \quad k = 2, 3, \ \dots, \ (N+1)/2$$

These numbers correspond to the energy in the spectrum of the signal. In particular, P_k corresponds to the energy level at frequency

$$\frac{k-1}{T} = \frac{k-1}{N\Delta} \quad k = 1, 2 \dots, \frac{N+1}{2}$$

Furthermore, note that there are only $(N + 1)/2 \approx T/(2\Delta)$ resolvable frequencies when N observations are taken. This is related to the Nyquist phenomenon, which is induced by discrete sampling of a continuous signal.

Similar relations hold for the case when N is even.

Finally, note that the Fourier transform has an (unnormalized) inverse that is implemented in `FFTRB`. The routine `FFTRF` is based on the real `FFT` in `FFTPACK`. The package `FFTPACK` was developed by Paul Swarztrauber at the National Center for Atmospheric Research.

Comments

1. Workspace may be explicitly provided, if desired, by use of `F2TRF/DF2TRF`. The reference is:

   `CALL F2TRF (N, SEQ, COEF, WFFTR)`

   The additional argument is

   WFFTR — Array of length 2`N` + 15 initialized by `FFTRI`. (Input)
   The initialization depends on `N`.

   If the Intel® Math Kernel Library or IBM Engineering and Scientific Subroutine Library is used, `WFFTR` is not referenced.

2. The routine `FFTRF` is most efficient when `N` is the product of small primes.

3. The arrays `COEF` and `SEQ` may be the same.

4. If `FFTRF/FFTRB` is used repeatedly with the same value of `N`, then call `FFTRI` followed by repeated calls to `F2TRF/F2TRB`. This is more efficient than repeated calls to `FFTRF/FFTRB`.

If the Intel® Math Kernel Library or IBM Engineering and Scientific Subroutine Library is used, parameters computed by `FFTRI` are not used. In this case, there is no need to call `FFTRI`.

Example

In this example, a pure cosine wave is used as a data vector, and its Fourier series is recovered. The Fourier series is a vector with all components zero except at the appropriate frequency where it has an N.

```
      USE FFTRF_INT
      USE CONST_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    N
      PARAMETER  (N=7)
!
      INTEGER    I, NOUT
      REAL       COEF(N), COS, FLOAT, TWOPI, SEQ(N)
      INTRINSIC  COS, FLOAT
      TWOPI = CONST('PI')
!
      TWOPI = 2.0*TWOPI
!                                 Get output unit number
      CALL UMACH (2, NOUT)
!                                 This loop fills out the data vector
!                                 with a pure exponential signal
      DO 10  I=1, N
         SEQ(I) = COS(FLOAT(I-1)*TWOPI/FLOAT(N))
   10 CONTINUE
!                                 Compute the Fourier transform of SEQ
      CALL FFTRF (N, SEQ, COEF)
!                                 Print results
      WRITE (NOUT,99998)
99998 FORMAT (9X, 'INDEX', 5X, 'SEQ', 6X, 'COEF')
      WRITE (NOUT,99999) (I, SEQ(I), COEF(I), I=1,N)
99999 FORMAT (1X, I11, 5X, F5.2, 5X, F5.2)
      END
```

Output

```
INDEX     SEQ       COEF
  1      1.00       0.00
  2      0.62       3.50
  3     -0.22       0.00
  4     -0.90       0.00
  5     -0.90       0.00
  6     -0.22       0.00
  7      0.62       0.00
```

FFTRB

more...

Computes the real periodic sequence from its Fourier coefficients.

Required Arguments

N — Length of the sequence to be transformed. (Input)

COEF — Array of length `N` containing the Fourier coefficients. (Input)

SEQ — Array of length `N` containing the periodic sequence. (Output)

FORTRAN 90 Interface

Generic: `CALL FFTRB (N, COEF, SEQ [, …])`

Specific: The specific interface names are `S_FFTRB` and `D_FFTRB`.

FORTRAN 77 Interface

Single: `CALL FFTRB (N, COEF, SEQ)`

Double: The double precision name is `DFFTRB`.

Description

The routine `FFTRB` is the unnormalized inverse of the routine `FFTRF`. This routine computes the discrete inverse Fourier transform of a real vector of size *N*. It uses the Intel® Math Kernel Library or IBM Engineering and Scientific Subroutine Library for the computation, if available. Otherwise, the method used is a variant of the Cooley-Tukey algorithm, which is most efficient when *N* is a product of small prime factors. If *N* satisfies this condition, then the computational effort is proportional to *N* log *N*.

Specifically, given an *N*-vector *c* = `COEF`, `FFTRB` returns in *s* = `SEQ`, if *N* is even:

$$s_m = c_1 + (-1)^{(m-1)} c_N + 2\sum_{n=2}^{N/2} c_{2n-2} \cos\frac{[(n-1)(m-1)2\pi]}{N} - 2\sum_{n=2}^{N/2} c_{2n-1} \sin\frac{[(n-1)(m-1)2\pi]}{N}$$

If *N* is odd:

$$s_m = c_1 + 2\sum_{n=2}^{(N+1)/2} c_{2n-2} \cos\frac{[(n-1)(m-1)2\pi]}{N} - 2\sum_{n=2}^{(N+1)/2} c_{2n-1} \sin\frac{[(n-1)(m-1)2\pi]}{N}$$

The routine `FFTRB` is based on the inverse real FFT in FFTPACK. The package FFTPACK was developed by Paul Swarztrauber at the National Center for Atmospheric Research.

Comments

1. Workspace may be explicitly provided, if desired, by use of `F2TRB/DF2TRB`. The reference is:

   `CALL F2TRB (N, COEF, SEQ, WFFTR)`

   The additional argument is

   WFFTR — Array of length 2`N` + 15 initialized by `FFTRI`. (Input)
   The initialization depends on `N`.

   If the Intel® Math Kernel Library or IBM Engineering and Scientific Subroutine Library is used, `WFFTR` is not referenced.

2. The routine `FFTRB` is most efficient when `N` is the product of small primes.

3. The arrays `COEF` and `SEQ` may be the same.

4. If `FFTRF/FFTRB` is used repeatedly with the same value of `N`, then call `FFTRI` followed by repeated calls to `F2TRF/F2TRB`. This is more efficient than repeated calls to `FFTRF/FFTRB`.

If the Intel® Math Kernel Library or IBM Engineering and Scientific Subroutine Library is used, parameters computed by `FFTRI` are not used. In this case, there is no need to call `FFTRI`.

Example

We compute the forward real FFT followed by the inverse operation. In this example, we first compute the Fourier transform

$$\hat{x} = COEF$$

of the vector x, where $x_j = (-1)^j$ for j = 1 to N. This vector

$$\hat{x}$$

is now input into FFTRB with the resulting output $s = Nx$, that is, $s_j = (-1)^j N$ for j = 1 to N.

```
      USE FFTRB_INT
      USE CONST_INT
      USE FFTRF_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    N
      PARAMETER  (N=7)
!
      INTEGER    I, NOUT
      REAL       COEF(N), FLOAT, SEQ(N), TWOPI, X(N)
      INTRINSIC  FLOAT
      TWOPI = CONST('PI')
!
      TWOPI = TWOPI
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Fill the data vector
      DO 10  I=1, N
         X(I) = FLOAT((-1)**I)
   10 CONTINUE
!                                  Compute the forward transform of X
      CALL FFTRF (N, X, COEF)
!                                  Print results
      WRITE (NOUT,99994)
      WRITE (NOUT,99995)
99994 FORMAT (9X, 'Result after forward transform')
99995 FORMAT (9X, 'INDEX', 5X, 'X', 8X, 'COEF')
      WRITE (NOUT,99996) (I, X(I), COEF(I), I=1,N)
99996 FORMAT (1X, I11, 5X, F5.2, 5X, F5.2)
!                                  Compute the backward transform of
!                                  COEF
      CALL FFTRB (N, COEF, SEQ)
!                                 Print results
      WRITE (NOUT,99997)
      WRITE (NOUT,99998)
99997 FORMAT (/, 9X, 'Result after backward transform')
99998 FORMAT (9X, 'INDEX', 4X, 'COEF', 6X, 'SEQ')
      WRITE (NOUT,99999) (I, COEF(I), SEQ(I), I=1,N)
99999 FORMAT (1X, I11, 5X, F5.2, 5X, F5.2)
      END
```

Output

```
Result after forward transform
INDEX     X         COEF
  1     -1.00     -1.00
  2      1.00     -1.00
  3     -1.00     -0.48
  4      1.00     -1.00
  5     -1.00     -1.25
  6      1.00     -1.00
  7     -1.00     -4.38
```

```
Result after backward transform
INDEX    COEF      SEQ
  1     -1.00     -7.00
  2     -1.00      7.00
  3     -0.48     -7.00
  4     -1.00      7.00
  5     -1.25     -7.00
  6     -1.00      7.00
  7     -4.38     -7.00
```

FFTRI

Computes parameters needed by FFTRF and FFTRB.

Required Arguments

N — Length of the sequence to be transformed. (Input)

WFFTR — Array of length 2N + 15 containing parameters needed by FFTRF and FFTRB. (Output)

FORTRAN 90 Interface

Generic: CALL FFTRI (N, WFFTR)

Specific: The specific interface names are S_FFTRI and D_FFTRI.

FORTRAN 77 Interface

Single: CALL FFTRI (N, WFFTR)

Double: The double precision name is DFFTRI.

Description

The routine FFTRI initializes the routines FFTRF and FFTRB. An efficient way to make multiple calls for the same *N* to routine FFTRF or FFTRB, is to use routine FFTRI for initialization. (In this case, replace FFTRF or FFTRB with F2TRF or F2TRB, respectively.) The routine FFTRI is based on the routine RFFTI in FFTPACK. The package FFTPACK was developed by Paul Swarztrauber at the National Center for Atmospheric Research.

If the Intel® Math Kernel Library or IBM Engineering and Scientific Subroutine Library is used, parameters computed by FFTRI are not used. In this case, there is no need to call FFTRI.

Comments

Different WFFTR arrays are needed for different values of N.

Example

In this example, we compute three distinct real FFTs by calling FFTRI once and then calling F2TRF three times.

```
      USE FFTRI_INT
      USE CONST_INT
      USE F2TRF_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    N
      PARAMETER  (N=7)
!
      INTEGER    I, K, NOUT
      REAL       COEF(N), COS, FLOAT, TWOPI, WFFTR(29), SEQ(N)
      INTRINSIC  COS, FLOAT
!
      TWOPI = CONST('PI')
      TWOPI = 2* TWOPI
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Set the work vector
      CALL FFTRI (N, WFFTR)
!
      DO 20  K=1, 3
!                                  This loop fills out the data vector
!                                  with a pure exponential signal
         DO 10  I=1, N
            SEQ(I) = COS(FLOAT(K*(I-1))*TWOPI/FLOAT(N))
   10 CONTINUE
!                                  Compute the Fourier transform of SEQ
         CALL F2TRF (N, SEQ, COEF, WFFTR)
!                                  Print results
         WRITE (NOUT,99998)
99998    FORMAT (/, 9X, 'INDEX', 5X, 'SEQ', 6X, 'COEF')
         WRITE (NOUT,99999) (I, SEQ(I), COEF(I), I=1,N)
99999    FORMAT (1X, I11, 5X, F5.2, 5X, F5.2)
!
   20 CONTINUE
      END
```

Output

```
INDEX     SEQ       COEF
  1       1.00      0.00
  2       0.62      3.50
  3      -0.22      0.00
  4      -0.90      0.00
  5      -0.90      0.00
  6      -0.22      0.00
  7       0.62      0.00


INDEX     SEQ       COEF
  1       1.00      0.00
  2      -0.22      0.00
  3      -0.90      0.00
  4       0.62      3.50
  5       0.62      0.00
  6      -0.90      0.00
  7      -0.22      0.00
```

```
 INDEX     SEQ       COEF
 1       1.00      0.00
 2      -0.90      0.00
 3       0.62      0.00
 4      -0.22      0.00
 5      -0.22      0.00
 6       0.62      3.50
 7      -0.90      0.00
```

FFTCF

more...

Computes the Fourier coefficients of a complex periodic sequence.

Required Arguments

N — Length of the sequence to be transformed. (Input)

SEQ — Complex array of length `N` containing the periodic sequence. (Input)

COEF — Complex array of length `N` containing the Fourier coefficients. (Output)

FORTRAN 90 Interface

Generic: `CALL FFTCF (N, SEQ, COEF)`

Specific: The specific interface names are `S_FFTCF` and `D_FFTCF`.

FORTRAN 77 Interface

Single: `CALL FFTCF (N, SEQ, COEF)`

Double: The double precision name is `DFFTCF`.

Description

The routine `FFTCF` computes the discrete complex Fourier transform of a complex vector of size *N*. It uses the Intel® Math Kernel Library, Sun Performance Library or IBM Engineering and Scientific Subroutine Library for the computation, if available. Otherwise, the method used is a variant of the Cooley-Tukey algorithm, which is most efficient when *N* is a product of small prime factors. If *N* satisfies this condition, then the computational effort is proportional to *N* log *N*. This considerable savings has historically led people to refer to this algorithm as the “fast Fourier transform” or FFT.

Specifically, given an *N*-vector *x*, `FFTCF` returns in *c* = `COEF`

$$c_m = \sum_{n=1}^{N} x_n e^{-2\pi i(n-1)(m-1)/N}$$

Furthermore, a vector of Euclidean norm *S* is mapped into a vector of norm

$$\sqrt{N}S$$

Finally, note that we can invert the Fourier transform as follows:

$$x_n = \frac{1}{N}\sum_{m=1}^{N} c_m e^{2\pi i(m-1)(n-1)/N}$$

This formula reveals the fact that, after properly normalizing the Fourier coefficients, one has the coefficients for a trigonometric interpolating polynomial to the data. An unnormalized inverse is implemented in `FFTCB`. `FFTCF` is based on the complex FFT in FFTPACK. The package FFTPACK was developed by Paul Swarztrauber at the National Center for Atmospheric Research.

Comments

1. Workspace may be explicitly provided, if desired, by use of `F2TCF/DF2TCF`. The reference is:

   `CALL F2TCF (N, SEQ, COEF, WFFTC, CPY)`

   The additional arguments are as follows:

   WFFTC — Real array of length 4 * `N` + 15 initialized by `FFTCI`. The initialization depends on `N`. (Input)

   CPY — Real array of length 2 * `N`. (Workspace)

   If the Intel® Math Kernel Library, Sun Performance Library or IBM Engineering and Scientific Subroutine Library is used, `WFFTC` and `CPY` are not referenced.

2. The routine `FFTCF` is most efficient when `N` is the product of small primes.

3. The arrays `COEF` and `SEQ` may be the same.

4. If `FFTCF/FFTCB` is used repeatedly with the same value of `N`, then call `FFTCI` followed by repeated calls to `F2TCF/F2TCB`. This is more efficient than repeated calls to `FFTCF/FFTCB`.

If the Intel® Math Kernel Library, Sun Performance Library or IBM Engineering and Scientific Subroutine Library is used, parameters computed by `FFTCI` are not used. In this case, there is no need to call `FFTCI`.

Example

In this example, we input a pure exponential data vector and recover its Fourier series, which is a vector with all components zero except at the appropriate frequency where it has an N. Notice that the norm of the input vector is

$$\sqrt{N}$$

but the norm of the output vector is N.

```
      USE FFTCF_INT
      USE CONST_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    N
      PARAMETER  (N=7)
!
      INTEGER    I, NOUT
      REAL       TWOPI
      COMPLEX    C, CEXP, COEF(N), H, SEQ(N)
      INTRINSIC  CEXP
!
      C     = (0.,1.)
      TWOPI = CONST('PI')
      TWOPI = 2.0 * TWOPI
!                                Here we compute (2*pi*i/N)*3.
      H = (TWOPI*C/N)*3.
!                                This loop fills out the data vector
!                                with a pure exponential signal of
!                                frequency 3.
      DO 10  I=1, N
         SEQ(I) = CEXP((I-1)*H)
   10 CONTINUE
!                                Compute the Fourier transform of SEQ
      CALL FFTCF (N, SEQ, COEF)
!                                Get output unit number and print
!                                results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99998)
99998 FORMAT (9X, 'INDEX', 8X, 'SEQ', 15X, 'COEF')
      WRITE (NOUT,99999) (I, SEQ(I), COEF(I), I=1,N)
99999 FORMAT (1X, I11, 5X,'(',F5.2,',',F5.2,')', &
                 5X,'(',F5.2,',',F5.2,')')
      END
```

Output

```
INDEX        SEQ                 COEF
  1     ( 1.00, 0.00)      ( 0.00, 0.00)
  2     (-0.90, 0.43)      ( 0.00, 0.00)
  3     ( 0.62,-0.78)      ( 0.00, 0.00)
  4     (-0.22, 0.97)      ( 7.00, 0.00)
  5     (-0.22,-0.97)      ( 0.00, 0.00)
  6     ( 0.62, 0.78)      ( 0.00, 0.00)
  7     (-0.90,-0.43)      ( 0.00, 0.00)
```

FFTCB

more...

Computes the complex periodic sequence from its Fourier coefficients.

Required Arguments

N — Length of the sequence to be transformed. (Input)

COEF — Complex array of length N containing the Fourier coefficients. (Input)

SEQ — Complex array of length N containing the periodic sequence. (Output)

FORTRAN 90 Interface

Generic: CALL FFTCB (N, COEF, SEQ)

Specific: The specific interface names are S_FFTCB and D_FFTCB.

FORTRAN 77 Interface

Single: CALL FFTCB (N, COEF, SEQ)

Double: The double precision name is DFFTCB.

Description

The routine FFTCB computes the inverse discrete complex Fourier transform of a complex vector of size *N*. It uses the Intel® Math Kernel Library, Sun Performance Library or IBM Engineering and Scientific Subroutine Library for the computation, if available. Otherwise, the method used is a variant of the Cooley-Tukey algorithm, which is most efficient when *N* is a product of small prime factors. If *N* satisfies this condition, then the computational effort is proportional to *N* log *N*. This considerable savings has historically led people to refer to this algorithm as the "fast Fourier transform" or FFT.

Specifically, given an *N*-vector *c* = COEF, FFTCB returns in *s* = SEQ

$$s_m = \sum_{n=1}^{N} c_n e^{2\pi i(n-1)(m-1)/N}$$

Furthermore, a vector of Euclidean norm *S* is mapped into a vector of norm

$$\sqrt{N}\,S$$

Finally, note that we can invert the inverse Fourier transform as follows:

$$c_n = \frac{1}{N}\sum_{m=1}^{N} s_m e^{-2\pi i(n-1)(m-1)/N}$$

This formula reveals the fact that, after properly normalizing the Fourier coefficients, one has the coefficients for a trigonometric interpolating polynomial to the data. `FFTCB` is based on the complex inverse FFT in FFTPACK. The package FFTPACK was developed by Paul Swarztrauber at the National Center for Atmospheric Research.

Comments

1. Workspace may be explicitly provided, if desired, by use of `F2TCB/DF2TCB`. The reference is:

   `CALL F2TCB (N, COEF, SEQ, WFFTC, CPY)`

   The additional arguments are as follows:

   WFFTC — Real array of length 4 * `N` + 15 initialized by `FFTCI`. The initialization depends on `N`. (Input)

   CPY — Real array of length 2 * `N`. (Workspace)

   If the Intel® Math Kernel Library, Sun Performance Library or IBM Engineering and Scientific Subroutine Library is used, `WFFTC` and `CPY` are not referenced.

2. The routine `FFTCB` is most efficient when `N` is the product of small primes.

3. The arrays `COEF` and `SEQ` may be the same.

4. If `FFTCF/FFTCB` is used repeatedly with the same value of `N`; then call `FFTCI` followed by repeated calls to `F2TCF/F2TCB`. This is more efficient than repeated calls to `FFTCF/FFTCB`.

If the Intel® Math Kernel Library, Sun Performance Library or IBM Engineering and Scientific Subroutine Library is used, parameters computed by `FFTCI` are not used. In this case, there is no need to call `FFTCI`.

Example

In this example, we first compute the Fourier transform of the vector x, where $x_j = j$ for j = 1 to N. Note that the norm of x is $(N[N + 1][2N + 1]/6)^{1/2}$, and hence, the norm of the transformed vector

$$\hat{x} = c$$

is $N([N + 1][2N + 1]/6)^{1/2}$. The vector

$$\hat{x}$$

is used as input into FFTCB with the resulting output $s = Nx$, that is, $s_j = jN$, for j = 1 to N.

```
      USE FFTCB_INT
      USE FFTCF_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    N
      PARAMETER  (N=7)
!
      INTEGER    I, NOUT
      COMPLEX    CMPLX, SEQ(N), COEF(N), X(N)
      INTRINSIC  CMPLX
!                                 This loop fills out the data vector
!                                 with X(I)=I, I=1,N
      DO 10  I=1, N
         X(I) = CMPLX(I,0)
   10 CONTINUE
!                                 Compute the forward transform of X
      CALL FFTCF (N, X, COEF)
!                                 Compute the backward transform of
!                                 COEF
      CALL FFTCB (N, COEF, SEQ)
!                                 Get output unit number
      CALL UMACH (2, NOUT)
!                                 Print results
      WRITE (NOUT,99998)
      WRITE (NOUT,99999) (I, X(I), COEF(I), SEQ(I), I=1,N)
99998 FORMAT (5X, 'INDEX', 9X, 'INPUT', 9X, 'FORWARD TRANSFORM', 3X, &
            'BACKWARD TRANSFORM')
99999 FORMAT (1X, I7, 7X,'(',F5.2,',',F5.2,')', &
                     7X,'(',F5.2,',',F5.2,')', &
                     7X,'(',F5.2,',',F5.2,')')
      END
```

Output

```
INDEX      INPUT         FORWARD TRANSFORM   BACKWARD TRANSFORM
 1       ( 1.00, 0.00)       (28.00, 0.00)       ( 7.00, 0.00)
 2       ( 2.00, 0.00)       (-3.50, 7.27)       (14.00, 0.00)
 3       ( 3.00, 0.00)       (-3.50, 2.79)       (21.00, 0.00)
 4       ( 4.00, 0.00)       (-3.50, 0.80)       (28.00, 0.00)
 5       ( 5.00, 0.00)       (-3.50,-0.80)       (35.00, 0.00)
 6       ( 6.00, 0.00)       (-3.50,-2.79)       (42.00, 0.00)
 7       ( 7.00, 0.00)       (-3.50,-7.27)       (49.00, 0.00)
```

FFTCI

Computes parameters needed by FFTCF and FFTCB.

Required Arguments

N — Length of the sequence to be transformed. (Input)

WFFTC — Array of length 4N + 15 containing parameters needed by FFTCF and FFTCB. (Output)

FORTRAN 90 Interface

Generic: CALL FFTCI (N, WFFTC)

Specific: The specific interface names are S_FFTCI and D_FFTCI.

FORTRAN 77 Interface

Single: CALL FFTCI (N, WFFTC)

Double: The double precision name is DFFTCI.

Description

The routine FFTCI initializes the routines FFTCF and FFTCB. An efficient way to make multiple calls for the same N to IMSL routine FFTCF or FFTCB is to use routine FFTCI for initialization. (In this case, replace FFTCF or FFTCB with F2TCF or F2TCB, respectively.) The routine FFTCI is based on the routine CFFTI in FFTPACK. The package FFTPACK was developed by Paul Swarztrauber at the National Center for Atmospheric Research.

If the Intel® Math Kernel Library, Sun Performance Library or IBM Engineering and Scientific Subroutine Library is used, parameters computed by FFTCI are not used. In this case, there is no need to call FFTCI.

Comments

Different WFFTC arrays are needed for different values of N.

Example

In this example, we compute a two-dimensional complex FFT by making one call to `FFTCI` followed by 2`N` calls to `F2TCF`.

```
      USE FFTCI_INT
      USE CONST_INT
      USE F2TCF_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                  SPECIFICATIONS FOR PARAMETERS
      INTEGER    N
      PARAMETER  (N=4)
!
      INTEGER    I, IR, IS, J, NOUT
      REAL       FLOAT, TWOPI, WFFTC(35), CPY(2*N)
      COMPLEX    CEXP, CMPLX, COEF(N,N), H, SEQ(N,N), TEMP
      INTRINSIC  CEXP, CMPLX, FLOAT
!
      TWOPI = CONST('PI')
      TWOPI = 2*TWOPI
      IR    = 3
      IS    = 1
!                                  Here we compute e**(2*pi*i/N)
      TEMP = CMPLX(0.0,TWOPI/FLOAT(N))
      H    = CEXP(TEMP)
!                                  Fill SEQ with data
      DO 20  I=1, N
         DO 10  J=1, N
            SEQ(I,J)  = H**((I-1)*(IR-1)+(J-1)*(IS-1))
   10 CONTINUE
   20 CONTINUE
!                                  Print out SEQ
!                                  Get output unit number
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99997)
      DO 30  I=1, N
         WRITE (NOUT,99998)  (SEQ(I,J),J=1,N)
   30 CONTINUE
!                                  Set initialization vector
      CALL FFTCI (N, WFFTC)
!                                  Transform the columns of SEQ
      DO 40  I=1, N
         CALL F2TCF (N, SEQ(1:,I), COEF(1:,I), WFFTC, CPY)
   40 CONTINUE
!                                  Take transpose of the result
      DO 60  I=1, N
         DO 50  J=I + 1, N
            TEMP      = COEF(I,J)
            COEF(I,J) = COEF(J,I)
            COEF(J,I) = TEMP
   50 CONTINUE
   60 CONTINUE
!                                  Transform the columns of this result
      DO 70  I=1, N
         CALL F2TCF (N, COEF(1:,I), SEQ(1:,I), WFFTC, CPY)
   70 CONTINUE
!                                  Take transpose of the result
      DO 90  I=1, N
         DO 80  J=I + 1, N
            TEMP     = SEQ(I,J)
            SEQ(I,J) = SEQ(J,I)
            SEQ(J,I) = TEMP
```

```
   80  CONTINUE
   90 CONTINUE
!                                  Print results
      WRITE (NOUT,99999)
      DO 100  I=1, N
         WRITE (NOUT,99998) (SEQ(I,J),J=1,N)
  100 CONTINUE
!
99997 FORMAT (1X, 'The input matrix is below')
99998 FORMAT (1X, 4(' (',F5.2,',',F5.2,')'))
99999 FORMAT (/, 1X, 'Result of two-dimensional transform')
      END
```

Output

```
The input matrix is below
 ( 1.00, 0.00) ( 1.00, 0.00) ( 1.00, 0.00) ( 1.00, 0.00)
 (-1.00, 0.00) (-1.00, 0.00) (-1.00, 0.00) (-1.00, 0.00)
 ( 1.00, 0.00) ( 1.00, 0.00) ( 1.00, 0.00) ( 1.00, 0.00)
 (-1.00, 0.00) (-1.00, 0.00) (-1.00, 0.00) (-1.00, 0.00)

Result of two-dimensional transform
 ( 0.00, 0.00) ( 0.00, 0.00) ( 0.00, 0.00) ( 0.00, 0.00)
 ( 0.00, 0.00) ( 0.00, 0.00) ( 0.00, 0.00) ( 0.00, 0.00)
 (16.00, 0.00) ( 0.00, 0.00) ( 0.00, 0.00) ( 0.00, 0.00)
 ( 0.00, 0.00) ( 0.00, 0.00) ( 0.00, 0.00) ( 0.00, 0.00)
```

FSINT

Computes the discrete Fourier sine transformation of an odd sequence.

Required Arguments

N — Length of the sequence to be transformed. It must be greater than 1. (Input)

SEQ — Array of length `N` containing the sequence to be transformed. (Input)

COEF — Array of length `N` + 1 containing the transformed sequence. (Output)

FORTRAN 90 Interface

Generic:	`CALL FSINT` (`N`, `SEQ`, `COEF`)
Specific:	The specific interface names are `S_FSINT` and `D_FSINT`.

FORTRAN 77 Interface

Single:	`CALL FSINT` (`N`, `SEQ`, `COEF`)
Double:	The double precision name is `DFSINT`.

Description

The routine `FSINT` computes the discrete Fourier sine transform of a real vector of size N. The method used is a variant of the Cooley-Tukey algorithm, which is most efficient when $N + 1$ is a product of small prime factors. If N satisfies this condition, then the computational effort is proportional to $N \log N$.

Specifically, given an N-vector s = `SEQ`, `FSINT` returns in c = `COEF`

$$c_m = 2\sum_{n=1}^{N} s_n \sin\left(\frac{mn\pi}{N+1}\right)$$

Finally, note that the Fourier sine transform is its own (unnormalized) inverse. The routine `FSINT` is based on the sine FFT in FFTPACK. The package FFTPACK was developed by Paul Swarztrauber at the National Center for Atmospheric Research.

Comments

1. Workspace may be explicitly provided, if desired, by use of F2INT/DF2INT. The reference is:

   CALL F2INT (N, SEQ, COEF, WFSIN)

   The additional argument is:

   WFSIN — Array of length INT(2.5 * N + 15) initialized by FSINI. The initialization depends on N. (Input)

2. The routine FSINT is most efficient when N + 1 is the product of small primes.

3. The routine FSINT is its own (unnormalized) inverse. Applying FSINT twice will reproduce the original sequence multiplied by 2 * (N + 1).

4. The arrays COEF and SEQ may be the same, if SEQ is also dimensioned at least N + 1.

5. COEF (N + 1) is needed as workspace.

6. If FSINT is used repeatedly with the same value of N, then call FSINI followed by repeated calls to F2INT. This is more efficient than repeated calls to FSINT.

Example

In this example, we input a pure sine wave as a data vector and recover its Fourier sine series, which is a vector with all components zero except at the appropriate frequency it has an *N*.

```
      USE FSINT_INT
      USE CONST_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    N
      PARAMETER  (N=7)
!
      INTEGER    I, NOUT
      REAL       COEF(N+1), FLOAT, PI, SIN, SEQ(N)
      INTRINSIC  FLOAT, SIN
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Fill the data vector SEQ
!                                  with a pure sine wave
      PI = CONST('PI')
      DO 10  I=1, N
         SEQ(I) = SIN(FLOAT(I)*PI/FLOAT(N+1))
   10 CONTINUE
!                                  Compute the transform of SEQ
      CALL FSINT (N, SEQ, COEF)
!                                  Print results
      WRITE (NOUT,99998)
      WRITE (NOUT,99999) (I, SEQ(I), COEF(I), I=1,N)
99998 FORMAT (9X, 'INDEX', 6X, 'SEQ', 7X, 'COEF')
99999 FORMAT (1X, I11, 5X, F6.2, 5X, F6.2)
      END
```

Output

```
INDEX       SEQ        COEF
  1        0.38        8.00
  2        0.71        0.00
  3        0.92        0.00
  4        1.00        0.00
  5        0.92        0.00
  6        0.71        0.00
  7        0.38        0.00
```

FSINI

Computes parameters needed by FSINT.

Required Arguments

N — Length of the sequence to be transformed. N must be greater than 1. (Input)

WFSIN — Array of length INT(2.5 * N + 15) containing parameters needed by FSINT. (Output)

FORTRAN 90 Interface

Generic: CALL FSINI (N, WFSIN)

Specific: The specific interface names are S_FSINI and D_FSINI.

FORTRAN 77 Interface

Single: CALL FSINI (N, WFSIN)

Double: The double precision name is DFSINI.

Description

The routine FSINI initializes the routine FSINT. An efficient way to make multiple calls for the same *N* to IMSL routine FSINT, is to use routine FSINI for initialization. (In this case, replace FSINT with F2INT.) The routine FSINI is based on the routine SINTI in FFTPACK. The package FFTPACK was developed by Paul Swarztrauber at the National Center for Atmospheric Research.

Comments

Different WFSIN arrays are needed for different values of N.

Example

In this example, we compute three distinct sine FFTs by calling FSINI once and then calling F2INT three times.

```
      USE FSINI_INT
      USE UMACH_INT
      USE CONST_INT
```

```
      USE F2INT_INT

      IMPLICIT   NONE
      INTEGER    N
      PARAMETER  (N=7)
!
      INTEGER    I, K, NOUT
      REAL       COEF(N+1), FLOAT, PI, SIN, WFSIN(32), SEQ(N)
      INTRINSIC  FLOAT, SIN
!                                 Get output unit number
      CALL UMACH (2, NOUT)
!                                 Initialize the work vector WFSIN
      CALL FSINI (N, WFSIN)
!                                 Different frequencies of the same
!                                 wave will be transformed
      DO 20  K=1, 3
!                                 Fill the data vector SEQ
!                                 with a pure sine wave
         PI = CONST('PI')
         DO 10  I=1, N
            SEQ(I) = SIN(FLOAT(K*I)*PI/FLOAT(N+1))
   10    CONTINUE
!                                 Compute the transform of SEQ
         CALL F2INT (N, SEQ, COEF, WFSIN)
!                                 Print results
         WRITE (NOUT,99998)
         WRITE (NOUT,99999) (I, SEQ(I), COEF(I), I=1,N)
   20 CONTINUE
99998 FORMAT (/, 9X, 'INDEX', 6X, 'SEQ', 7X, 'COEF')
99999 FORMAT (1X, I11, 5X, F6.2, 5X, F6.2)
      END
```

Output

```
INDEX      SEQ        COEF
  1       0.38        8.00
  2       0.71        0.00
  3       0.92        0.00
  4       1.00        0.00
  5       0.92        0.00
  6       0.71        0.00
  7       0.38        0.00

INDEX      SEQ        COEF
  1       0.71        0.00
  2       1.00        8.00
  3       0.71        0.00
  4       0.00        0.00
  5      -0.71        0.00
  6      -1.00        0.00
  7      -0.71        0.00

INDEX      SEQ        COEF
  1       0.92        0.00
  2       0.71        0.00
  3      -0.38        8.00
  4      -1.00        0.00
  5      -0.38        0.00
  6       0.71        0.00
  7       0.92        0.00
```

FCOST

Computes the discrete Fourier cosine transformation of an even sequence.

Required Arguments

N — Length of the sequence to be transformed. It must be greater than 1. (Input)

SEQ — Array of length N containing the sequence to be transformed. (Input)

COEF — Array of length N containing the transformed sequence. (Output)

FORTRAN 90 Interface

Generic: CALL FCOST (N, SEQ, COEF)

Specific: The specific interface names are S_FCOST and D_FCOST.

FORTRAN 77 Interface

Single: CALL FCOST (N, SEQ, COEF)

Double: The double precision name is DFCOST.

Description

The routine FCOST computes the discrete Fourier cosine transform of a real vector of size *N*. It uses the IBM Engineering and Scientific Subroutine Library for the computation, if available. Otherwise, the method used is a variant of the Cooley-Tukey algorithm , which is most efficient when $N - 1$ is a product of small prime factors. If *N* satisfies this condition, then the computational effort is proportional to $N \log N$.

Specifically, given an *N*-vector *s* = SEQ, FCOST returns in *c* = COEF

$$c_m = 2\sum_{n=2}^{N-1} s_n \cos\left[\frac{(m-1)(n-1)\pi}{N-1}\right] + s_1 + s_N(-1)^{(m-1)}$$

Finally, note that the Fourier cosine transform is its own (unnormalized) inverse. Two applications of FCOST to a vector *s* produces (2*N* 2)*s*. The routine FCOST is based on the cosine FFT in FFTPACK. The package FFTPACK was developed by Paul Swarztrauber at the National Center for Atmospheric Research.

Comments

1. Workspace may be explicitly provided, if desired, by use of F2OST/DF2OST. The reference is:

   CALL F2OST (N, SEQ, COEF, WFCOS)

   The additional argument is

   WFCOS — Array of length 3 * N + 15 initialized by FCOSI. The initialization depends on N. (Input)

   If the IBM Engineering and Scientific Subroutine Library is used, WFCOS is not referenced.

2. The routine FCOST is most efficient when N 1 is the product of small primes.

3. The routine FCOST is its own (unnormalized) inverse. Applying FCOST twice will reproduce the original sequence multiplied by 2 * (N − 1).

4. The arrays COEF and SEQ may be the same.

5. If FCOST is used repeatedly with the same value of N, then call FCOSI followed by repeated calls to F2OST. This is more efficient than repeated calls to FCOST.

If the IBM Engineering and Scientific Subroutine Library is used, parameters computed by FCOSI are not used. In this case, there is no need to call FCOSI.

Example

In this example, we input a pure cosine wave as a data vector and recover its Fourier cosine series, which is a vector with all components zero except at the appropriate frequency it has an $N-1$.

```
      USE FCOST_INT
      USE CONST_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    N
      PARAMETER  (N=7)
!
      INTEGER    I, NOUT
      REAL       COEF(N), COS, FLOAT, PI, SEQ(N)
      INTRINSIC  COS, FLOAT
!
      CALL UMACH (2, NOUT)
!                                 Fill the data vector SEQ
!                                 with a pure cosine wave
      PI = CONST('PI')
      DO 10  I=1, N
         SEQ(I) = COS(FLOAT(I-1)*PI/FLOAT(N-1))
   10 CONTINUE
!                                 Compute the transform of SEQ
      CALL FCOST (N, SEQ, COEF)
!                                 Print results
      WRITE (NOUT,99998)
      WRITE (NOUT,99999) (I, SEQ(I), COEF(I), I=1,N)
```

```
99998 FORMAT (9X, 'INDEX', 6X, 'SEQ', 7X, 'COEF')
99999 FORMAT (1X, I11, 5X, F6.2, 5X, F6.2)
      END
```

Output

```
INDEX      SEQ        COEF
  1       1.00        0.00
  2       0.87        6.00
  3       0.50        0.00
  4       0.00        0.00
  5      -0.50        0.00
  6      -0.87        0.00
  7      -1.00        0.00
```

FCOSI

Computes parameters needed by FCOST.

Required Arguments

N — Length of the sequence to be transformed. N must be greater than 1. (Input)

WFCOS — Array of length 3N + 15 containing parameters needed by FCOST. (Output)

FORTRAN 90 Interface

Generic: CALL FCOSI (N, WFCOS)

Specific: The specific interface names are S_FCOSI and D_FCOSI.

FORTRAN 77 Interface

Single: CALL FCOSI (N, WFCOS)

Double: The double precision name is DFCOSI.

Description

The routine FCOSI initializes the routine FCOST. An efficient way to make multiple calls for the same *N* to IMSL routine FCOST is to use routine FCOSI for initialization. (In this case, replace FCOST with F2OST.) The routine FCOSI is based on the routine COSTI in FFTPACK. The package FFTPACK was developed by Paul Swarztrauber at the National Center for Atmospheric Research.

If the IBM Engineering and Scientific Subroutine Library is used, parameters computed by FCOSI are not used. In this case, there is no need to call FCOSI.

Comments

Different WFCOS arrays are needed for different values of N.

Example

In this example, we compute three distinct cosine FFTs by calling `FCOSI` once and then calling `F2OST` three times.

```
      USE FCOSI_INT
      USE CONST_INT
      USE F2OST_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    N
      PARAMETER  (N=7)
!
      INTEGER    I, K, NOUT
      REAL       COEF(N), COS, FLOAT, PI, WFCOS(36), SEQ(N)
      INTRINSIC  COS, FLOAT
!                                 Get output unit number
      CALL UMACH (2, NOUT)
!                                 Initialize the work vector WFCOS
      CALL FCOSI (N, WFCOS)
!                                 Different frequencies of the same
!                                 wave will be transformed
      PI = CONST('PI')
      DO 20  K=1, 3
!                                 Fill the data vector SEQ
!                                 with a pure cosine wave
         DO 10  I=1, N
            SEQ(I) = COS(FLOAT(K*(I-1))*PI/FLOAT(N-1))
   10    CONTINUE
!                                 Compute the transform of SEQ
         CALL F2OST (N, SEQ, COEF, WFCOS)
!                                 Print results
         WRITE (NOUT,99998)
         WRITE (NOUT,99999) (I, SEQ(I), COEF(I), I=1,N)
   20 CONTINUE
99998 FORMAT (/, 9X, 'INDEX', 6X, 'SEQ', 7X, 'COEF')
99999 FORMAT (1X, I11, 5X, F6.2, 5X, F6.2)
      END
```

Output

```
INDEX      SEQ        COEF
  1        1.00       0.00
  2        0.87       6.00
  3        0.50       0.00
  4        0.00       0.00
  5       -0.50       0.00
  6       -0.87       0.00
  7       -1.00       0.00

INDEX      SEQ        COEF
  1        1.00       0.00
  2        0.50       0.00
  3       -0.50       6.00
  4       -1.00       0.00
  5       -0.50       0.00
  6        0.50       0.00
  7        1.00       0.00

INDEX      SEQ        COEF
  1        1.00       0.00
```

```
    2        0.00        0.00
    3       -1.00        0.00
    4        0.00        6.00
    5        1.00        0.00
    6        0.00        0.00
    7       -1.00        0.00
```

QSINF

Computes the coefficients of the sine Fourier transform with only odd wave numbers.

Required Arguments

N — Length of the sequence to be transformed. (Input)

SEQ — Array of length `N` containing the sequence. (Input)

COEF — Array of length `N` containing the Fourier coefficients. (Output)

FORTRAN 90 Interface

Generic: `CALL QSINF` (`N`, `SEQ`, `COEF`)

Specific: The specific interface names are `S_QSINF` and `D_QSINF`.

FORTRAN 77 Interface

Single: `CALL QSINF` (`N`, `SEQ`, `COEF`)

Double: The double precision name is `DQSINF`.

Description

The routine `QSINF` computes the discrete Fourier quarter sine transform of a real vector of size *N*. The method used is a variant of the Cooley-Tukey algorithm, which is most efficient when *N* is a product of small prime factors. If *N* satisfies this condition, then the computational effort is proportional to *N* log *N*.

Specifically, given an N-vector *s* = `SEQ`, `QSINF` returns in *c* = `COEF`

$$c_m = 2\sum_{n=1}^{N-1} s_n \sin\left[\frac{(2m-1)n\pi}{2N}\right] + s_N(-1)^{m-1}$$

Finally, note that the Fourier quarter sine transform has an (unnormalized) inverse, which is implemented in the IMSL routine `QSINB`. The routine `QSINF` is based on the quarter sine FFT in FFTPACK. The package FFTPACK was developed by Paul Swarztrauber at the National Center for Atmospheric Research.

Comments

1. Workspace may be explicitly provided, if desired, by use of Q2INF/DQ2INF. The reference is:

   CALL Q2INF (N, SEQ, COEF, WQSIN)

   The additional argument is:

   WQSIN — Array of length 3 * N + 15 initialized by QSINI. The initialization depends on N. (Input)

2. The routine QSINF is most efficient when N is the product of small primes.

3. The arrays COEF and SEQ may be the same.

4. If QSINF/QSINB is used repeatedly with the same value of N, then call QSINI followed by repeated calls to Q2INF/Q2INB. This is more efficient than repeated calls to QSINF/QSINB.

Example

In this example, we input a pure quarter sine wave as a data vector and recover its Fourier quarter sine series.

```
      USE QSINF_INT
      USE CONST_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    N
      PARAMETER  (N=7)
!
      INTEGER    I, NOUT
      REAL       COEF(N), FLOAT, PI, SIN, SEQ(N)
      INTRINSIC  FLOAT, SIN
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Fill the data vector SEQ
!                                  with a pure sine wave
      PI = CONST('PI')
      DO 10  I=1, N
         SEQ(I) = SIN(FLOAT(I)*(PI/2.0)/FLOAT(N))
   10 CONTINUE
!                                  Compute the transform of SEQ
      CALL QSINF (N, SEQ, COEF)
!                                  Print results
      WRITE (NOUT,99998)
      WRITE (NOUT,99999) (I, SEQ(I), COEF(I), I=1,N)
99998 FORMAT (9X, 'INDEX', 6X, 'SEQ', 7X, 'COEF')
99999 FORMAT (1X, I11, 5X, F6.2, 5X, F6.2)
      END
```

Output

```
INDEX       SEQ         COEF
  1        0.22         7.00
  2        0.43         0.00
  3        0.62         0.00
  4        0.78         0.00
```

```
     5        0.90        0.00
     6        0.97        0.00
     7        1.00        0.00
```

QSINB

Computes a sequence from its sine Fourier coefficients with only odd wave numbers.

Required Arguments

N — Length of the sequence to be transformed. (Input)

COEF — Array of length `N` containing the Fourier coefficients. (Input)

SEQ — Array of length `N` containing the sequence. (Output)

FORTRAN 90 Interface

Generic: `CALL QSINB (N, COEF, SEQ)`

Specific: The specific interface names are `S_QSINB` and `D_QSINB`.

FORTRAN 77 Interface

Single: `CALL QSINB (N, COEF, SEQ)`

Double: The double precision name is `DQSINB`.

Description

The routine `QSINB` computes the discrete (unnormalized) inverse Fourier quarter sine transform of a real vector of size *N*. The method used is a variant of the Cooley-Tukey algorithm, which is most efficient when *N* is a product of small prime factors. If *N* satisfies this condition, then the computational effort is proportional to *N* log *N*.

Specifically, given an *N*-vector c = `COEF`, `QSINB` returns in s = `SEQ`

$$s_m = 4\sum_{n=1}^{N} c_n \sin\left(\frac{(2n-1)m\pi}{2N}\right)$$

Furthermore, a vector x of length *N* that is first transformed by `QSINF` and then by `QSINB` will be returned by `QSINB` as $4Nx$. The routine `QSINB` is based on the inverse quarter sine FFT in FFTPACK which was developed by Paul Swarztrauber at the National Center for Atmospheric Research.

Comments

1. Workspace may be explicitly provided, if desired, by use of Q2INB/DQ2INB. The reference is:

   CALL Q2INB (N, SEQ, COEF, WQSIN)

   The additional argument is:

   WQSIN — array of length 3 * N + 15 initialized by QSINI. The initialization depends on N.(Input)

2. The routine QSINB is most efficient when N is the product of small primes.

3. The arrays COEF and SEQ may be the same.

4. If QSINF/QSINB is used repeatedly with the same value of N, then call QSINI followed by repeated calls to Q2INF/Q2INB. This is more efficient than repeated calls to QSINF/QSINB.

Example

In this example, we first compute the quarter wave sine Fourier transform *c* of the vector *x* where $x_n = n$ for $n = 1$ to N. We then compute the inverse quarter wave Fourier transform of *c* which is $4Nx = s$.

```
      USE QSINB_INT
      USE QSINF_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    N
      PARAMETER  (N=7)
!
      INTEGER    I, NOUT
      REAL       FLOAT, SEQ(N), COEF(N), X(N)
      INTRINSIC  FLOAT
!                                 Get output unit number
      CALL UMACH (2, NOUT)
!                                 Fill the data vector X
!                                 with X(I) = I, I=1,N
      DO 10  I=1, N
         X(I) = FLOAT(I)
   10 CONTINUE
!                                 Compute the forward transform of X
      CALL QSINF (N, X, COEF)
!                                 Compute the backward transform of W
      CALL QSINB (N, COEF, SEQ)
!C                                 Print results
      WRITE (NOUT,99998)
      WRITE (NOUT,99999) (X(I), COEF(I), SEQ(I), I=1,N)
99998 FORMAT (5X, 'INPUT', 5X, 'FORWARD TRANSFORM', 3X, 'BACKWARD ', &
            'TRANSFORM')
99999 FORMAT (3X, F6.2, 10X, F6.2, 15X, F6.2)
      END
```

Output

```
INPUT     FORWARD TRANSFORM   BACKWARD TRANSFORM
```

```
  1.00            39.88                28.00
  2.00            -4.58                56.00
  3.00             1.77                84.00
  4.00            -1.00               112.00
  5.00             0.70               140.00
  6.00            -0.56               168.00
  7.00             0.51               196.00
```

QSINI

Computes parameters needed by QSINF and QSINB.

Required Arguments

N — Length of the sequence to be transformed. (Input)

WQSIN — Array of length 3N + 15 containing parameters needed by QSINF and QSINB. (Output)

FORTRAN 90 Interface

Generic: CALL QSINI (N, WQSIN)

Specific: The specific interface names are S_QSINI and D_QSINI.

FORTRAN 77 Interface

Single: CALL QSINI (N, WQSIN)

Double: The double precision name is DQSINI.

Description

The routine QSINI initializes the routines QSINF and QSINB. An efficient way to make multiple calls for the same *N* to IMSL routine QSINF or QSINB is to use routine QSINI for initialization. (In this case, replace QSINF or QSINB with Q2INF or Q2INB, respectively.) The routine QSINI is based on the routine SINQI in FFTPACK. The package FFTPACK was developed by Paul Swarztrauber at the National Center for Atmospheric Research.

Comments

Different WQSIN arrays are needed for different values of N.

Example

In this example, we compute three distinct quarter sine transforms by calling QSINI once and then calling Q2INF three times.

```
      USE QSINI_INT
```

```
      USE CONST_INT
      USE Q2INF_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    N
      PARAMETER  (N=7)
!
      INTEGER    I, K, NOUT
      REAL       COEF(N), FLOAT, PI, SIN, WQSIN(36), SEQ(N)
      INTRINSIC  FLOAT, SIN
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Initialize the work vector WQSIN
      CALL QSINI (N, WQSIN)
!                                  Different frequencies of the same
!                                  wave will be transformed
      PI = CONST('PI')
      DO 20  K=1, 3
!                                  Fill the data vector SEQ
!                                  with a pure sine wave
         DO 10  I=1, N
            SEQ(I) = SIN(FLOAT((2*K-1)*I)*(PI/2.0)/FLOAT(N))
   10    CONTINUE
!                                  Compute the transform of SEQ
         CALL Q2INF (N, SEQ, COEF, WQSIN)
!                                  Print results
         WRITE (NOUT,99998)
         WRITE (NOUT,99999) (I, SEQ(I), COEF(I), I=1,N)
   20 CONTINUE
99998 FORMAT (/, 9X, 'INDEX', 6X, 'SEQ', 7X, 'COEF')
99999 FORMAT (1X, I11, 5X, F6.2, 5X, F6.2)
      END
```

Output

```
INDEX      SEQ       COEF
  1        0.22      7.00
  2        0.43      0.00
  3        0.62      0.00
  4        0.78      0.00
  5        0.90      0.00
  6        0.97      0.00
  7        1.00      0.00

INDEX      SEQ       COEF
  1        0.62      0.00
  2        0.97      7.00
  3        0.90      0.00
  4        0.43      0.00
  5       -0.22      0.00
  6       -0.78      0.00
  7       -1.00      0.00

INDEX      SEQ       COEF
  1        0.90      0.00
  2        0.78      0.00
  3       -0.22      7.00
  4       -0.97      0.00
  5       -0.62      0.00
  6        0.43      0.00
  7        1.00      0.00
```

QCOSF

Computes the coefficients of the cosine Fourier transform with only odd wave numbers.

Required Arguments

N — Length of the sequence to be transformed. (Input)

SEQ — Array of length `N` containing the sequence. (Input)

COEF — Array of length `N` containing the Fourier coefficients. (Output)

FORTRAN 90 Interface

Generic: `CALL QCOSF (N, SEQ, COEF [, …])`

Specific: The specific interface names are `S_QCOSF` and `D_QCOSF`.

FORTRAN 77 Interface

Single: `CALL QCOSF (N, SEQ, COEF)`

Double: The double precision name is `DQCOSF`.

Description

The routine `QCOSF` computes the discrete Fourier quarter cosine transform of a real vector of size *N*. The method used is a variant of the Cooley-Tukey algorithm, which is most efficient when *N* is a product of small prime factors. If *N* satisfies this condition, then the computational effort is proportional to *N* log *N*.

Specifically, given an *N*-vector *s* = `SEQ`, `QCOSF` returns in *c* = `COEF`

$$c_m = s_1 + 2\sum_{n=2}^{N} s_n \cos\left(\frac{(2m-1)(n-1)\pi}{2N}\right)$$

Finally, note that the Fourier quarter cosine transform has an (unnormalized) inverse which is implemented in `QCOSB`. The routine `QCOSF` is based on the quarter cosine FFT in FFTPACK. The package FFTPACK was developed by Paul Swarztrauber at the National Center for Atmospheric Research.

Comments

1. Workspace may be explicitly provided, if desired, by use of Q2OSF/DQ2OSF. The reference is:

   CALL Q2OSF (N, SEQ, COEF, WQCOS)

   The additional argument is:

   WQCOS — Array of length 3 * N + 15 initialized by QCOSI. The initialization depends on N. (Input)

2. The routine QCOSF is most efficient when N is the product of small primes.

3. The arrays COEF and SEQ may be the same.

4. If QCOSF/QCOSB is used repeatedly with the same value of N, then call QCOSI followed by repeated calls to Q2OSF/Q2OSB. This is more efficient than repeated calls to QCOSF/QCOSB.

Example

In this example, we input a pure quarter cosine wave as a data vector and recover its Fourier quarter cosine series.

```
      USE QCOSF_INT
      USE CONST_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    N
      PARAMETER  (N=7)
!
      INTEGER    I, NOUT
      REAL       COEF(N), COS, FLOAT, PI, SEQ(N)
      INTRINSIC  COS, FLOAT
!                                 Get output unit number
      CALL UMACH (2, NOUT)
!                                 Fill the data vector SEQ
!                                 with a pure cosine wave
      PI = CONST('PI')
      DO 10  I=1, N
            SEQ(I) = COS(FLOAT(I-1)*(PI/2.0)/FLOAT(N))
   10    CONTINUE

!                                 Compute the transform of SEQ
         Call QCOSF (N, SEQ, COEF)
!                                  Print results
         WRITE (NOUT,99998)
         WRITE (NOUT,99999) (I, SEQ(I), COEF(I), I=1,N)
99998 FORMAT (9X, 'INDEX', 6X, 'SEQ', 7X, 'COEF')
99999 FORMAT (1X, I11, 5X, F6.2, 5X, F6.2)
      END
```

Output

```
INDEX      SEQ        COEF
  1        1.00       7.00
```

```
    2       0.97       0.00
    3       0.90       0.00
    4       0.78       0.00
    5       0.62       0.00
    6       0.43       0.00
    7       0.22       0.00
```

QCOSB

Computes a sequence from its cosine Fourier coefficients with only odd wave numbers.

Required Arguments

N — Length of the sequence to be transformed. (Input)

COEF — Array of length `N` containing the Fourier coefficients. (Input)

SEQ — Array of length `N` containing the sequence. (Output)

FORTRAN 90 Interface

Generic: `CALL QCOSB (N, COEF, SEQ)`

Specific: The specific interface names are `S_QCOSB` and `D_QCOSB`.

FORTRAN 77 Interface

Single: `CALL QCOSB (N, COEF, SEQ)`

Double: The double precision name is `DQCOSB`.

Description

The routine `QCOSB` computes the discrete (unnormalized) inverse Fourier quarter cosine transform of a real vector of size *N*. The method used is a variant of the Cooley-Tukey algorithm, which is most efficient when *N* is a product of small prime factors. If *N* satisfies this condition, then the computational effort is proportional to *N* log *N*. Specifically, given an *N*-vector c = `COEF`, `QCOSB` returns in s = `SEQ`

$$s_m = 4\sum_{n=1}^{N} c_n \cos\left(\frac{(2n-1)(m-1)\pi}{2N}\right)$$

Furthermore, a vector x of length *N* that is first transformed by `QCOSF` and then by `QCOSB` will be returned by `QCOSB` as $4Nx$. The routine `QCOSB` is based on the inverse quarter cosine FFT in FFTPACK. The package FFTPACK was developed by Paul Swarztrauber at the National Center for Atmospheric Research.

Comments

1. Workspace may be explicitly provided, if desired, by use of `Q2OSB/DQ2OSB`. The reference is:

   `CALL Q2OSB (N, COEF, SEQ, WQCOS)`

   The additional argument is:

   WQCOS — Array of length 3 * `N` + 15 initialized by `QCOSI`. The initialization depends on `N`. (Input)

2. The routine `QCOSB` is most efficient when `N` is the product of small primes.

3. The arrays `COEF` and `SEQ` may be the same.

4. If `QCOSF/QCOSB` is used repeatedly with the same value of `N`, then call `QCOSI` followed by repeated calls to `Q2OSF/Q2OSB`. This is more efficient than repeated calls to `QCOSF/QCOSB`.

Example

In this example, we first compute the quarter wave cosine Fourier transform c of the vector x, where $x_n = n$ for $n = 1$ to N. We then compute the inverse quarter wave Fourier transform of c which is $4Nx = s$.

```
      USE QCOSB_INT
      USE QCOSF_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    N
      PARAMETER  (N=7)
!
      INTEGER    I, NOUT
      REAL       FLOAT, SEQ(N), COEF(N), X(N)
      INTRINSIC  FLOAT
!                                 Get output unit number
      CALL UMACH (2, NOUT)
!                                 Fill the data vector X
!                                 with X(I) = I, I=1,N
      DO 10  I=1, N
         X(I) = FLOAT(I)
   10 CONTINUE
!                                 Compute the forward transform of X
      CALL QCOSF (N, X, COEF)
!                                 Compute the backward transform of
!                                 COEF
      CALL QCOSB (N, COEF, SEQ)
!                                 Print results
      WRITE (NOUT,99998)
      DO 20  I=1, N
         WRITE (NOUT,99999) X(I), COEF(I), SEQ(I)
   20 CONTINUE
99998 FORMAT (5X, 'INPUT', 5X, 'FORWARD TRANSFORM', 3X, 'BACKWARD ', &
            'TRANSFORM')
99999 FORMAT (3X, F6.2, 10X, F6.2, 15X, F6.2)
      END
```

Output

```
INPUT     FORWARD TRANSFORM   BACKWARD TRANSFORM
1.00           31.12               28.00
2.00          -27.45               56.00
3.00           10.97               84.00
4.00           -9.00              112.00
5.00            4.33              140.00
6.00           -3.36              168.00
7.00            0.40              196.00
```

QCOSI

Computes parameters needed by QCOSF and QCOSB.

Required Arguments

N — Length of the sequence to be transformed. (Input)

WQCOS — Array of length 3N + 15 containing parameters needed by QCOSF and QCOSB. (Output)

FORTRAN 90 Interface

Generic: CALL QCOSI (N, WQCOS)

Specific: The specific interface names are S_QCOSI and D_QCOSI.

FORTRAN 77 Interface

Single: CALL QCOSI (N, WQCOS)

Double: The double precision name is DQCOSI.

Description

The routine QCOSI initializes the routines QCOSF and QCOSB. An efficient way to make multiple calls for the same *N* to IMSL routine QCOSF or QCOSB is to use routine QCOSI for initialization. (In this case, replace QCOSF or QCOSB with Q2OSF or Q2OSB , respectively.) The routine QCOSI is based on the routine COSQI in FFTPACK, which was developed by Paul Swarztrauber at the National Center for Atmospheric Research.

Comments

Different WQCOS arrays are needed for different values of N.

Example

In this example, we compute three distinct quarter cosine transforms by calling QCOSI once and then calling Q2OSF three times.

```
      USE QCOSI_INT
```

```
      USE CONST_INT
      USE Q2OSF_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    N
      PARAMETER  (N=7)
!
      INTEGER    I, K, NOUT
      REAL       COEF(N), COS, FLOAT, PI, WQCOS(36), SEQ(N)
      INTRINSIC  COS, FLOAT
!                                 Get output unit number
      CALL UMACH (2, NOUT)
!                                 Initialize the work vector WQCOS
      CALL QCOSI (N, WQCOS)
!                                 Different frequencies of the same
!                                 wave will be transformed
      PI = CONST('PI')
      DO 20  K=1, 3
!                                 Fill the data vector SEQ
!                                 with a pure cosine wave
         DO 10  I=1, N
            SEQ(I) = COS(FLOAT((2*K-1)*(I-1))*(PI/2.0)/FLOAT(N))
   10    CONTINUE
!                                 Compute the transform of SEQ
         CALL Q2OSF (N, SEQ, COEF, WQCOS)
!                                 Print results
         WRITE (NOUT,99998)
         WRITE (NOUT,99999) (I, SEQ(I), COEF(I), I=1,N)
   20 CONTINUE
99998 FORMAT (/, 9X, 'INDEX', 6X, 'SEQ', 7X, 'COEF')
99999 FORMAT (1X, I11, 5X, F6.2, 5X, F6.2)
      END
```

Output

```
INDEX      SEQ       COEF
  1       1.00       7.00
  2       0.97       0.00
  3       0.90       0.00
  4       0.78       0.00
  5       0.62       0.00
  6       0.43       0.00
  7       0.22       0.00

INDEX      SEQ       COEF
  1       1.00       0.00
  2       0.78       7.00
  3       0.22       0.00
  4      -0.43       0.00
  5      -0.90       0.00
  6      -0.97       0.00
  7      -0.62       0.00

INDEX      SEQ       COEF
  1       1.00       0.00
  2       0.43       0.00
  3      -0.62       7.00
  4      -0.97       0.00
  5      -0.22       0.00
  6       0.78       0.00
  7       0.90       0.00
```

FFT2D

more...

Computes Fourier coefficients of a complex periodic two-dimensional array.

Required Arguments

A — `NRA` by `NCA` complex matrix containing the periodic data to be transformed. (Input)

COEF — `NRA` by `NCA` complex matrix containing the Fourier coefficients of `A`. (Output)

Optional Arguments

NRA — The number of rows of `A`. (Input)
Default: `NRA` = size (`A`,1).

NCA — The number of columns of `A`. (Input)
Default: `NCA` = size (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = size (`A`,1).

LDCOEF — Leading dimension of `COEF` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDCOEF` = size `(COEF`,1`)`.

FORTRAN 90 Interface

Generic: `CALL FFT2D` (`A`, `COEF [, …])`

Specific: The specific interface names are `S_FFT2D` and `D_FFT2D`.

FORTRAN 77 Interface

Single: CALL FFT2D (NRA, NCA, A, LDA, COEF, LDCOEF)

Double: The double precision name is DFFT2D.

Description

The routine FFT2D computes the discrete complex Fourier transform of a complex two dimensional array of size (NRA = N) × (NCA = M). It uses the Intel® Math Kernel Library, Sun Performance Library or IBM Engineering and Scientific Subroutine Library for the computation, if available. Otherwise, the method used is a variant of the Cooley-Tukey algorithm , which is most efficient when N and M are each products of small prime factors. If N and M satisfy this condition, then the computational effort is proportional to $N\,M \log N\,M$. This considerable savings has historically led people to refer to this algorithm as the "fast Fourier transform" or FFT.

Specifically, given an $N \times M$ array a, FFT2D returns in c = COEF

$$c_{jk} = \sum_{n=1}^{N} \sum_{m=1}^{M} a_{nm} e^{-2\pi i(j-1)(n-1)/N} e^{-2\pi i(k-1)(m-1)/M}$$

Furthermore, a vector of Euclidean norm S is mapped into a vector of norm

$$\sqrt{NM}\,S$$

Finally, note that an unnormalized inverse is implemented in FFT2B. The routine FFT2D is based on the complex FFT in FFTPACK. The package FFTPACK was developed by Paul Swarztrauber at the National Center for Atmospheric Research.

Comments

1. Workspace may be explicitly provided, if desired, by use of F2T2D/DF2T2D. The reference is:

   CALL F2T2D (NRA, NCA, A, LDA, COEF, LDCOEF, WFF1, WFF2, CWK, CPY)

   The additional arguments are as follows:

   WFF1 — Real array of length 4 * NRA + 15 initialized by FFTCI. The initialization depends on NRA. (Input)

   WFF2 — Real array of length 4 * NCA + 15 initialized by FFTCI. The initialization depends on NCA. (Input)

   CWK — Complex array of length 1. (Workspace)

   CPY — Real array of length 2 * MAX (NRA, NCA). (Workspace)

If the Intel® Math Kernel Library, Sun Performance Library or IBM Engineering and Scientific Subroutine Library is used, `WFFT1`, `WFF2`, `CWK`, and `CPY` are not referenced.

2. The routine `FFT2D` is most efficient when `NRA` and `NCA` are the product of small primes.

3. The arrays `COEF` and `A` may be the same.

4. If `FFT2D/FFT2B` is used repeatedly, with the same values for `NRA` and `NCA`, then use `FFTCI` to fill `WFF1`(`N` = `NRA`) and `WFF2`(`N` = `NCA`). Follow this with repeated calls to `F2T2D/F2T2B`. This is more efficient than repeated calls to `FFT2D/FFT2B`.

If the Intel® Math Kernel Library, Sun Performance Library or IBM Engineering and Scientific Subroutine Library is used, parameters computed by `FFTCI` are not used. In this case, there is no need to call `FFTCI`.

Example

In this example, we compute the Fourier transform of the pure frequency input for a 5 × 4 array

$$a_{nm} = e^{2\pi i(n-1)2/N} e^{2\pi i(m-1)3/M}$$

for $1 \le n \le 5$ and $1 \le m \le 4$ using the IMSL routine `FFT2D`. The result

$$\hat{a} = c$$

has all zeros except in the (3, 4) position.

```
      USE FFT2D_INT
      USE CONST_INT
      USE WRCRN_INT

      IMPLICIT   NONE
      INTEGER    I, IR, IS, J, NCA, NRA
      REAL       FLOAT, TWOPI
      COMPLEX    A(5,4), C, CEXP, CMPLX, COEF(5,4), H
      CHARACTER  TITLE1*26, TITLE2*26
      INTRINSIC  CEXP, CMPLX, FLOAT
!
      TITLE1 = 'The input matrix is below '
      TITLE2 = 'The output matrix is below'
      NRA    = 5
      NCA    = 4
      IR     = 3
      IS     = 4
!                                  Fill A with initial data
      TWOPI = CONST('PI')
      TWOPI = 2.0*TWOPI
      C     = CMPLX(0.0,1.0)
      H     = CEXP(TWOPI*C)
      DO 10  I=1, NRA
         DO 10  J=1, NCA
            A(I,J) = CEXP(TWOPI*C*((FLOAT((I-1)*(IR-1))/FLOAT(NRA)+ &
                     FLOAT((J-1)*(IS-1))/FLOAT(NCA))))
   10 CONTINUE
```

```
!
      CALL WRCRN (TITLE1, A)
!
      CALL FFT2D (A, COEF)
!
      CALL WRCRN (TITLE2, COEF)
!
      END
```

Output

```
                  The input matrix is below
                  1                 2                 3                 4
1  ( 1.000, 0.000)  ( 0.000,-1.000)  (-1.000, 0.000)  ( 0.000, 1.000)
2  (-0.809, 0.588)  ( 0.588, 0.809)  ( 0.809,-0.588)  (-0.588,-0.809)
3  ( 0.309,-0.951)  (-0.951,-0.309)  (-0.309, 0.951)  ( 0.951, 0.309)
4  ( 0.309, 0.951)  ( 0.951,-0.309)  (-0.309,-0.951)  (-0.951, 0.309)
5  (-0.809,-0.588)  (-0.588, 0.809)  ( 0.809, 0.588)  ( 0.588,-0.809)

                   The Output matrix is below
                  1                 2                 3                 4
1  (  0.00,  0.00)  (  0.00,  0.00)  (  0.00,  0.00)  (  0.00,  0.00)
2  (  0.00,  0.00)  (  0.00,  0.00)  (  0.00,  0.00)  (  0.00,  0.00)
3  (  0.00,  0.00)  (  0.00,  0.00)  (  0.00,  0.00)  ( 20.00,  0.00)
4  (  0.00,  0.00)  (  0.00,  0.00)  (  0.00,  0.00)  (  0.00,  0.00)
5  (  0.00,  0.00)  (  0.00,  0.00)  (  0.00,  0.00)  (  0.00,  0.00)
```

FFT2B

more...

Computes the inverse Fourier transform of a complex periodic two-dimensional array.

Required Arguments

COEF — NRCOEF by NCCOEF complex array containing the Fourier coefficients to be transformed. (Input)

A — NRCOEF by NCCOEF complex array containing the Inverse Fourier coefficients of COEF. (Output)

Optional Arguments

NRCOEF — The number of rows of COEF. (Input)
Default: NRCOEF = size (COEF,1).

NCCOEF — The number of columns of COEF. (Input)
Default: NCCOEF = size (COEF,2).

LDCOEF — Leading dimension of COEF exactly as specified in the dimension statement of the calling program. (Input)
Default: LDCOEF = size (COEF,1).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

FORTRAN 90 Interface

Generic: CALL FFT2B (COEF, A [, …])

Specific: The specific interface names are S_FFT2B and D_FFT2B.

FORTRAN 77 Interface

Single: CALL FFT2B (NRCOEF, NCCOEF, COEF, LDCOEF, A, LDA)

Double: The double precision name is DFFT2B.

Description

The routine FFT2B computes the inverse discrete complex Fourier transform of a complex two-dimensional array of size (NRCOEF = N) × (NCCOEF = M). It uses the Intel® Math Kernel Library, Sun Performance Library or IBM Engineering and Scientific Subroutine Library for the computation, if available. Otherwise, the method used is a variant of the Cooley-Tukey algorithm , which is most efficient when N and M are both products of small prime factors. If N and M satisfy this condition, then the computational effort is proportional to $N M \log N M$. This considerable savings has historically led people to refer to this algorithm as the “fast Fourier transform” or FFT.

Specifically, given an $N \times M$ array c = COEF, FFT2B returns in a

$$a_{jk} = \sum_{n=1}^{N} \sum_{m=1}^{M} c_{nm} e^{2\pi i (j-1)(n-1)/N} e^{2\pi i (k-1)(m-1)/M}$$

Furthermore, a vector of Euclidean norm S is mapped into a vector of norm

$$S\sqrt{NM}$$

Finally, note that an unnormalized inverse is implemented in FFT2D. The routine FFT2B is based on the complex FFT in FFTPACK. The package FFTPACK was developed by Paul Swarztrauber at the National Center for Atmospheric Research.

Comments

1. Workspace may be explicitly provided, if desired, by use of F2T2B/DF2T2B. The reference is:

   CALL F2T2B (NRCOEF, NCCOEF, A, LDA, COEF, LDCOEF, WFF1, WFF2, CWK, CPY)

   The additional arguments are as follows:

   WFF1 — Real array of length 4 * NRCOEF + 15 initialized by FFTCI. The initialization depends on NRCOEF. (Input)

   WFF2 — Real array of length 4 * NCCOEF + 15 initialized by FFTCI. The initialization depends on NCCOEF. (Input)

   CWK — Complex array of length 1. (Workspace)

   CPY — Real array of length 2 * MAX(NRCOEF, NCCOEF). (Workspace)

If the Intel® Math Kernel Library, Sun Performance Library or IBM Engineering and Scientific Subroutine Library is used, `WFF1`, `WFF2`, `CWK`, and `CPY` are not referenced.

2. The routine `FFT2B` is most efficient when `NRCOEF` and `NCCOEF` are the product of small primes.

3. The arrays `COEF` and `A` may be the same.

4. If `FFT2D`/`FFT2B` is used repeatedly, with the same values for `NRCOEF` and `NCCOEF`, then use `FFTCI` to fill `WFF1`(N = `NRCOEF`) and `WFF2`(N = `NCCOEF`). Follow this with repeated calls to `F2T2D`/`F2T2B`. This is more efficient than repeated calls to `FFT2D`/`FFT2B`.

If the Intel® Math Kernel Library, Sun Performance Library or IBM Engineering and Scientific Subroutine Library is used, parameters computed by `FFTCI` are not used. In this case, there is no need to call `FFTCI`.

Example

In this example, we first compute the Fourier transform of the 5 × 4 array

$$x_{nm} = n + 5(m - 1)$$

for $1 \le n \le 5$ and $1 \le m \le 4$ using the IMSL routine `FFT2D`. The result

$$\hat{x} = c$$

is then inverted by a call to `FFT2B`. Note that the result is an array a satisfying $a = (5)(4)x = 20x$. In general, `FFT2B` is an unnormalized inverse with expansion factor $N\,M$.

```
      USE FFT2B_INT
      USE FFT2D_INT
      USE WRCRN_INT

      IMPLICIT   NONE
      INTEGER    M, N, NCA, NRA
      COMPLEX    CMPLX, X(5,4), A(5,4), COEF(5,4)
      CHARACTER  TITLE1*26, TITLE2*26, TITLE3*26
      INTRINSIC  CMPLX
!
      TITLE1 = 'The input matrix is below '
      TITLE2 = 'After FFT2D               '
      TITLE3 = 'After FFT2B               '
      NRA    = 5
      NCA    = 4
!                                 Fill X with initial data
      DO 20  N=1, NRA
         DO 10  M=1, NCA
            X(N,M) = CMPLX(FLOAT(N+5*M-5),0.0)
   10    CONTINUE
   20 CONTINUE
!
      CALL WRCRN (TITLE1, X)
!
      CALL FFT2D (X, COEF)
!
```

```
      CALL WRCRN (TITLE2, COEF)
!
      CALL FFT2B (COEF, A)
!
      CALL WRCRN (TITLE3, A)
!
      END
```

Output

```
                 The input matrix is below
                 1                2                3                4
1  (  1.00,  0.00)  (  6.00,  0.00)  ( 11.00,  0.00)  ( 16.00,  0.00)
2  (  2.00,  0.00)  (  7.00,  0.00)  ( 12.00,  0.00)  ( 17.00,  0.00)
3  (  3.00,  0.00)  (  8.00,  0.00)  ( 13.00,  0.00)  ( 18.00,  0.00)
4  (  4.00,  0.00)  (  9.00,  0.00)  ( 14.00,  0.00)  ( 19.00,  0.00)
5  (  5.00,  0.00)  ( 10.00,  0.00)  ( 15.00,  0.00)  ( 20.00,  0.00)

                              After FFT2D
                 1                2                3                4
1  ( 210.0,   0.0)  ( -50.0,  50.0)  ( -50.0,   0.0)  ( -50.0, -50.0)
2  ( -10.0,  13.8)  (   0.0,   0.0)  (   0.0,   0.0)  (   0.0,   0.0)
3  ( -10.0,   3.2)  (   0.0,   0.0)  (   0.0,   0.0)  (   0.0,   0.0)
4  ( -10.0,  -3.2)  (   0.0,   0.0)  (   0.0,   0.0)  (   0.0,   0.0)
5  ( -10.0, -13.8)  (   0.0,   0.0)  (   0.0,   0.0)  (   0.0,   0.0)

                              After FFT2B
                 1                2                3                4
1  (  20.0,   0.0)  ( 120.0,   0.0)  ( 220.0,   0.0)  ( 320.0,   0.0)
2  (  40.0,   0.0)  ( 140.0,   0.0)  ( 240.0,   0.0)  ( 340.0,   0.0)
3  (  60.0,   0.0)  ( 160.0,   0.0)  ( 260.0,   0.0)  ( 360.0,   0.0)
4  (  80.0,   0.0)  ( 180.0,   0.0)  ( 280.0,   0.0)  ( 380.0,   0.0)
5  ( 100.0,   0.0)  ( 200.0,   0.0)  ( 300.0,   0.0)  ( 400.0,   0.0)
```

FFT3F

more...

Computes Fourier coefficients of a complex periodic three-dimensional array.

Required Arguments

A — Three-dimensional complex matrix containing the data to be transformed. (Input)

B — Three-dimensional complex matrix containing the Fourier coefficients of `A`. (Output)
The matrices `A` and `B` may be the same.

Optional Arguments

N1 — Limit on the first subscript of matrices `A` and `B`. (Input)
Default: `N1` = size(`A`, 1)

N2 — Limit on the second subscript of matrices `A` and `B`. (Input)
Default: `N2` = size(`A`, 2)

N3 — Limit on the third subscript of matrices `A` and `B`. (Input)
Default: `N3` = size(`A`, 3)

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = size (`A`,1).

MDA — Middle dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `MDA` = size (`A`,2).

LDB — Leading dimension of `B` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDB` = size (`B`,1).

MDB — Middle dimension of B exactly as specified in the dimension statement of the calling program. (Input)
Default: MDB = size (B,2).

FORTRAN 90 Interface

Generic: CALL FFT3F (A, B [, …])

Specific: The specific interface names are S_FFT3F and D_FFT3F.

FORTRAN 77 Interface

Single: CALL FFT3F (N1, N2, N3, A, LDA, MDA, B, LDB, MDB)

Double: The double precision name is DFFT3F.

Description

The routine FFT3F computes the forward discrete complex Fourier transform of a complex three-dimensional array of size (N1 = *N*) × (N2 = *M*) × (N3 = *L*). It uses the Intel® Math Kernel Library, Sun Performance Library or IBM Engineering and Scientific Subroutine Library for the computation, if available. Otherwise, the method used is a variant of the Cooley-Tukey algorithm , which is most efficient when *N*, *M*, and *L* are each products of small prime factors. If *N*, *M*, and *L* satisfy this condition, then the computational effort is proportional to *N M L* log *N M L*. This considerable savings has historically led people to refer to this algorithm as the "fast Fourier transform" or FFT.

Specifically, given an *N* × *M* × *L* array *a*, FFT3F returns in *c* = COEF

$$c_{jkl} = \sum_{n=1}^{N}\sum_{m=1}^{M}\sum_{l=1}^{L} a_{nml} e^{-2\pi i(j-1)(n-1)/N} e^{-2\pi i(k-1)(m-1)/M} e^{-2\pi i(k-1)(l-1)/L}$$

Furthermore, a vector of Euclidean norm *S* is mapped into a vector of norm

$$\sqrt{NML}\,S$$

Finally, note that an unnormalized inverse is implemented in FFT3B. The routine FFT3F is based on the complex FFT in FFTPACK. The package FFTPACK was developed by Paul Swarztrauber at the National Center for Atmospheric Research.

Comments

1. Workspace may be explicitly provided, if desired, by use of F2T3F/DF2T3F. The reference is:

CALL F2T3F (N1, N2, N3, A, LDA, MDA, B, LDB, MDB, WFF1, WFF2, WFF3, CPY)

The additional arguments are as follows:

WFF1 — Real array of length 4 * N1 + 15 initialized by FFTCI. The initialization depends on N1. (Input)

WFF2 — Real array of length 4 * N2 + 15 initialized by FFTCI. The initialization depends on N2. (Input)

WFF3 — Real array of length 4 * N3 + 15 initialized by FFTCI. The initialization depends on N3. (Input)

CPY — Real array of size 2 * MAX(N1, N2, N3). (Workspace)

If the Intel® Math Kernel Library, Sun Performance Library or IBM Engineering and Scientific Subroutine Library is used, WFF1, WFF2, WFF3, and CPY are not referenced.

2. The routine FFT3F is most efficient when N1, N2, and N3 are the product of small primes.

3. If FFT3F/FFT3B is used repeatedly with the same values for N1, N2 and N3, then use FFTCI to fill WFF1(N = N1), WFF2(N = N2), and WFF3(N = N3). Follow this with repeated calls to F2T3F/F2T3B. This is more efficient than repeated calls to FFT3F/FFT3B.

If the Intel® Math Kernel Library, Sun Performance Library or IBM Engineering and Scientific Subroutine Library is used, parameters computed by FFTCI are not used. In this case, there is no need to call FFTCI.

Example

In this example, we compute the Fourier transform of the pure frequency input for a $2 \times 3 \times 4$ array

$$a_{nml} = e^{2\pi i(n-1)1/2} e^{2\pi i(m-1)2/3} e^{2\pi i(l-1)2/4}$$

for $1 \leq n \leq 2$, $1 \leq m \leq 3$, and $1 \leq l \leq 4$ using the IMSL routine FFT3F. The result

$$\hat{a} = c$$

has all zeros except in the (2, 3, 3) position.

```
      USE FFT3F_INT
      USE UMACH_INT
      USE CONST_INT

      IMPLICIT   NONE
      INTEGER    LDA, LDB, MDA, MDB, NDA, NDB
      PARAMETER  (LDA=2, LDB=2, MDA=3, MDB=3, NDA=4, NDB=4)
!                                 SPECIFICATIONS FOR LOCAL VARIABLES
      INTEGER    I, J, K, L, M, N, N1, N2, N3, NOUT
      REAL       PI
      COMPLEX    A(LDA,MDA,NDA), B(LDB,MDB,NDB), C, H
!                                 SPECIFICATIONS FOR INTRINSICS
      INTRINSIC  CEXP, CMPLX
```

```
      COMPLEX    CEXP, CMPLX
!                                SPECIFICATIONS FOR SUBROUTINES
!                                SPECIFICATIONS FOR FUNCTIONS
!                                Get output unit number
      CALL UMACH (2, NOUT)
      PI = CONST('PI')
      C  = CMPLX(0.0,2.0*PI)
!                                Set array A
      DO 30  N=1, 2
         DO 20  M=1, 3
            DO 10  L=1, 4
               H         = C*(N-1)*1/2 + C*(M-1)*2/3 + C*(L-1)*2/4
               A(N,M,L) = CEXP(H)
   10       CONTINUE
   20    CONTINUE
   30 CONTINUE
!
      CALL FFT3F (A, B)
!
      WRITE (NOUT,99996)
      DO 50  I=1, 2
         WRITE (NOUT,99998) I
         DO 40  J=1, 3
            WRITE (NOUT,99999) (A(I,J,K),K=1,4)
   40    CONTINUE
   50 CONTINUE
!
      WRITE (NOUT,99997)
      DO 70  I=1, 2
         WRITE (NOUT,99998) I
         DO 60  J=1, 3
            WRITE (NOUT,99999) (B(I,J,K),K=1,4)
   60    CONTINUE
   70 CONTINUE
!
99996 FORMAT (13X, 'The input for FFT3F is')
99997 FORMAT (/, 13X, 'The results from FFT3F are')
99998 FORMAT (/, ' Face no. ', I1)
99999 FORMAT (1X, 4('(',F6.2,',',F6.2,')',3X))
      END
```

Output

```
             The input for FFT3F is

Face no. 1
(  1.00,  0.00)   ( -1.00,  0.00)   (  1.00,  0.00)   ( -1.00,  0.00)
( -0.50, -0.87)   (  0.50,  0.87)   ( -0.50, -0.87)   (  0.50,  0.87)
( -0.50,  0.87)   (  0.50, -0.87)   ( -0.50,  0.87)   (  0.50, -0.87)

Face no. 2
( -1.00,  0.00)   (  1.00,  0.00)   ( -1.00,  0.00)   (  1.00,  0.00)
(  0.50,  0.87)   ( -0.50, -0.87)   (  0.50,  0.87)   ( -0.50, -0.87)
(  0.50, -0.87)   ( -0.50,  0.87)   (  0.50, -0.87)   ( -0.50,  0.87)

The results from FFT3F are

Face no. 1
(  0.00,  0.00)   (  0.00,  0.00)   (  0.00,  0.00)   (  0.00,  0.00)
(  0.00,  0.00)   (  0.00,  0.00)   (  0.00,  0.00)   (  0.00,  0.00)
(  0.00,  0.00)   (  0.00,  0.00)   (  0.00,  0.00)   (  0.00,  0.00)

Face no. 2
(  0.00,  0.00)   (  0.00,  0.00)   (  0.00,  0.00)   (  0.00,  0.00)
(  0.00,  0.00)   (  0.00,  0.00)   (  0.00,  0.00)   (  0.00,  0.00)
```

```
 (  0.00,  0.00)   (  0.00,  0.00)   ( 24.00,  0.00)   (  0.00,  0.00)
```

FFT3B

more...

Computes the inverse Fourier transform of a complex periodic three-dimensional array.

Required Arguments

A — Three-dimensional complex matrix containing the data to be transformed. (Input)

B — Three-dimensional complex matrix containing the inverse Fourier coefficients of A. (Output)
The matrices A and B may be the same.

Optional Arguments

N1 — Limit on the first subscript of matrices A and B. (Input)
Default: N1 = size (A,1).

N2 — Limit on the second subscript of matrices A and B. (Input)
Default: N2 = size (A,2).

N3 — Limit on the third subscript of matrices A and B. (Input)
Default: N3 = size (A,3).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

MDA — Middle dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: MDA = size (A,2).

LDB — Leading dimension of B exactly as specified in the dimension statement of the calling program. (Input)
Default: LDB = size (B,1).

MDB — Middle dimension of `B` exactly as specified in the dimension statement of the calling program. (Input)
Default: `MDB` = size `(B,2)`.

FORTRAN 90 Interface

Generic: `CALL FFT3B (A, B [, …])`

Specific: The specific interface names are `S_FFT3B` and `D_FFT3B`.

FORTRAN 77 Interface

Single: `CALL FFT3B (N1, N2, N3, A, LDA, MDA, B, LDB, MDB)`

Double: The double precision name is `DFFT3B`.

Description

The routine `FFT3B` computes the inverse discrete complex Fourier transform of a complex three-dimensional array of size (`N1` = *N*) × (`N2` = *M*) × (`N3` = *L*). It uses the Intel® Math Kernel Library, Sun Performance Library or IBM Engineering and Scientific Subroutine Library for the computation, if available. Otherwise, the method used is a variant of the Cooley-Tukey algorithm, which is most efficient when *N*, *M*, and *L* are each products of small prime factors. If *N*, *M*, and *L* satisfy this condition, then the computational effort is proportional to *N M L* log *N M L*. This considerable savings has historically led people to refer to this algorithm as the “fast Fourier transform” or FFT.

Specifically, given an $N \times M \times L$ array *a*, `FFT3B` returns in *b*

$$b_{jkl} \sum_{n=1}^{N} \sum_{m=1}^{M} \sum_{l=1}^{L} a_{nml} e^{2\pi i (j-1)(n-1)/N} e^{2\pi i (k-1)(m-1)/M} e^{2\pi i (k-1)(l-1)/L}$$

Furthermore, a vector of Euclidean norm *S* is mapped into a vector of norm

$$\sqrt{NML}\, S$$

Finally, note that an unnormalized inverse is implemented in `FFT3F`. The routine `FFT3B` is based on the complex FFT in FFTPACK. The package FFTPACK was developed by Paul Swarztrauber at the National Center for Atmospheric Research.

Comments

1. Workspace may be explicitly provided, if desired, by use of `F2T3B/DF2T3B`. The reference is:

CALL F2T3B (N1, N2, N3, A, LDA, MDA, B, LDB, MDB, WFF1, WFF2, WFF3, CPY)

The additional arguments are as follows:

WFF1 — Real array of length 4 * N1 + 15 initialized by FFTCI. The initialization depends on N1. (Input)

WFF2 — Real array of length 4 * N2 + 15 initialized by FFTCI. The initialization depends on N2. (Input)

WFF3 — Real array of length 4 * N3 + 15 initialized by FFTCI. The initialization depends on N3. (Input)

CPY — Real array of size 2 * MAX(N1, N2, N3). (Workspace)

If the Intel® Math Kernel Library, Sun Performance Library or IBM Engineering and Scientific Subroutine Library is used, WFF1, WFF2, WFF3, and CPY are not referenced.

2. The routine FFT3B is most efficient when N1, N2, and N3 are the product of small primes.

3. If FFT3F/FFT3B is used repeatedly with the same values for N1, N2 and N3, then use FFTCI to fill WFF1(N = N1), WFF2(N = N2), and WFF3(N = N3). Follow this with repeated calls to F2T3F/F2T3B. This is more efficient than repeated calls to FFT3F/FFT3B.

If the Intel® Math Kernel Library, Sun Performance Library or IBM Engineering and Scientific Subroutine Library is used, parameters computed by FFTCI are not used. In this case, there is no need to call FFTCI.

Example

In this example, we compute the Fourier transform of the 2 × 3 × 4 array

$$x_{nml} = n + 2(m-1) + 2(3)(l-1)$$

for $1 \le n \le 2$, $1 \le m \le 3$, and $1 \le l \le 4$ using the IMSL routine FFT3F. The result

$$a = \hat{x}$$

is then inverted using FFT3B. Note that the result is an array b satisfying $b = 2(3)(4)x = 24x$. In general, FFT3B is an unnormalized inverse with expansion factor $N\,M\,L$.

```
      USE FFT3B_INT
      USE FFT3F_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    LDA, LDB, MDA, MDB, NDA, NDB
      PARAMETER  (LDA=2, LDB=2, MDA=3, MDB=3, NDA=4, NDB=4)
!                                  SPECIFICATIONS FOR LOCAL VARIABLES
      INTEGER    I, J, K, L, M, N, N1, N2, N3, NOUT
      COMPLEX    A(LDA,MDA,NDA), B(LDB,MDB,NDB), X(LDB,MDB,NDB)
!                                  SPECIFICATIONS FOR INTRINSICS
      INTRINSIC  CEXP, CMPLX
```

```
      COMPLEX    CEXP, CMPLX
!                                  SPECIFICATIONS FOR SUBROUTINES
!                                  Get output unit number
      CALL UMACH (2, NOUT)
      N1 = 2
      N2 = 3
      N3 = 4
!                                  Set array X
      DO 30  N=1, 2
         DO 20  M=1, 3
            DO 10  L=1, 4
               X(N,M,L) = N + 2*(M-1) + 2*3*(L-1)
   10       CONTINUE
   20    CONTINUE
   30 CONTINUE
!
      CALL FFT3F (X, A)
      CALL FFT3B (A, B)
!
      WRITE (NOUT,99996)
      DO 50  I=1, 2
         WRITE (NOUT,99998) I
         DO 40  J=1, 3
            WRITE (NOUT,99999) (X(I,J,K),K=1,4)
   40    CONTINUE
   50 CONTINUE
!
      WRITE (NOUT,99997)
      DO 70  I=1, 2
         WRITE (NOUT,99998) I
         DO 60  J=1, 3
            WRITE (NOUT,99999) (A(I,J,K),K=1,4)
   60    CONTINUE
   70 CONTINUE
!
      WRITE (NOUT, 99995)
      DO 90  I=1, 2
         WRITE (NOUT,99998) I
         DO 80  J=1, 3
            WRITE (NOUT,99999) (B(I,J,K),K=1,4)
   80    CONTINUE
   90 CONTINUE
99995 FORMAT (13X, 'The unnormalized inverse is')
99996 FORMAT (13X, 'The input for FFT3F is')
99997 FORMAT (/, 13X, 'The results from FFT3F are')
99998 FORMAT (/, ' Face no. ', I1)
99999 FORMAT (1X, 4('(',F6.2,',',F6.2,')',3X))
      END
```

Output

```
            The input for FFT3F is

Face no. 1
(  1.00,  0.00)   (  7.00,  0.00)   ( 13.00,  0.00)   ( 19.00,  0.00)
(  3.00,  0.00)   (  9.00,  0.00)   ( 15.00,  0.00)   ( 21.00,  0.00)
(  5.00,  0.00)   ( 11.00,  0.00)   ( 17.00,  0.00)   ( 23.00,  0.00)

Face no. 2
(  2.00,  0.00)   (  8.00,  0.00)   ( 14.00,  0.00)   ( 20.00,  0.00)
(  4.00,  0.00)   ( 10.00,  0.00)   ( 16.00,  0.00)   ( 22.00,  0.00)
(  6.00,  0.00)   ( 12.00,  0.00)   ( 18.00,  0.00)   ( 24.00,  0.00)

The results from FFT3F are
```

```
Face no. 1
(300.00,  0.00)   (-72.00, 72.00)   (-72.00,  0.00)   (-72.00,-72.00)
(-24.00, 13.86)   (  0.00,  0.00)   (  0.00,  0.00)   (  0.00,  0.00)
(-24.00,-13.86)   (  0.00,  0.00)   (  0.00,  0.00)   (  0.00,  0.00)

Face no. 2
(-12.00,  0.00)   (  0.00,  0.00)   (  0.00,  0.00)   (  0.00,  0.00)
(  0.00,  0.00)   (  0.00,  0.00)   (  0.00,  0.00)   (  0.00,  0.00)
(  0.00,  0.00)   (  0.00,  0.00)   (  0.00,  0.00)   (  0.00,  0.00)

The unnormalized inverse is
Face no. 1
( 24.00,  0.00)   (168.00,  0.00)   (312.00,  0.00)   (456.00,  0.00)
( 72.00,  0.00)   (216.00,  0.00)   (360.00,  0.00)   (504.00,  0.00)
(120.00,  0.00)   (264.00,  0.00)   (408.00,  0.00)   (552.00,  0.00)

Face no. 2
( 48.00,  0.00)   (192.00,  0.00)   (336.00,  0.00)   (480.00,  0.00)
( 96.00,  0.00)   (240.00,  0.00)   (384.00,  0.00)   (528.00,  0.00)
(144.00,  0.00)   (288.00,  0.00)   (432.00,  0.00)   (576.00,  0.00)
```

RCONV

more...

Computes the convolution of two real vectors.

Required Arguments

X — Real vector of length `NX`. (Input)

Y — Real vector of length `NY`. (Input)

Z — Real vector of length `NZ` ontaining the convolution of `X` and `Y`. (Output)

ZHAT — Real vector of length `NZ` containing the discrete Fourier transform of `Z`. (Output)

Optional Arguments

IDO — Flag indicating the usage of `RCONV`. (Input)
Default: `IDO` = 0.

IDO	Usage
0	If this is the only call to `RCONV`.
If `RCONV` is called multiple times in sequence with the same `NX`, `NY`, and `IPAD`, `IDO` should be set to	
1	on the first call
2	on the intermediate calls
3	on the final call

NX — Length of the vector `X`. (Input)
Default: `NX` = size `(X,1)`.

NY — Length of the vector `Y`. (Input)
Default: `NY` = size `(Y,1)`.

IPAD — `IPAD` should be set to zero for periodic data or to one for nonperiodic data. (Input)
Default: `IPAD` = 0.

NZ — Length of the vector `Z`. (Input/Output)
Upon input: When `IPAD` is zero, `NZ` must be at least `MAX(NX, NY)`. When `IPAD` is one, `NZ` must be greater than or equal to the smallest integer greater than or equal to (`NX` + `NY` − 1) of the form $(2^{\alpha}) * (3^{\beta}) * (5^{\gamma})$ where alpha, beta, and gamma are nonnegative integers. Upon output, the value for `NZ` that was used by `RCONV`.
Default: NZ = size (Z,1).

FORTRAN 90 Interface

Generic: `CALL RCONV (X, Y, Z, ZHAT [, …])`

Specific: The specific interface names are `S_RCONV` and `D_RCONV`.

FORTRAN 77 Interface

Single: `CALL RCONV (IDO, NX, X, NY, Y, IPAD, NZ, Z, ZHAT)`

Double: The double precision name is `DRCONV`.

Description

The routine `RCONV` computes the discrete convolution of two sequences *x* and *y*. More precisely, let n_x be the length of *x* and n_y denote the length of *y*. If a circular convolution is desired, then `IPAD` must be set to zero. We set

$$n_z := \max\{n_x, n_y\}$$

and we pad out the shorter vector with zeroes. Then, we compute

$$z_i = \sum_{j=1}^{n_z} x_{i-j+1} y_j$$

where the index on *x* is interpreted as a positive number between 1 and n_z, modulo n_z.

The technique used to compute the z_i's is based on the fact that the (complex discrete) Fourier transform maps convolution into multiplication. Thus, the Fourier transform of *z* is given by

$$\hat{z}(n) = \hat{x}(n)\hat{y}(n)$$

where

$$\hat{z}(n) = \sum_{m=1}^{n_z} z_m e^{-2\pi i(m-1)(n-1)/n_z}$$

The technique used here to compute the convolution is to take the discrete Fourier transform of *x* and *y*, multiply the results together component-wise, and then take the inverse transform of this product. It is very important to make sure that n_z is a product of small primes if `IPAD` is set to zero. If n_z is a product of small primes, then the computational effort will be proportional to $n_z \log(n_z)$. If `IPAD` is one, then a good value is chosen for n_z so that the Fourier transforms are efficient and $n_z \geq n_x + n_y - 1$. This will mean that both vectors will be padded with zeroes.

We point out that no complex transforms of *x* or *y* are taken since both sequences are real, we can take real transforms and simulate the complex transform above. This can produce a savings of a factor of six in time as well as save space over using the complex transform.

Comments

1. Workspace may be explicitly provided, if desired, by use of `R2ONV/DR2ONV`. The reference is:

   `CALL R2ONV(IDO, NX, X, NY, Y, IPAD, NZ, Z, ZHAT, XWK, YWK, WK)`

   The additional arguments are as follows:

   XWK — Real work array of length `NZ`.

   YWK — Real work array of length `NZ`.

   WK — Real work arrary of length 2 * `NZ` + 15.

2. Informational error

Type	Code	Description
4	1	The length of the vector *z* must be large enough to hold the results. An acceptable length is returned in `NZ`.

Example

In this example, we compute both a periodic and a non-periodic convolution. The idea here is that one can compute a moving average of the type found in digital filtering using this routine. The averaging operator in this case is especially simple and is given by averaging five consecutive points in the sequence. The periodic case tries to recover a noisy sin function by averaging five nearby values. The nonperiodic case tries to recover the values of an exponential function contaminated by noise. The large error for the last value printed has to do with the fact that the convolution is averaging the zeroes in the “pad” rather than function values. Notice that the signal size is 100, but we only report the errors at ten points.

```
      USE IMSL_LIBRARIES

      IMPLICIT   NONE
      INTEGER    NFLTR, NY, A
      PARAMETER  (NFLTR=5, NY=100)
!
      INTEGER    I, IPAD, K, MOD, NOUT, NZ
      REAL       ABS, EXP, F1, F2, FLOAT, FLTR(NFLTR), &
                FLTRER, ORIGER, SIN, TOTAL1, TOTAL2, TWOPI, X, &
                Y(NY), Z(2*(NFLTR+NY-1)), ZHAT(2*(NFLTR+NY-1))
      INTRINSIC  ABS, EXP, FLOAT, MOD, SIN
!                                DEFINE FUNCTIONS
      F1(X) = SIN(X)
      F2(X) = EXP(X)
!
      CALL RNSET (1234579)
      CALL UMACH (2, NOUT)
      TWOPI = CONST('PI')
      TWOPI = 2.0*TWOPI
!                                 SET UP THE FILTER
      DO 10  I=1, 5
         FLTR(I) = 0.2
   10 CONTINUE
!                                 SET UP Y-VECTOR FOR THE PERIODIC
!                                 CASE.
      DO 20  I=1, NY
         X    = TWOPI*FLOAT(I-1)/FLOAT(NY-1)
         Y(I) = RNUNF()
         Y(I) = F1(X) + 0.5*Y(I) - 0.25
   20 CONTINUE
!                                 CALL THE CONVOLUTION ROUTINE FOR THE
!                                 PERIODIC CASE.
      NZ = 2*(NFLTR+NY-1)
      CALL RCONV (FLTR, Y, Z, ZHAT, IPAD=0, NZ=NZ)
!                                 PRINT RESULTS
      WRITE (NOUT,99993)
      WRITE (NOUT,99995)
      TOTAL1 = 0.0
      TOTAL2 = 0.0
      DO 30  I=1, NY
!                                 COMPUTE THE OFFSET FOR THE Z-VECTOR
         IF (I .GE. NY-1) THEN
            K = I - NY + 2
         ELSE
            K = I + 2
         END IF
!
         X      = TWOPI*FLOAT(I-1)/FLOAT(NY-1)
         ORIGER = ABS(Y(I)-F1(X))
         FLTRER = ABS(Z(K)-F1(X))
         IF (MOD(I,11) .EQ. 1) WRITE (NOUT,99997) X, F1(X), ORIGER, &
            FLTRER
         TOTAL1 = TOTAL1 + ORIGER
         TOTAL2 = TOTAL2 + FLTRER
   30 CONTINUE
      WRITE (NOUT,99998) TOTAL1/FLOAT(NY)
      WRITE (NOUT,99999) TOTAL2/FLOAT(NY)
!                                 SET UP Y-VECTOR FOR THE NONPERIODIC
!                                 CASE.
      DO 40  I=1, NY
         A    = FLOAT(I-1)/FLOAT(NY-1)
         Y(I) = RNUNF()
         Y(I) = F2(A) + 0.5*Y(I) - 0.25
   40 CONTINUE
!                                 CALL THE CONVOLUTION ROUTINE FOR THE
```

```
!                                 NONPERIODIC CASE.
      NZ = 2*(NFLTR+NY-1)
      CALL RCONV (FLTR, Y, Z, ZHAT, IPAD=1)
!                                 PRINT RESULTS
      WRITE (NOUT,99994)
      WRITE (NOUT,99996)
      TOTAL1 = 0.0
      TOTAL2 = 0.0
      DO 50  I=1, NY
         X      = FLOAT(I-1)/FLOAT(NY-1)
         ORIGER = ABS(Y(I)-F2(X))
         FLTRER = ABS(Z(I+2)-F2(X))
         IF (MOD(I,11) .EQ. 1) WRITE (NOUT,99997) X, F2(X), ORIGER, &
            FLTRER
         TOTAL1 = TOTAL1 + ORIGER
         TOTAL2 = TOTAL2 + FLTRER
   50 CONTINUE
      WRITE (NOUT,99998) TOTAL1/FLOAT(NY)
      WRITE (NOUT,99999) TOTAL2/FLOAT(NY)
99993 FORMAT (' Periodic Case')
99994 FORMAT (/,' Nonperiodic Case')
99995 FORMAT (8X, 'x', 9X, 'sin(x)', 6X, 'Original Error', 5X, &
            'Filtered Error')
99996 FORMAT (8X, 'x', 9X, 'exp(x)', 6X, 'Original Error', 5X, &
            'Filtered Error')
99997 FORMAT (1X, F10.4, F13.4, 2F18.4)
99998 FORMAT (' Average absolute error before filter:', F10.5)
99999 FORMAT (' Average absolute error after filter:', F11.5)
      END
```

Output

```
Periodic Case
    x          sin(x)      Original Error     Filtered Error
 0.0000       0.0000            0.0811             0.0587
 0.6981       0.6428            0.0226             0.0781
 1.3963       0.9848            0.1526             0.0529
 2.0944       0.8660            0.0959             0.0125
 2.7925       0.3420            0.1747             0.0292
 3.4907      -0.3420            0.1035             0.0238
 4.1888      -0.8660            0.0402             0.0595
 4.8869      -0.9848            0.0673             0.0798
 5.5851      -0.6428            0.1044             0.0074
 6.2832       0.0000            0.0154             0.0018
 Average absolute error before filter:   0.12481
 Average absolute error after filter:    0.04778

Nonperiodic Case
    x          exp(x)      Original Error     Filtered Error
 0.0000       1.0000            0.1476             0.3915
 0.1111       1.1175            0.0537             0.0326
 0.2222       1.2488            0.1278             0.0932
 0.3333       1.3956            0.1136             0.0987
 0.4444       1.5596            0.1617             0.0964
 0.5556       1.7429            0.0071             0.0662
 0.6667       1.9477            0.1248             0.0713
 0.7778       2.1766            0.1556             0.0158
 0.8889       2.4324            0.1529             0.0696
 1.0000       2.7183            0.2124             1.0562
 Average absolute error before filter:   0.12538
 Average absolute error after filter:    0.07764
```

CCONV

more...

Computes the convolution of two complex vectors.

Required Arguments

X — Complex vector of length `NX`. (Input)

Y — Complex vector of length `NY`. (Input)

Z — Complex vector of length `NZ` containing the convolution of `X` and `Y`. (Output)

ZHAT — Complex vector of length `NZ` containing the discrete complex Fourier transform of `Z`. (Output)

Optional Arguments

IDO — Flag indicating the usage of `CCONV`. (Input)
Default: `IDO` = 0.

IDO	Usage
0	If this is the only call to `CCONV`.
If `CCONV` is called multiple times in sequence with the same `NX`, `NY`, and `IPAD`, `IDO` should be set to:	
1	on the first call
2	on the intermediate calls
3	on the final call

NX — Length of the vector `X`. (Input)
Default: `NX` = size `(X,1)`.

NY — Length of the vector `Y`. (Input)
Default: `NY` = size `(Y,1)`.

IPAD — IPAD should be set to zero for periodic data or to one for nonperiodic data. (Input)
Default: IPAD =0.

NZ — Length of the vector Z. (Input/Output)
Upon input: When IPAD is zero, NZ must be at least MAX(NX, NY). When IPAD is one, NZ must be greater than or equal to the smallest integer greater than or equal to (NX + NY − 1) of the form $(2^{\alpha}) * (3^{\beta}) * (5^{\gamma})$ where alpha, beta, and gamma are nonnegative integers. Upon output, the value for NZ that was used by CCONV.
Default: NZ = size (Z,1).

FORTRAN 90 Interface

Generic: CALL CCONV (X, Y, Z, ZHAT [, …])

Specific: The specific interface names are S_CCONV and D_CCONV.

FORTRAN 77 Interface

Single: CALL CCONV (IDO, NX, X, NY, Y, IPAD, NZ, Z, ZHAT)

Double: The double precision name is DCCONV.

Description

The subroutine CCONV computes the discrete convolution of two complex sequences x and y. More precisely, let n_x be the length of x and n_y denote the length of y. If a circular convolution is desired, then IPAD must be set to zero. We set

$$n_z := \max\{n_x, n_y\}$$

and we pad out the shorter vector with zeroes. Then, we compute

$$z_i = \sum_{j=1}^{n_z} x_{i-j+1} y_j$$

where the index on x is interpreted as a positive number between 1 and n_z, modulo n_z.

The technique used to compute the z_i's is based on the fact that the (complex discrete) Fourier transform maps convolution into multiplication. Thus, the Fourier transform of z is given by

$$\hat{z}(n) = \hat{x}(n)\hat{y}(n)$$

where

$$\hat{z}(n) = \sum_{m=1}^{n_z} z_m e^{-2\pi i(m-1)(n-1)/n_z}$$

The technique used here to compute the convolution is to take the discrete Fourier transform of *x* and *y*, multiply the results together component-wise, and then take the inverse transform of this product. It is very important to make sure that n_z is a product of small primes if `IPAD` is set to zero. If n_z is a product of small primes, then the computational effort will be proportional to $n_z \log(n_z)$. If `IPAD` is one, then a a good value is chosen for n_z so that the Fourier transforms are efficient and $n_z \ge n_x + n_y - 1$. This will mean that both vectors will be padded with zeroes.

Comments

1. Workspace may be explicitly provided, if desired, by use of `C2ONV/DC2ONV`. The reference is:

   `CALL C2ONV (IDO, NX, X, NY, Y, IPAD, NZ, Z, ZHAT, XWK, YWK, WK)`

   The additional arguments are as follows:

   XWK — Complex work array of length `NZ`.

   YWK — Complex work array of length `NZ`.

   WK — Real work array of length 6 * `NZ` + 15.

2. Informational error

Type	Code	Description
4	1	The length of the vector `Z` must be large enough to hold the results. An acceptable length is returned in `NZ`.

Example

In this example, we compute both a periodic and a non-periodic convolution. The idea here is that one can compute a moving average of the type found in digital filtering using this routine. The averaging operator in this case is especially simple and is given by averaging five consecutive points in the sequence. The periodic case tries to recover a noisy function $f_1(x) = \cos(x) + i \sin(x)$ by averaging five nearby values. The nonperiodic case tries to recover the values of the function $f_2(x) = e^x f_1(x)$ contaminated by noise. The large error for the first and last value printed has to do with the fact that the convolution is averaging the zeroes in the "pad" rather than function values. Notice that the signal size is 100, but we only report the errors at ten points.

```
      USE IMSL_LIBRARIES

      IMPLICIT   NONE
      INTEGER    NFLTR, NY
      PARAMETER  (NFLTR=5, NY=100)
```

```
!
      INTEGER    I, IPAD, K, MOD, NOUT, NZ
      REAL       CABS, COS, EXP, FLOAT, FLTRER, ORIGER,  &
                SIN, TOTAL1, TOTAL2, TWOPI, X, T1, T2
      COMPLEX    CMPLX, F1, F2, FLTR(NFLTR), Y(NY), Z(2*(NFLTR+NY-1)), &
                ZHAT(2*(NFLTR+NY-1))
      INTRINSIC  CABS, CMPLX, COS, EXP, FLOAT, MOD, SIN
!                                DEFINE FUNCTIONS
      F1(X) = CMPLX(COS(X),SIN(X))
      F2(X) = EXP(X)*CMPLX(COS(X),SIN(X))
!
      CALL RNSET (1234579)
      CALL UMACH (2, NOUT)
      TWOPI = CONST('PI')
      TWOPI = 2.0*TWOPI
!                                 SET UP THE FILTER
      CALL CSET(NFLTR,(0.2,0.0),FLTR,1)
!                                 SET UP Y-VECTOR FOR THE PERIODIC
!                                 CASE.
      DO 20  I=1, NY
         X    = TWOPI*FLOAT(I-1)/FLOAT(NY-1)
         T1   = RNUNF()
         T2   = RNUNF()
         Y(I) = F1(X) + CMPLX(0.5*T1-0.25,0.5*T2-0.25)
   20 CONTINUE
!                                 CALL THE CONVOLUTION ROUTINE FOR THE
!                                 PERIODIC CASE.
      NZ = 2*(NFLTR+NY-1)
      CALL CCONV (FLTR, Y, Z, ZHAT)
!                                 PRINT RESULTS
      WRITE (NOUT,99993)
      WRITE (NOUT,99995)
      TOTAL1 = 0.0
      TOTAL2 = 0.0
      DO 30  I=1, NY
!                                 COMPUTE THE OFFSET FOR THE Z-VECTOR
         IF (I .GE. NY-1) THEN
            K = I - NY + 2
         ELSE
            K = I + 2
         END IF
!
         X      = TWOPI*FLOAT(I-1)/FLOAT(NY-1)
         ORIGER = CABS(Y(I)-F1(X))
         FLTRER = CABS(Z(K)-F1(X))
         IF (MOD(I,11) .EQ. 1) WRITE (NOUT,99997) X, F1(X), ORIGER, &
            FLTRER
         TOTAL1 = TOTAL1 + ORIGER
         TOTAL2 = TOTAL2 + FLTRER
   30 CONTINUE
      WRITE (NOUT,99998) TOTAL1/FLOAT(NY)
      WRITE (NOUT,99999) TOTAL2/FLOAT(NY)
!                                 SET UP Y-VECTOR FOR THE NONPERIODIC
!                                 CASE.
      DO 40  I=1, NY
         X    = FLOAT(I-1)/FLOAT(NY-1)
         T1   = RNUNF()
         T2   = RNUNF()
         Y(I) = F2(X) + CMPLX(0.5*T1-0.25,0.5*T2-0.25)
   40 CONTINUE
!                                 CALL THE CONVOLUTION ROUTINE FOR THE
!                                 NONPERIODIC CASE.
      NZ = 2*(NFLTR+NY-1)
      CALL CCONV (FLTR, Y, Z, ZHAT, IPAD=1)
!                                 PRINT RESULTS
      WRITE (NOUT,99994)
```

```
      WRITE (NOUT,99996)
      TOTAL1 = 0.0
      TOTAL2 = 0.0
      DO 50  I=1, NY
         X      = FLOAT(I-1)/FLOAT(NY-1)
         ORIGER = CABS(Y(I)-F2(X))
         FLTRER = CABS(Z(I+2)-F2(X))
         IF (MOD(I,11) .EQ. 1) WRITE (NOUT,99997) X, F2(X), ORIGER, &
            FLTRER
         TOTAL1 = TOTAL1 + ORIGER
         TOTAL2 = TOTAL2 + FLTRER
   50 CONTINUE
      WRITE (NOUT,99998) TOTAL1/FLOAT(NY)
      WRITE (NOUT,99999) TOTAL2/FLOAT(NY)
99993 FORMAT (' Periodic Case')
99994 FORMAT (/, ' Nonperiodic Case')
99995 FORMAT (8X, 'x', 15X, 'f1(x)', 8X, 'Original Error', 5X, &
            'Filtered Error')
99996 FORMAT (8X, 'x', 15X, 'f2(x)', 8X, 'Original Error', 5X, &
            'Filtered Error')
99997 FORMAT (1X, F10.4, 5X, '(', F7.4, ',', F8.4, ' )', 5X, F8.4, &
            10X, F8.4)
99998 FORMAT (' Average absolute error before filter:', F11.5)
99999 FORMAT (' Average absolute error after filter:', F12.5)
      END
```

Output

```
Periodic Case
 x               f1(x)          Original Error     Filtered Error
 0.0000     ( 1.0000,  0.0000 )        0.1666             0.0773
 0.6981     ( 0.7660,  0.6428 )        0.1685             0.1399
 1.3963     ( 0.1736,  0.9848 )        0.1756             0.0368
 2.0944     (-0.5000,  0.8660 )        0.2171             0.0142
 2.7925     (-0.9397,  0.3420 )        0.1147             0.0200
 3.4907     (-0.9397, -0.3420 )        0.0998             0.0331
 4.1888     (-0.5000, -0.8660 )        0.1137             0.0586
 4.8869     ( 0.1736, -0.9848 )        0.2217             0.0843
 5.5851     ( 0.7660, -0.6428 )        0.1831             0.0744
 6.2832     ( 1.0000,  0.0000 )        0.3234             0.0893
 Average absolute error before filter:    0.19315
 Average absolute error after filter:     0.08296

Nonperiodic Case
 x               f2(x)          Original Error     Filtered Error
 0.0000     ( 1.0000,  0.0000 )        0.0783             0.4336
 0.1111     ( 1.1106,  0.1239 )        0.2434             0.0477
 0.2222     ( 1.2181,  0.2752 )        0.1819             0.0584
 0.3333     ( 1.3188,  0.4566 )        0.0703             0.1267
 0.4444     ( 1.4081,  0.6706 )        0.1458             0.0868
 0.5556     ( 1.4808,  0.9192 )        0.1946             0.0930
 0.6667     ( 1.5307,  1.2044 )        0.1458             0.0734
 0.7778     ( 1.5508,  1.5273 )        0.1815             0.0690
 0.8889     ( 1.5331,  1.8885 )        0.0805             0.0193
 1.0000     ( 1.4687,  2.2874 )        0.2396             1.1708
 Average absolute error before filter:    0.18549
 Average absolute error after filter:     0.09636
```

RCORL

more...

Computes the correlation of two real vectors.

Required Arguments

X — Real vector of length `N`. (Input)

Y — Real vector of length `N`. (Input)

Z — Real vector of length `NZ` containing the correlation of `X` and `Y`. (Output)

ZHAT — Real vector of length `NZ` containing the discrete Fourier transform of `Z`. (Output)

Optional Arguments

IDO — Flag indicating the usage of `RCORL`. (Input)
Default: `IDO` = 0.

IDO	Usage
0	If this is the only call to `RCORL`.
If `RCORL` is called multiple times in sequence with the same `NX`, `NY`, and `IPAD`, `IDO` should be set to:	
1	on the first call
2	on the intermediate calls
3	on the final call

N — Length of the `X` and `Y` vectors. (Input)
Default: `N` = size `(X,1)`.

IPAD — `IPAD` should be set as follows. (Input)
Default: `IPAD` = 0.

IPAD	Value
IPAD	0 for periodic data with X and Y different.
IPAD	1 for nonperiodic data with X and Y different.
IPAD	2 for periodic data with X and Y identical.
IPAD	3 for nonperiodic data with X and Y identical.

NZ — Length of the vector Z. (Input/Output)
Upon input: When IPAD is zero or two, NZ must be at least (2 * N − 1). When IPAD is one or three, NZ must be greater than or equal to the smallest integer greater than or equal to (2 * N − 1) of the form (2^{α}) * (3^{β}) * (5^{γ}) where alpha, beta, and gamma are nonnegative integers. Upon output, the value for NZ that was used by RCORL.
Default: NZ = size (Z,1).

FORTRAN 90 Interface

Generic: CALL RCORL (X, Y, Z, ZHAT [, …])

Specific: The specific interface names are S_RCORL and D_RCORL.

FORTRAN 77 Interface

Single: CALL RCORL (IDO, N, X, Y, IPAD, NZ, Z, ZHAT)

Double: The double precision name is DRCORL.

Description

The subroutine RCORL computes the discrete correlation of two sequences *x* and *y*. More precisely, let *n* be the length of *x* and *y*. If a circular correlation is desired, then IPAD must be set to zero (for *x* and *y* distinct) and two (for *x* = *y*). We set (on output)

$$\begin{aligned} n_z &= n && \text{if IPAD} = 0,2 \\ n_z &= 2^{\alpha}3^{\beta}5^{\gamma} \geq 2n-1 && \text{if IPAD} = 1,3 \end{aligned}$$

where α, β, γ are nonnegative integers yielding the smallest number of the type $2^{\alpha}3^{\beta}5^{\gamma}$ satisfying the inequality. Once n_z is determined, we pad out the vectors with zeroes. Then, we compute

$$z_i = \sum_{j=1}^{n_z} x_{i+j-1} y_j$$

where the index on x is interpreted as a positive number between one and n_z, modulo n_z. Note that this means that

$$z_{n_z - k}$$

contains the correlation of $x(\cdot - k - 1)$ with y as $k = 0, 1, \ldots, n_z/2$. Thus, if $x(k - 1) = y(k)$ for all k, then we would expect

$$z_{n_z}$$

to be the largest component of z.

The technique used to compute the z_i's is based on the fact that the (complex discrete) Fourier transform maps correlation into multiplication. Thus, the Fourier transform of z is given by

$$\hat{z}_j = \hat{x}_j \overline{\hat{y}_j}$$

where

$$\hat{z}_j = \sum_{m=1}^{n_z} z_m e^{-2\pi i (m-1)(j-1)/n_z}$$

Thus, the technique used here to compute the correlation is to take the discrete Fourier transform of x and the conjugate of the discrete Fourier transform of y, multiply the results together component-wise, and then take the inverse transform of this product. It is very important to make sure that n_z is a product of small primes if `IPAD` is set to zero or two. If n_z is a product of small primes, then the computational effort will be proportional to $n_z \log(n_z)$. If `IPAD` is one or three, then a good value is chosen for n_z so that the Fourier transforms are efficient and $n_z \geq 2n - 1$. This will mean that both vectors will be padded with zeroes.

We point out that no complex transforms of x or y are taken since both sequences are real, and we can take real transforms and simulate the complex transform above. This can produce a savings of a factor of six in time as well as save space over using the complex transform.

Comments

1. Workspace may be explicitly provided, if desired, by use of `R2ORL/DR2ORL`. The reference is:

   `CALL R2ORL (IDO, N, X, Y, IPAD, NZ, Z, ZHAT, XWK, YWK, WK)`

The additional arguments are as follows:

XWK — Real work array of length NZ.

YWK — Real work array of length NZ.

WK — Real work arrary of length 2 * NZ + 15.

2. Informational error

Type	Code	Description
4	1	The length of the vector Z must be large enough to hold the results. An acceptable length is returned in NZ.

Example

In this example, we compute both a periodic and a non-periodic correlation between two distinct signals *x* and *y*. In the first case we have 100 equally spaced points on the interval [0, 2π] and $f_1(x) = \sin(x)$. We define *x* and *y* as follows

$$x_i = f_1\left(2\pi\frac{i-1}{n-1}\right) \qquad i = 1, \ldots, n$$
$$y_i = f_1\left(2\pi\frac{i-1}{n-1} + \frac{\pi}{2}\right) \qquad i = 1, \ldots, n$$

Note that the maximum value of *z* (the correlation of *x* with *y*) occurs at *i* = 26, which corresponds to the offset.

The nonperiodic case uses the function $f_2(x) = \sin(x^2)$. The two input signals are on the interval [0, 4π].

$$x_i = f_2\left(4\pi\frac{i-1}{n-1}\right) \qquad i = 1, \ldots, n$$
$$y_i = f_2\left(4\pi\frac{i-1}{n-1} + \pi\right) \qquad i = 1, \ldots, n$$

The offset of *x* to *y* is again (roughly) 26 and this is where *z* has its maximum value.

```
      USE IMSL_LIBRARIES

      IMPLICIT   NONE
      INTEGER    N
      PARAMETER  (N=100)
!
      INTEGER    I, IPAD, K, NOUT, NZ
      REAL       A, F1, F2, FLOAT, PI, SIN, X(N), XNORM, &
                Y(N), YNORM, Z(4*N), ZHAT(4*N)
      INTRINSIC  FLOAT, SIN
!                                 Define functions
      F1(A) = SIN(A)
      F2(A) = SIN(A*A)
!
      CALL UMACH (2, NOUT)
      PI = CONST('pi')
!                                  Set up the vectors for the
!                                  periodic case.
      DO 10  I=1, N
```

```
          X(I) = F1(2.0*PI*FLOAT(I-1)/FLOAT(N-1))
          Y(I) = F1(2.0*PI*FLOAT(I-1)/FLOAT(N-1)+PI/2.0)
   10 CONTINUE
!                                  Call the correlation routine for the
!                                  periodic case.
      NZ = 2*N
      CALL RCORL (X, Y, Z, ZHAT)
!                                  Find the element of Z with the
!                                  largest normalized value.
      XNORM = SNRM2(N,X,1)
      YNORM = SNRM2(N,Y,1)
      DO 20  I=1, N
         Z(I) = Z(I)/(XNORM*YNORM)
   20 CONTINUE
      K = ISMAX(N,Z,1)
!                                  Print results for the periodic
!                                  case.
      WRITE (NOUT,99995)
      WRITE (NOUT,99994)
      WRITE (NOUT,99997)
      WRITE (NOUT,99998) K
      WRITE (NOUT,99999) K, Z(K)
!                                  Set up the vectors for the
!                                  nonperiodic case.
      DO 30  I=1, N
         X(I) = F2(4.0*PI*FLOAT(I-1)/FLOAT(N-1))
         Y(I) = F2(4.0*PI*FLOAT(I-1)/FLOAT(N-1)+PI)
   30 CONTINUE
!                                  Call the correlation routine for the
!                                  nonperiodic case.
      NZ = 4*N
      CALL RCORL (X, Y, Z, ZHAT, IPAD=1)
!                                  Find the element of Z with the
!                                  largest normalized value.
      XNORM = SNRM2(N,X,1)
      YNORM = SNRM2(N,Y,1)
      DO 40  I=1, N
         Z(I) = Z(I)/(XNORM*YNORM)
   40 CONTINUE
      K = ISMAX(N,Z,1)
!                                  Print results for the nonperiodic
!                                  case.
      WRITE (NOUT,99996)
      WRITE (NOUT,99994)
      WRITE (NOUT,99997)
      WRITE (NOUT,99998) K
      WRITE (NOUT,99999) K, Z(K)
99994 FORMAT (1X, 28('-'))
99995 FORMAT (' Case #1: Periodic data')
99996 FORMAT (/, ' Case #2: Nonperiodic data')
99997 FORMAT (' The element of Z with the largest normalized ')
99998 FORMAT (' value is Z(', I2, ').')
99999 FORMAT (' The normalized value of Z(', I2, ') is', F6.3)
      END
```

Output

```
Example #1: Periodic case
----------------------------
The element of Z with the largest normalized value is Z(26).
The normalized value of Z(26) is 1.000

Example #2: Nonperiodic case
----------------------------
The element of Z with the largest normalized value is Z(26).
```

```
The normalized value of Z(26) is 0.661
```

CCORL

more...

Computes the correlation of two complex vectors.

Required Arguments

X — Complex vector of length `N`. (Input)

Y — Complex vector of length `N`. (Input)

Z — Complex vector of length `NZ` containing the correlation of `X` and `Y`. (Output)

ZHAT — Complex vector of length `NZ` containing the inverse discrete complex Fourier transform of `Z`. (Output)

Optional Arguments

IDO — Flag indicating the usage of `CCORL`. (Input)
Default: `IDO` = 0.

IDO	**Usage**
0	If this is the only call to `CCORL`.
If `CCORL` is called multiple times in sequence with the same `NX`, `NY`, and `IPAD`, `IDO` should be set to:	
1	on the first call
2	on the intermediate calls
3	on the final call

N — Length of the `X` and `Y` vectors. (Input)
Default: `N` = size `(X,1)`.

IPAD — IPAD should be set as follows. (Input)

IPAD = 0 for periodic data with X and Y different. IPAD = 1 for nonperiodic data with X and Y different. IPAD = 2 for periodic data with X and Y identical. IPAD = 3 for nonperiodic data with X and Y identical.

Default: IPAD = 0.

NZ — Length of the vector Z. (Input/Output)

Upon input: When IPAD is zero or two, NZ must be at least (2 * N − 1). When IPAD is one or three, NZ must be greater than or equal to the smallest integer greater than or equal to (2 * N − 1) of the form (2^{α}) * (3^{β}) * (5^{γ}) where alpha, beta, and gamma are nonnegative integers. Upon output, the value for NZ that was used by CCORL.

Default: NZ = size (Z,1).

FORTRAN 90 Interface

Generic: CALL CCORL (X, Y, Z, ZHAT [, …])

Specific: The specific interface names are S_CCORL and D_CCORL.

FORTRAN 77 Interface

Single: CALL CCORL (IDO, N, X, Y, IPAD, NZ, Z, ZHAT)

Double: The double precision name is DCCORL.

Description

The subroutine CCORL computes the discrete correlation of two complex sequences *x* and *y*. More precisely, let *n* be the length of *x* and *y*. If a circular correlation is desired, then IPAD must be set to zero (for *x* and *y* distinct) and two (for *x* = *y*). We set (on output)

$$\begin{aligned} n_z &= n && \text{if IPAD} = 0{,}2 \\ n_z &= 2^{\alpha}3^{\beta}5^{\gamma} \geq 2n - 1 && \text{if IPAD} = 1{,}3 \end{aligned}$$

where α, β, γ are nonnegative integers yielding the smallest number of the type $2^{\alpha}3^{\beta}5^{\gamma}$ satisfying the inequality. Once n_z is determined, we pad out the vectors with zeroes. Then, we compute

$$z_i = \sum_{j=1}^{n_z} x_{i+j-1} \overline{y}_j$$

where the index on x is interpreted as a positive number between one and n_z, modulo n_z. Note that this means that

$$z_{n_z - k}$$

contains the correlation of $x(\cdot - k - 1)$ with y as $k = 0, 1, \ldots, n_z/2$. Thus, if $x(k - 1) = y(k)$ for all k, then we would expect

$$\Re\, z_{n_z}$$

to be the largest component of $\Re z$.

The technique used to compute the z_i's is based on the fact that the (complex discrete) Fourier transform maps correlation into multiplication. Thus, the Fourier transform of z is given by

$$\hat{z}_j = \hat{x}_j \overline{\hat{y}_j}$$

where

$$\hat{z}_j = \sum_{m=1}^{n_z} z_m e^{-2\pi i (m-1)(j-1)/n_z}$$

Thus, the technique used here to compute the correlation is to take the discrete Fourier transform of x and the conjugate of the discrete Fourier transform of y, multiply the results together component-wise, and then take the inverse transform of this product. It is very important to make sure that n_z is a product of small primes if `IPAD` is set to zero or two. If n_z is a product of small primes, then the computational effort will be proportional to $n_z \log(n_z)$. If `IPAD` is one or three, then a good value is chosen for n_z so that the Fourier transforms are efficient and $n_z \geq 2n - 1$. This will mean that both vectors will be padded with zeroes.

Comments

1. Workspace may be explicitly provided, if desired, by use of `C2ORL/DC2ORL`. The reference is:

   `CALL C2ORL (IDO, N, X, Y, IPAD, NZ, Z, ZHAT, XWK, YWK, WK)`

   The additional arguments are as follows:

   XWK — Complex work array of length `NZ`.

   YWK — Complex work array of length `NZ`.

WK — Real work array of length 6 * `NZ` + 15.

2. Informational error

Type	Code	Description
4	1	The length of the vector `Z` must be large enough to hold the results. An acceptable length is returned in `NZ`.

Example

In this example, we compute both a periodic and a non-periodic correlation between two distinct signals *x* and *y*. In the first case, we have 100 equally spaced points on the interval [0, 2π] and $f_1(x) = \cos(x) + i \sin(x)$. We define *x* and *y* as follows

$$x_i = f_1(2\pi \tfrac{i-1}{n-1}) \qquad i = 1, \ldots, n$$
$$y_i = f_1(2\pi \tfrac{i-1}{n-1} + \tfrac{\pi}{2}) \qquad i = 1, \ldots, n$$

Note that the maximum value of *z* (the correlation of *x* with *y*) occurs at $i = 26$, which corresponds to the offset.

The nonperiodic case uses the function $f_2(x) = \cos(x^2) + i \sin(x^2)$. The two input signals are on the interval [0, 4π].

$$x_i = f_2(4\pi \tfrac{i-1}{n-1}) \qquad i = 1, \ldots, n$$
$$y_i = f_2(4\pi \tfrac{i-1}{n-1} + \pi) \qquad i = 1, \ldots, n$$

The offset of *x* to *y* is again (roughly) 26 and this is where *z* has its maximum value.

```
      USE IMSL_LIBRARIES

      IMPLICIT   NONE
      INTEGER    N
      PARAMETER  (N=100)
!
      INTEGER    I, IPAD, K, NOUT, NZ
      REAL       A, COS, F1, F2, FLOAT, PI, SIN, &
                XNORM, YNORM, ZREAL1(4*N)
      COMPLEX    CMPLX, X(N), Y(N), Z(4*N), ZHAT(4*N)
      INTRINSIC  CMPLX, COS, FLOAT, SIN
!                                 Define functions
      F1(A) = CMPLX(COS(A),SIN(A))
      F2(A) = CMPLX(COS(A*A),SIN(A*A))
!
      CALL RNSET (1234579)
      CALL UMACH (2, NOUT)
      PI = CONST('pi')
!                                  Set up the vectors for the
!                                  periodic case.
      DO 10  I=1, N
         X(I) = F1(2.0*PI*FLOAT(I-1)/FLOAT(N-1))
         Y(I) = F1(2.0*PI*FLOAT(I-1)/FLOAT(N-1)+PI/2.0)
   10 CONTINUE
!                                  Call the correlation routine for the
```

```
!                                  periodic case.
      NZ = 2*N
      CALL CCORL (X, Y, Z, ZHAT, IPAD=0, NZ=NZ)
!                                  Find the element of Z with the
!                                  largest normalized real part.
      XNORM = SCNRM2(N,X,1)
      YNORM = SCNRM2(N,Y,1)
      DO 20  I=1, N
         ZREAL1(I) = REAL(Z(I))/(XNORM*YNORM)
   20 CONTINUE
      K = ISMAX(N,ZREAL1,1)
!                                  Print results for the periodic
!                                  case.
      WRITE (NOUT,99995)
      WRITE (NOUT,99994)
      WRITE (NOUT,99997)
      WRITE (NOUT,99998) K
      WRITE (NOUT,99999) K, ZREAL1(K)
!                                  Set up the vectors for the
!                                  nonperioddic case.
      DO 30  I=1, N
         X(I) = F2(4.0*PI*FLOAT(I-1)/FLOAT(N-1))
         Y(I) = F2(4.0*PI*FLOAT(I-1)/FLOAT(N-1)+PI)
   30 CONTINUE
!                                  Call the correlation routine for the
!                                  nonperiodic case.
      NZ = 4*N
      CALL CCORL (X, Y, Z, ZHAT, IPAD=1, NZ=NZ)
!                                  Find the element of z with the
!                                  largest normalized real part.
      XNORM = SCNRM2(N,X,1)
      YNORM = SCNRM2(N,Y,1)
      DO 40  I=1, N
         ZREAL1(I) = REAL(Z(I))/(XNORM*YNORM)
   40 CONTINUE
      K = ISMAX(N,ZREAL1,1)
!                                  Print results for the nonperiodic
!                                  case.
      WRITE (NOUT,99996)
      WRITE (NOUT,99994)
      WRITE (NOUT,99997)
      WRITE (NOUT,99998) K
      WRITE (NOUT,99999) K, ZREAL1(K)
99994 FORMAT (1X, 28('-'))
99995 FORMAT (' Case #1: periodic data')
99996 FORMAT (/, ' Case #2: nonperiodic data')
99997 FORMAT (' The element of Z with the largest normalized ')
99998 FORMAT (' real part is Z(', I2, ').')
99999 FORMAT (' The normalized value of real(Z(', I2, ')) is', F6.3)
      END
```

Output

```
Example #1: periodic case
----------------------------
The element of Z with the largest normalized real part is Z(26).
The normalized value of real(Z(26)) is 1.000

Example #2: nonperiodic case
----------------------------
The element of Z with the largest normalized real part is Z(26).
The normalized value of real(Z(26)) is 0.638
```

INLAP

Computes the inverse Laplace transform of a complex function.

Required Arguments

F — User-supplied `FUNCTION` to which the inverse Laplace transform will be computed. The form is `F(Z)`, where

`Z` – Complex argument. (Input)

`F` – The complex function value. (Output)

`F` must be declared `EXTERNAL` in the calling program. `F` should also be declared `COMPLEX`.

T — Array of length `N` containing the points at which the inverse Laplace transform is desired. (Input) `T(I)` must be greater than zero for all `I`.

FINV — Array of length `N` whose `I`-th component contains the approximate value of the Laplace transform at the point `T(I)`. (Output)

Optional Arguments

N — Number of points at which the inverse Laplace transform is desired. (Input)
Default: `N` = size `(T,1)`.

ALPHA — An estimate for the maximum of the real parts of the singularities of `F`. If unknown, set `ALPHA` = 0. (Input)
Default: `ALPHA` = 0.0.

KMAX — The number of function evaluations allowed for each `T(I)`. (Input)
Default: `KMAX` = 500.

RELERR — The relative accuracy desired. (Input)
Default: `RELERR` = 1.1920929e-5 for single precision and 2.22d-10 for double precision.

FORTRAN 90 Interface

Generic: `CALL INLAP (F, T, FINV [, …])`

Specific: The specific interface names are `S_INLAP` and `D_INLAP`.

FORTRAN 77 Interface

Single: CALL INLAP (F, N, T, ALPHA, RELERR, KMAX, FINV)

Double: The double precision name is DINLAP.

Description

The routine INLAP computes the inverse Laplace transform of a complex-valued function. Recall that if *f* is a function that vanishes on the negative real axis, then we can define the Laplace transform of *f* by

$$L[f](s) := \int_0^{\infty} e^{-sx} f(x)\,dx$$

It is assumed that for some value of *s* the integrand is absolutely integrable.

The computation of the inverse Laplace transform is based on applying the epsilon algorithm to the complex Fourier series obtained as a discrete approximation to the inversion integral. The initial algorithm was proposed by K.S. Crump (1976) but was significantly improved by de Hoog et al. (1982). Given a complex-valued transform $F(s) = L[f](s)$, the trapezoidal rule gives the approximation to the inverse transform

$$g(t) = \left(e^{\alpha t}/T\right) \Re \left\{ \frac{1}{2} F(\alpha) + \sum_{k=1}^{\infty} F\left(\alpha + \frac{ik\pi}{T}\right) \exp\left(\frac{ik\pi t}{T}\right) \right\}$$

This is the real part of the sum of a complex power series in $z = \exp(i\pi t/T)$, and the algorithm accelerates the convergence of the partial sums of this power series by using the epsilon algorithm to compute the corresponding diagonal Pade approximants. The algorithm attempts to choose the order of the Pade approximant to obtain the specified relative accuracy while not exceeding the maximum number of function evaluations allowed. The parameter α is an estimate for the maximum of the real parts of the singularities of *F*, and an incorrect choice of α may give false convergence. Even in cases where the correct value of α is unknown, the algorithm will attempt to estimate an acceptable value. Assuming satisfactory convergence, the discretization error $E := g - f$ satisfies

$$E = \sum_{n=1}^{\infty} e^{-2n\alpha T} f(2nT + t)$$

It follows that if $|f(t)| \le Me^{\beta t}$, then we can estimate the expression above to obtain (for $0 \le t \le 2T$)

$$E \le Me^{\alpha t} / \left(e^{2T(\alpha-\beta)} - 1\right)$$

Comments

Informational errors

Type	Code	Description
4	1	The algorithm was not able to achieve the accuracy requested within KMAX function evaluations for some T(I).
4	2	Overflow is occurring for a particular value of T.

Example

We invert the Laplace transform of the simple function $(s - 1)^{-2}$ and print the computed answer, the true solution and the difference at five different points. The correct inverse transform is xe^{x}.

```
      USE INLAP_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    I, KMAX, N, NOUT
      REAL       ALPHA, DIF(5), EXP, FINV(5), FLOAT, RELERR, T(5), &
                TRUE(5)
      COMPLEX    F
      INTRINSIC  EXP, FLOAT
      EXTERNAL   F
!                                 Get output unit number
      CALL UMACH (2, NOUT)
!
      DO 10  I=1, 5
         T(I) = FLOAT(I) - 0.5
   10 CONTINUE
      N      = 5
      ALPHA  = 1.0E0
      RELERR = 5.0E-4
      CALL INLAP (F, T, FINV, ALPHA=ALPHA, RELERR=RELERR)
!                                 Evaluate the true solution and the
!                                 difference
      DO 20  I=1, 5
         TRUE(I)  = T(I)*EXP(T(I))
         DIF(I) = TRUE(I) - FINV(I)
   20 CONTINUE
!
      WRITE (NOUT,99999) (T(I),FINV(I),TRUE(I),DIF(I),I=1,5)
99999 FORMAT (7X, 'T', 8X, 'FINV', 9X, 'TRUE', 9X, 'DIFF', /, &
            5(1X,E9.1,3X,1PE10.3,3X,1PE10.3,3X,1PE10.3,/))
      END
!
      COMPLEX FUNCTION F (S)
      COMPLEX    S
      F = 1./(S-1.)**2
      RETURN
      END
```

Output

```
     T        FINV         TRUE         DIFF
0.5E+00    8.244E-01    8.244E-01   -4.768E-06
1.5E+00    6.723E+00    6.723E+00   -3.481E-05
2.5E+00    3.046E+01    3.046E+01   -1.678E-04
3.5E+00    1.159E+02    1.159E+02   -6.027E-04
4.5E+00    4.051E+02    4.051E+02   -2.106E-03
```

SINLP

Computes the inverse Laplace transform of a smooth complex function.

Required Arguments

F — User-supplied FUNCTION to which the inverse Laplace transform will be computed. The form is F(Z), where

Z — Complex argument. (Input)

F — The complex function value. (Output)

F must be declared EXTERNAL in the calling program. F must also be declared COMPLEX.

T — Vector of length N containing points at which the inverse Laplace transform is desired. (Input) T(I) must be greater than zero for all I.

FINV — Vector of length N whose I-th component contains the approximate value of the inverse Laplace transform at the point T(I). (Output)

Optional Arguments

N — The number of points at which the inverse Laplace transform is desired. (Input)
Default: N = size (T,1).

SIGMA0 — An estimate for the maximum of the real parts of the singularities of F. (Input)
If unknown, set SIGMA0 = 0.0.
Default: SIGMA0 = 0.e0.

EPSTOL — The required absolute uniform pseudo accuracy for the coefficients and inverse Laplace transform values. (Input)
Default: EPSTOL = 1.1920929e-5 for single precision and 2.22d-10 for double precision.

ERRVEC — Vector of length eight containing diagnostic information. (Output)
All components depend on the intermediately generated Laguerre coefficients. See *Comments*.

FORTRAN 90 Interface

Generic: CALL SINLP (F, T, FINV [, …])

Specific: The specific interface names are S_SINLP and D_SINLP.

FORTRAN 77 Interface

Single: CALL SINLP (F, N, T, SIGMA0, EPSTOL, ERRVEC, FINV)

Double: The double precision name is DSINLP.

Description

The routine SINLP computes the inverse Laplace transform of a complex-valued function. Recall that if *f* is a function that vanishes on the negative real axis, then we can define the Laplace transform of *f* by

$$L[f](s) := \int_0^\infty e^{-sx} f(x)\,dx$$

It is assumed that for some value of *s* the integrand is absolutely integrable.

The computation of the inverse Laplace transform is based on a modification of Weeks' method (see W.T. Weeks (1966)) due to B.S. Garbow et. al. (1988). This method is suitable when *f* has continuous derivatives of all orders on [0, ∞). In this situation, this routine should be used in place of the IMSL routine INLAP. It is especially efficient when multiple function values are desired. In particular, given a complex-valued function *F*(*s*) = *L*[*f*](*s*), we can expand *f* in a Laguerre series whose coefficients are determined by *F*. This is fully described in B.S. Garbow et. al. (1988) and Lyness and Giunta (1986).

The algorithm attempts to return approximations *g*(*t*) to *f*(*t*) satisfying

$$\left|\frac{g(t) - f(t)}{e^{\sigma t}}\right| < \varepsilon$$

where **ε** := EPSTOL and **σ** := SIGMA > SIGMA0. The expression on the left is called the pseudo error. An estimate of the pseudo error is available in ERRVEC(1).

The first step in the method is to transform *F* to **ϕ** where

$$\phi(z) = \frac{b}{1-z} F\left(\frac{b}{1-z} - \frac{b}{2} + \sigma\right)$$

Then, if *f* is smooth, it is known that **ϕ** is analytic in the unit disc of the complex plane and hence has a Taylor series expansion

$$\phi(z) = \sum_{s=0}^{\infty} a_s z^s$$

which converges for all *z* whose absolute value is less than the radius of convergence R_c. This number is estimated in ERRVEC(6). In ERRVEC(5), we estimate the smallest number *K* which satisfies

$$|a_s| < \frac{K}{R^s}$$

for all $R < R_c$.

The coefficients of the Taylor series for ϕ can be used to expand f in a Laguerre series

$$f(t) = e^{\sigma t} \sum_{s=0}^{\infty} a_s e^{-bt/2} L_s(bt)$$

Comments

1. Workspace may be explicitly provided, if desired, by use of S2NLP/DS2NLP. The reference is:

   CALL S2NLP (F, N, T, SIGMA0, EPSTOL, ERRVEC, FINV, SIGMA, BVALUE, MTOP, WK, IFLOVC)

   The additional arguments are as follows:

   SIGMA — The first parameter of the Laguerre expansion. If SIGMA is not greater than SIGMA0, it is reset to SIGMA0 + 0.7. (Input)

   BVALUE — The second parameter of the Laguerre expansion. If BVALUE is less than 2.0 * (SIGMA − SIGMA0), it is reset to 2.5 * (SIGMA − SIGMA0). (Input)

   MTOP — An upper limit on the number of coefficients to be computed in the Laguerre expansion. MTOP must be a multiple of four. Note that the maximum number of Laplace transform evaluations is MTOP/2 + 2. (Default: 1024.) (Input)

   WK — Real work vector of length 9 * MTOP/4.

   IFLOVC — Integer vector of length N, the I-th component of which contains the overflow/underflow indicator for the computed value of FINV(I). (Output) See Comment 3.

2. Informational errors

Type	Code	Description
1	1	Normal termination, but with estimated error bounds slightly larger than EPSTOL. Note, however, that the actual errors on the final results may be smaller than EPSTOL as bounds independent of T are pessimistic.
3	2	Normal calculation, terminated early at the roundoff error level estimate because this estimate exceeds the required accuracy (usually due to overly optimistic expectation by the user about attainable accuracy).
4	3	The decay rate of the coefficients is too small. It may improve results to use S2NLP and increase MTOP.

Type	Code	Description
4	4	The decay rate of the coefficients is too small. In addition, the roundoff error level is such that required accuracy cannot be reached.
4	5	No error bounds are returned as the behavior of the coefficients does not enable reasonable prediction. Results are probably wrong. Check the value of SIGMA0. In this case, each of ERRVEC(J), J = 1, …, 5, is set to −1.0.

3. The following are descriptions of the vectors ERRVEC and IFLOVC.

ERRVEC — Real vector of length eight.

ERRVEC(1) = Overall estimate of the pseudo error, ERRVEC(2) + ERRVEC(3) + ERRVEC(4). Pseudo error = absolute error / exp(sigma * tvalue).

ERRVEC(2) = Estimate of the pseudo discretization error.

ERRVEC(3) = Estimate of the pseudo truncation error.

ERRVEC(4) = Estimate of the pseudo condition error on the basis of minimal noise levels in the function values.

ERRVEC(5) = K, the coefficient of the decay function for ACOEF, the coefficients of the Laguerre expansion.

ERRVEC(6) = R, the base of the decay function for ACOEF. Here abs(ACOEF (J + 1)).LE.K/R**J for J.GE.MACT/2, where MACT is the number of Laguerre coefficients actually computed.

ERRVEC(7) = ALPHA, the logarithm of the largest ACOEF.

ERRVEC(8) = BETA, the logarithm of the smallest nonzero ACOEF.

IFLOVC — Integer vector of length N containing the overflow/underflow indicators for FINV. For each I, the value of IFLOVC(I) signifies the following.

0 = Normal termination.

1 = The value of the inverse Laplace transform is found to be too large to be representable; FINV(I) is set to AMACH(6).

−1 = The value of the inverse Laplace transform is found to be too small to be representable; FINV(I) is set to 0.0.

2 = The value of the inverse Laplace transform is estimated to be too large, even before the series expansion, to be representable; FINV(I) is set to AMACH(6).

−2 = The value of the inverse Laplace transform is estimated to be too small, even before the series expansion, to be representable; FINV(I) is set to 0.0.

Example

We invert the Laplace transform of the simple function $(s - 1)^{-2}$ and print the computed answer, the true solution, and the difference at five different points. The correct inverse transform is xe^x.

```
      USE SINLP_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    I, NOUT
      REAL       DIF(5), ERRVEC(8), EXP, FINV(5), FLOAT, RELERR, &
                SIGMA0, T(5), TRUE(5), EPSTOL
      COMPLEX    F
      INTRINSIC  EXP, FLOAT
      EXTERNAL   F
!                                 Get output unit number
      CALL UMACH (2, NOUT)
!
      DO 10  I=1, 5
         T(I) = FLOAT(I) - 0.5
   10 CONTINUE
      SIGMA0 = 1.0E0
      RELERR = 5.0E-4
      EPSTOL = 1.0E-4
      CALL SINLP (F, T, FINV, SIGMA0=SIGMA0, EPSTOL=RELERR)
!                                 Evaluate the true solution and the
!                                 difference
      DO 20  I=1, 5
         TRUE(I) = T(I)*EXP(T(I))
         DIF(I) = TRUE(I) - FINV(I)
   20 CONTINUE
!
      WRITE (NOUT,99999) (T(I),FINV(I),TRUE(I),DIF(I),I=1,5)
99999 FORMAT (7X, 'T', 8X, 'FINV', 9X, 'TRUE', 9X, 'DIFF', /, &
            5(1X,E9.1,3X,1PE10.3,3X,1PE10.3,3X,1PE10.3,/))
      END
!
      COMPLEX FUNCTION F (S)
      COMPLEX    S
!
      F = 1./(S-1.)**2
      RETURN
      END
```

Output

```
      T         FINV         TRUE         DIFF
 0.5E+00    8.244E-01    8.244E-01   -2.086E-06
 1.5E+00    6.723E+00    6.723E+00   -8.583E-06
 2.5E+00    3.046E+01    3.046E+01    0.000E+00
 3.5E+00    1.159E+02    1.159E+02    2.289E-05
 4.5E+00    4.051E+02    4.051E+02   -2.136E-04
```

Nonlinear Equations

Routines

Usage Notes

Zeros of a Polynomial

A polynomial function of degree *n* can be expressed as follows:

$$p(z) = a_n z^n + a_{n-1} z^{n-1} + \ldots + a_1 z + a_0$$

where $a_n \neq 0$.

There are three routines for zeros of a polynomial. The routines ZPLRC and ZPORC find zeros of the polynomial with real coefficients while the routine ZPOCC finds zeros of the polynomial with complex coefficients.

The Jenkins-Traub method is used for the routines ZPORC and ZPOCC; whereas ZPLRC uses the Laguerre method. Both methods perform well in comparison with other methods. The Jenkins-Traub algorithm usually runs faster than the Laguerre method. Furthermore, the routine ZANLY in the next section can also be used for the complex polynomial.

Zero(s) of a Function

The routines ZANLY and ZREAL use Müller's method to find the zeros of a complex analytic function and real zeros of a real function, respectively. The routine ZBREN finds a zero of a real function, using an algorithm that is a combination of interpolation and bisection. This algorithm requires the user to supply two points such that the function values at these two points have opposite sign. For functions where it is difficult to obtain two such points, ZUNI or ZREAL can be used.

Root of System of Equations

A system of equations can be stated as follows:

$$f_i(x) = 0, \text{ for } i = 1, 2, \ldots, n$$

where $x \in \mathbf{R}^n$.

The routines NEQNF and NEQNJ use a modified Powell hybrid method to find a zero of a system of nonlinear equations. The difference between these two routines is that the Jacobian is estimated by a finite-difference method in NEQNF, whereas the user has to provide the Jacobian for NEQNJ. It is advised that the Jacobian-checking routine, CHJAC (see *Chapter 8, "Optimization"*), be used to ensure the accuracy of the user-supplied Jacobian.

The routines NEQBF and NEQBJ use a secant method with Broyden's update to find a zero of a system of nonlinear equations. The difference between these two routines is that the Jacobian is estimated by a finite-difference method in NEQBF; whereas the user has to provide the Jacobian for NEQBJ. For more details, see Dennis and Schnabel (1983, Chapter 8).

ZPLRC

Finds the zeros of a polynomial with real coefficients using Laguerre's method.

Required Arguments

COEFF — Vector of length NDEG + 1 containing the coefficients of the polynomial in increasing order by degree. (Input)
The polynomial is
COEFF(NDEG + 1) * Z**NDEG + COEFF(NDEG) * Z**(NDEG – 1) + ... + COEFF(1).

ROOT — Complex vector of length NDEG containing the zeros of the polynomial. (Output)

Optional Arguments

NDEG — Degree of the polynomial. 1 ≤ NDEG ≤ 100 (Input)
Default: NDEG = size (COEFF,1) – 1.

FORTRAN 90 Interface

Generic: CALL ZPLRC (COEFF, ROOT [, ...])

Specific: The specific interface names are S_ZPLRC and D_ZPLRC.

FORTRAN 77 Interface

Single: CALL ZPLRC (NDEG, COEFF, ROOT)

Double: The double precision name is DZPLRC.

Description

Routine ZPLRC computes the *n* zeros of the polynomial

$$p(z) = a_n z^n + a_{n-1} z^{n-1} + \ldots + a_1 z + a_0$$

where the coefficients a_i for i = 0, 1, ..., n are real and n is the degree of the polynomial.

The routine `ZPLRC` is a modification of B.T. Smith's routine `ZERPOL` (Smith 1967) that uses Laguerre's method. Laguerre's method is cubically convergent for isolated zeros and linearly convergent for multiple zeros. The maximum length of the step between successive iterates is restricted so that each new iterate lies inside a region about the previous iterate known to contain a zero of the polynomial. An iterate is accepted as a zero when the polynomial value at that iterate is smaller than a computed bound for the rounding error in the polynomial value at that iterate. The original polynomial is deflated after each real zero or pair of complex zeros is found. Subsequent zeros are found using the deflated polynomial.

Comments

Informational errors

Type	**Code**	**Description**
3	1	The first several coefficients of the polynomial are equal to zero. Several of the last roots will be set to machine infinity to compensate for this problem.
3	2	Fewer than `NDEG` zeros were found. The `ROOT` vector will contain the value for machine infinity in the locations that do not contain zeros.

Example

This example finds the zeros of the third-degree polynomial

$$p(z) = z^3 - 3z^2 + 4z - 2$$

where *z* is a complex variable.

```
      USE ZPLRC_INT
      USE WRCRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    NDEG
      PARAMETER  (NDEG=3)
!
      REAL       COEFF(NDEG+1)
      COMPLEX    ZERO(NDEG)
!                                 Set values of COEFF
!                                 COEFF = (-2.0  4.0 -3.0  1.0)
!
      DATA COEFF/-2.0, 4.0, -3.0, 1.0/
!
      CALL ZPLRC (COEFF, ZERO, NDEG)
!
      CALL WRCRN ('The zeros found are', ZERO, 1, NDEG, 1)
!
      END
```

Output

```
                The zeros found are
               1                2                 3
  ( 1.000, 1.000)  ( 1.000,-1.000)  ( 1.000, 0.000)
```

ZPORC

Finds the zeros of a polynomial with real coefficients using the Jenkins-Traub three-stage algorithm.

Required Arguments

COEFF — Vector of length `NDEG` + 1 containing the coefficients of the polynomial in increasing order by degree. (Input)
The polynomial is
`COEFF`(`NDEG` + 1)`*Z**NDEG` + `COEFF`(`NDEG`) `* Z**`(`NDEG` –1) + … + `COEFF`(1).

ROOT — Complex vector of length `NDEG` containing the zeros of the polynomial. (Output)

Optional Arguments

NDEG — Degree of the polynomial. 1 ≤ `NDEG` ≤ 100 (Input)
Default: `NDEG` = size (`COEFF`,1) – 1.

FORTRAN 90 Interface

Generic: `CALL ZPORC (COEFF, ROOT [, …])`

Specific: The specific interface names are `S_ZPORC` and `D_ZPORC`.

FORTRAN 77 Interface

Single: `CALL ZPORC (NDEG, COEFF, ROOT)`

Double: The double precision name is `DZPORC`.

Description

Routine `ZPORC` computes the *n* zeros of the polynomial

$$p(z) = a_n z^n + a_{n-1} z^{n-1} + \ldots + a_1 z + a_0$$

where the coefficients a_i for *i* = 0, 1, …, *n* are real and *n* is the degree of the polynomial.

The routine ZPORC uses the Jenkins-Traub three-stage algorithm (Jenkins and Traub 1970; Jenkins 1975). The zeros are computed one at a time for real zeros or two at a time for complex conjugate pairs. As the zeros are found, the real zero or quadratic factor is removed by polynomial deflation.

Comments

Informational errors

Type	Code	Description
3	1	The first several coefficients of the polynomial are equal to zero. Several of the last roots will be set to machine infinity to compensate for this problem.
3	2	Fewer than NDEG zeros were found. The ROOT vector will contain the value for machine infinity in the locations that do not contain zeros.

Example

This example finds the zeros of the third-degree polynomial

$$p(z) = z^3 - 3z^2 + 4z - 2$$

where z is a complex variable.

```
      USE ZPORC_INT
      USE WRCRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    NDEG
      PARAMETER  (NDEG=3)
!
      REAL       COEFF(NDEG+1)
      COMPLEX    ZERO(NDEG)
!                                 Set values of COEFF
!                                 COEFF = (-2.0  4.0 -3.0  1.0)
!
      DATA COEFF/-2.0, 4.0, -3.0, 1.0/
!
      CALL ZPORC (COEFF, ZERO)
!
      CALL WRCRN ('The zeros found are', ZERO, 1, NDEG, 1)
!
      END
```

Output

```
              The zeros found are
             1                 2                 3
( 1.000, 0.000)  ( 1.000, 1.000)  ( 1.000,-1.000)
```

ZPOCC

Finds the zeros of a polynomial with complex coefficients.

Required Arguments

COEFF — Complex vector of length NDEG + 1 containing the coefficients of the polynomial in increasing order by degree. (Input)
The polynomial is
COEFF(NDEG + 1) * Z**NDEG + COEFF(NDEG) * Z**(NDEG – 1) + ... + COEFF(1).

ROOT — Complex vector of length NDEG containing the zeros of the polynomial. (Output)

Optional Arguments

NDEG – Degree of the polynomial. 1 ≤ NDEG < 50 (Input)
Default: NDEG = size (COEFF,1) – 1.

FORTRAN 90 Interface

Generic: CALL ZPOCC (COEFF, ROOT [, …])

Specific: The specific interface names are S_ZPOCC and D_ZPOCC.

FORTRAN 77 Interface

Single: CALL ZPOCC (NDEG, COEFF, ROOT)

Double: The double precision name is DZPOCC.

Description

Routine ZPOCC computes the *n* zeros of the polynomial

$$p(z) = a_n z^n + a_{n-1} z^{n-1} + \dots + a_1 z + a_0$$

where the coefficients a_i for $i = 0, 1, \dots, n$ are complex and n is the degree of the polynomial.

The routine ZPOCC uses the Jenkins-Traub three-stage complex algorithm (Jenkins and Traub 1970, 1972). The zeros are computed one at a time in roughly increasing order of modulus. As each zero is found, the polynomial is deflated to one of lower degree.

Comments

Informational errors

Type	Code	Description
3	1	The first several coefficients of the polynomial are equal to zero. Several of the last roots will be set to machine infinity to compensate for this problem.
3	2	Fewer than NDEG zeros were found. The ROOT vector will contain the value for machine infinity in the locations that do not contain zeros.

Example

This example finds the zeros of the third-degree polynomial

$$p(z) = z^3 - (3 + 6i)z^2 - (8 - 12i)z + 10$$

where z is a complex variable.

```
      USE ZPOCC_INT
      USE WRCRN_INT

      IMPLICIT   NONE
!                                  Declare variables
      INTEGER    NDEG
      PARAMETER  (NDEG=3)
!
      COMPLEX    COEFF(NDEG+1), ZERO(NDEG)
!                                  Set values of COEFF
!                                  COEFF = ( 10.0 +  0.0i )
!                                          ( -8.0 + 12.0i )
!                                          ( -3.0 -  6.0i )
!                                          (  1.0 +  0.0i )
!
      DATA COEFF/(10.0,0.0), (-8.0,12.0), (-3.0,-6.0), (1.0,0.0)/
!
      CALL ZPOCC (COEFF, ZERO)
!
      CALL WRCRN ('The zeros found are', ZERO, 1, NDEG, 1)
!
      END
```

Output

```
              The zeros found are
             1                 2                 3
( 1.000, 1.000)  ( 1.000, 2.000)  ( 1.000, 3.000)
```

ZANLY

Finds the zeros of a univariate complex function using Müller's method.

Required Arguments

F — User-supplied COMPLEX FUNCTION to compute the value of the function of which the zeros will be found. The form is F(Z), where

Z — The complex value at which the function is evaluated. (Input)
Z should not be changed by F.

F — The computed complex function value at the point Z. (Output)

F must be declared EXTERNAL in the calling program.

Z — A complex vector of length NKNOWN + NNEW. (Output)
Z(1), …, Z(NKNOWN) contain the known zeros. Z(NKNOWN + 1), …, Z(NKNOWN + NNEW) contain the new zeros found by ZANLY. If ZINIT is not needed, ZINIT and Z can share the same storage locations.

Optional Arguments

ERRABS — First stopping criterion. (Input)
Let FP(Z) = F(Z)/P where P = (Z − Z(1)) * (Z – Z(2)) *…* (Z − Z(K – 1)) and Z(1), …, Z(K – 1) are previously found zeros. If (CABS(F(Z)).LE.ERRABS.AND.CABS(FP(Z)).LE.ERRABS), then Z is accepted as a zero.
Default: ERRABS = 1.e-4 for single precision and 1.d-8 for double precision.

ERRREL — Second stopping criterion is the relative error. (Input)
A zero is accepted if the difference in two successive approximations to this zero is within ERRREL. ERRREL must be less than 0.01; otherwise, 0.01 will be used.
Default: ERRREL = 1.e-4 for single precision and 1.d-8 for double precision.

NKNOWN — The number of previously known zeros, if any, that must be stored in ZINIT(1), …, ZINIT(NKNOWN) prior to entry to ZANLY. (Input)
NKNOWN must be set equal to zero if no zeros are known.
Default: NKNOWN = 0.

NNEW — The number of new zeros to be found by ZANLY. (Input)
Default: NNEW = 1.

NGUESS — The number of initial guesses provided. (Input)
These guesses must be stored in ZINIT(NKNOWN + 1), …, ZINIT(NKNOWN + NGUESS). NGUESS must be set equal to zero if no guesses are provided.
Default: NGUESS = 0.

ITMAX — The maximum allowable number of iterations per zero. (Input)
Default: ITMAX = 100.

ZINIT — A complex vector of length NKNOWN + NNEW. (Input)
ZINIT(1), …, ZINIT(NKNOWN) must contain the known zeros. ZINIT(NKNOWN + 1), …, ZINIT(NKNOWN + NNEW) may, on user option, contain initial guesses for the NNEW new zeros that are to be computed. If the user does not provide an initial guess, zero is used.

INFO — An integer vector of length NKNOWN + NNEW. (Output)
INFO(J) contains the number of iterations used in finding the J-th zero when convergence was achieved. If convergence was not obtained in ITMAX iterations, INFO(J) will be greater than ITMAX.

FORTRAN 90 Interface

Generic: CALL ZANLY (F, Z [, …])

Specific: The specific interface names are S_ZANLY and D_ZANLY.

FORTRAN 77 Interface

Single: CALL ZANLY (F, ERRABS, ERRREL, NKNOWN, NNEW, NGUESS, ZINIT, ITMAX, Z, INFO)

Double: The double precision name is DZANLY.

Description

Müller's method with deflation is used. It assumes that the complex function *f(z)* has at least two continuous derivatives. For more details, see Müller (1965).

Comments

1. Informational error

Type	Code	Description
3	1	Failure to converge within ITMAX iterations for at least one of the NNEW new roots.

2. Routine ZANLY always returns the last approximation for zero J in Z(J). If the convergence criterion is satisfied, then INFO(J) is less than or equal to ITMAX. If the convergence criterion is not satisfied, then INFO(J) is set to either ITMAX + 1 or ITMAX + K, with K greater than 1. INFO(J) = ITMAX + 1 indicates that ZANLY did not obtain convergence in the allowed number of iterations. In this case, the user may wish to set ITMAX to a larger value. INFO(J) = ITMAX + K means that convergence was obtained (on iteration K) for the deflated function FP(Z) = F(Z)/((Z - Z(1))...(Z - Z(J - 1))) but failed for F(Z). In this case, better initial guesses might help or it might be necessary to relax the convergence criterion.

Example

This example finds the zeros of the equation $f(z) = z^3 + 5z^2 + 9z + 45$, where z is a complex variable.

```
      USE ZANLY_INT
      USE WRCRN_INT

      IMPLICIT   NONE
!                                  Declare variables
      INTEGER    INFO(3), NGUESS, NNEW
      COMPLEX    F, Z(3), ZINIT(3)
      EXTERNAL   F
!                                  Set the guessed zero values in ZINIT
!
!                                  ZINIT = (1.0+1.0i 1.0+1.0i 1.0+1.0i)
      DATA ZINIT/3*(1.0,1.0)/
!                                  Set values for all input parameters
      NNEW   = 3
      NGUESS = 3
!                                  Find the zeros of F
      CALL ZANLY (F, Z, NNEW=NNEW, NGUESS=NGUESS, &
                 ZINIT=ZINIT, INFO=INFO)
!                                  Print results
      CALL WRCRN ('The zeros are', Z)
      END
!                                  External complex function
      COMPLEX FUNCTION F (Z)
      COMPLEX    Z
!
      F = Z**3 + 5.0*Z**2 + 9.0*Z + 45.0
      RETURN
      END
```

Output

```
              The zeros are
             1                 2                 3
 ( 0.000, 3.000)  ( 0.000,-3.000)  (-5.000, 0.000)
```

ZUNI

Finds a zero of a real univariate function.

Required Arguments

F — User-supplied function of which a zero will be found. The form is F(X [,…]), where:

Function Return Value

F — The computed function value at the point X. (Output)

Required Arguments

X — The point at which the function is evaluated. (Input)
X should not be changed by F.

Optional Arguments

FCN_DATA — A derived type, s_fcn_data, which may be used to pass additional information to/from the user-supplied function. For a detailed description of this argument see FCN_DATA below.

F must be declared EXTERNAL in the calling program.

A — See B. (Input/Output)

B — Two points at which the user-supplied function can be evaluated. (Input/Output)
On input, if F(A) and F(B) are of opposite sign, the zero will be found in the interval [A, B] and on output B will contain the value of X at which F(X)=0. If F(A)*F(B) > 0, and A ≠ B then a search along the *x* number line is initiated for a point at which there is a sign change and |B − A| will be used in setting the step size for the initial search. If A = B on entry then the search is started as described in the description section below. On output, B is the abscissa at which |F(x)| had the smallest value. If F(B) ≠ 0 on output, A will contain the nearest abscissa to output B at which F(x) was evaluated and found to have the opposite sign from F(B).

Optional Arguments

TOL— Error tolerance. (Input)
If TOL > 0.0, the zero is to be isolated to an interval of length less than TOL.

If TOL < 0.0, an x is desired for which |F(x)| is ≤ |TOL|.

If TOL = 0.0, the iteration continues until the zero of F(x) is isolated as accurately as possible.

Default: TOL = 0.0.

MAXFN — The number of function evaluations. (Input/Output)

On input, MAXFN specifies an upper bound on the number of function evaluations required for convergence. Set MAXFN to 0 if the number of function evaluations is to be unbounded. On output, MAXFN will contain the actual number of function evaluations used.

Default: MAXFN = 0 so the number of function evaluations is unbounded.

FCN_DATA — A derived type, s_fcn_data, which may be used to pass additional information to/from the user-supplied function.

The derived type, s_fcn_data, is defined as:

```
type s_fcn_data
    real(kind(1e0)), pointer, dimension(:) :: rdata
    integer, pointer, dimension(:) :: idata
 end type
```

in module mp_types. The double precision counterpart to s_fcn_data is named d_fcn_data. The user must include a use mp_types statement in the calling program to define this derived type. Note that if this optional argument is used then this argument must also be used in the user-supplied function. (Input/Output)

FORTRAN 90 Interface

Generic: CALL ZUNI (F, A, B [, …])

Specific: The specific interface names are S_ZUNI and D_ZUNI.

Description

ZUNI is based on the JPL Library routine SZERO. The algorithm used is attributed to Dr. Fred T. Krogh, JPL, 1972. Tests have shown ZUNI to require fewer function evaluations, on average, than a number of other algorithms for finding a zero of a continuous function. Also, unlike ZBREN which restricts the user to supplying points A and B such that f(A) and f(B) are opposite in sign, ZUNI will accept any two points A and B and initiate a search on the number line for an x such that $f(x) = 0$ when there is no sign difference between f(A) and f(B). In either case, B is updated with a new value on each successive iteration. The algorithm description follows.

When $f(\mathrm{A}) \times f(\mathrm{B}) > 0$ at the initial point, iterates for x are generated according to the formula $x = x_{\min} + (x_{\min} - x_{\max}) \times \rho$, where the subscript "min" is associated with the (f, x) pair that has the smallest value for $|f|$, the subscript "max" is associated with the (f, x) pair that has the largest value for $|f|$, and ρ is 8 if $r = f_{\min} / (f_{\max} - f_{\min}) \geq 8$, else $\rho = \max(\kappa/4, r)$, where κ is a count of the number of iterations that have been taken without finding fs with opposite signs. If A and B have the same value initially, then the next x is a distance $0.008 + |x_{\min}|/4$ from $x_{\min}$ taken toward 0. (If A = B = 0, the next x is -.008.)

Let x_1 and x_2 denote the first two x values that give f values with different signs. Let $\alpha < \beta$ be the two values of x that bracket the zero as tightly as is known. Thus $\alpha = x_1$ or $\alpha = x_2$ and β is the other when computing x_3. The next point, x_3, is generated by treating x as the linear function $q(f)$ that interpolates the points $(f(x_1), x_1)$ and $(f(x_2), x_2)$, and then computing $x_3 = q(0)$, subject to the condition that $\alpha + \varepsilon \leq x_3 \leq \beta - \varepsilon$, where $\varepsilon = 0.875 \times max($`TOL`, machine precision). (This condition on x_3 with updated values for α and β is also applied to future iterates.)

Let $x_4, x_5, \ldots, x_m$ denote the abscissae on the following iterations. Let $a = x_m$, $b = x_{m-1}$, and $c = x_{m-2}$. Either α or β (defined as above) will coincide with a, and β will frequently coincide with either b or c. Let $p(x)$ be the quadratic polynomial in x that passes through the values of f evaluated at a, b, and c. Let $q(f)$ be the quadratic polynomial in f that passes through the points $(f(a), a)$, $(f(b), b)$, and $f(c), c)$.

Let $\zeta = \alpha$ or β, selected so that $\zeta \neq a$. If the sign of f has changed in the last 4 iterations and $p'(a) \times q'(f(a))$ and $p'(\zeta) \times q'(f(\zeta))$ are both in the interval [1/4, 4], then x is set to $q(0)$. (Note that if p is replaced by f and q is replaced by x, then both products have the value 1.) Otherwise x is set to $a - (a - \zeta)(\phi/(1+\phi))$, where ϕ is selected based on past behavior and is such that $0 < \phi$. If the sign of f () does not change for an extended period, ϕ gets large.

Comments

Informational error

Type	Code	Description
4	1	The error tolerance criteria was not satisfied. `B` contains the abscissa at which |`F(x)`| had the smallest value.

Example

This example finds a zero of the function

$$f(x) = x^2 + x - 2$$

in the interval [– 10.0, 0.0].

```
      USE ZUNI_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    NOUT, MAXFN
      REAL       A, B, F
      EXTERNAL   F
!                                 Set values of A, B, MAXFN
      A      = -10.0
      B      = 0.0
      MAXFN  = 0
```

```
!
      CALL UMACH (2, NOUT)
!                                  Find zero of F
      CALL ZUNI (F, A, B, MAXFN=MAXFN)
!
      WRITE (NOUT,99999) B, MAXFN
99999 FORMAT ('  The best approximation to the zero of F is equal to', &
             F5.1, '.', /, '  The number of function evaluations', &
             ' required was ', I2, '.', //)
!
      END
!
      REAL FUNCTION F (X)
      REAL       X
!
      F = X*X + X - 2.0
      RETURN
      END
```

Output

```
The best approximation to the zero of F is equal to -2.0.
The number of function evaluations required was 10.
```

ZBREN

Finds a zero of a real function that changes sign in a given interval.

Required Arguments

F — User-supplied FUNCTION to compute the value of the function of which a zero will be found. The form is F(X), where

X — The point at which the function is evaluated. (Input)
X should not be changed by F.

F — The computed function value at the point X. (Output)
F must be declared EXTERNAL in the calling program.

A — See B. (Input/Output)

B — On input, the user must supply two points, A and B, such that F(A) and F(B) are opposite in sign. (Input/Output)
On output, both A and B are altered. B will contain the best approximation to the zero of F.

Optional Arguments

ERRABS — First stopping criterion. (Input)
A zero, B, is accepted if ABS(F(B)) is less than or equal to ERRABS. ERRABS may be set to zero.
Default: ERRABS = 1.e-4 for single precision and 1.d-8 for double precision.

ERRREL — Second stopping criterion is the relative error. (Input)
A zero is accepted if the change between two successive approximations to this zero is within ERRREL.
Default: ERRREL = 1.e-4 for single precision and 1.d-8 for double precision.

MAXFN — On input, MAXFN specifies an upper bound on the number of function evaluations required for convergence. (Input/Output)
On output, MAXFN will contain the actual number of function evaluations used.
Default: MAXFN = 100.

FORTRAN 90 Interface

Generic: CALL ZBREN (F, A, B [, …])

Specific: The specific interface names are S_ZBREN and D_ZBREN.

FORTRAN 77 Interface

Single: CALL ZBREN (F, ERRABS, ERRREL, A, B, MAXFN)

Double: The double precision name is DZBREN.

Description

The algorithm used by ZBREN is a combination of linear interpolation, inverse quadratic interpolation, and bisection. Convergence is usually superlinear and is never much slower than the rate for the bisection method. See Brent (1971) for a more detailed account of this algorithm.

Comments

1. Informational error

Type	Code	Description
4	1	Failure to converge in MAXFN function evaluations.

2. On exit from ZBREN without any error message, A and B satisfy the following:

   F(A)F(B) $\le$ 0.0

   |F(B)| $\le$ |F(A)|, and

   either |F(B)| $\le$ ERRABS or

   |A−B| $\le$ max(|B|, 0.1) * ERRREL

   The presence of 0.1 in the stopping criterion causes leading zeros to the right of the decimal point to be counted as significant digits. Scaling may be required in order to accurately determine a zero of small magnitude.

3. ZBREN is guaranteed to convergence within K function evaluations, where K = $(\ln((B - A)/D) + 1.0)^2$, and

$$\left(D = \min_{x \in (A,B)} \left(\max\left(|x|, 0.1\right) * \mathrm{ERRREL}\right)\right)$$

   This is an upper bound on the number of evaluations. Rarely does the actual number of evaluations used by ZBREN exceed

$$\sqrt{K}$$

   D can be computed as follows:

```
P = AMAX1(0.1, AMIN1(|A|, |B|))
IF((A - 0.1) * (B - 0.1) < 0.0) P = 0.1,
D = P * ERRREL
```

Example

This example finds a zero of the function

$$f(x) = x^2 + x - 2$$

in the interval (– 10.0, 0.0).

```
      USE ZBREN_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                  Declare variables
      REAL       ERRABS, ERRREL
!
      INTEGER    NOUT, MAXFN
      REAL       A, B, F
      EXTERNAL   F
!                                  Set values of A, B, ERRABS,
!                                  ERRREL, MAXFN
      A      = -10.0
      B      = 0.0
      ERRABS = 0.0
      ERRREL = 0.001
      MAXFN  = 100
!
      CALL UMACH (2, NOUT)
!                                  Find zero of F
      CALL ZBREN (F, A, B, ERRABS=ERRABS, ERRREL=ERRREL, MAXFN=MAXFN)
!
      WRITE (NOUT,99999) B, MAXFN
99999 FORMAT ('  The best approximation to the zero of F is equal to', &
            F5.1, '.', /, '  The number of function evaluations', &
            ' required was ', I2, '.', //)
!
      END
!
      REAL FUNCTION F (X)
      REAL       X
!
      F = X**2 + X - 2.0
      RETURN
      END
```

Output

```
The best approximation to the zero of F is equal to -2.0.
The number of function evaluations required was 12.
```

ZREAL

Finds the real zeros of a real function using Müller's method.

Required Arguments

F — User-supplied FUNCTION to compute the value of the function of which a zero will be found. The form is

F(X), where

X – The point at which the function is evaluated. (Input)
X should not be changed by F.

F – The computed function value at the point X. (Output)

F must be declared EXTERNAL in the calling program.

X — A vector of length NROOT. (Output)
X contains the computed zeros.

Optional Arguments

ERRABS — First stopping criterion. (Input)
A zero X(I) is accepted if ABS(F(X(I)).LT. ERRABS.
Default: ERRABS = 1.e-4 for single precision and 1.d-8 for double precision.

ERRREL — Second stopping criterion is the relative error. (Input)
A zero X(I) is accepted if the relative change of two successive approximations to X(I) is less than ERRREL.
Default: ERRREL = 1.e-4 for single precision and 1.d-8 for double precision.

EPS — See ETA. (Input)
Default: EPS = 1.e-4 for single precision and 1.d-8 for double precision.

ETA — Spread criteria for multiple zeros. (Input)
If the zero X(I) has been computed and ABS(X(I) – X(J)).LT.EPS, where X(J) is a previously computed zero, then the computation is restarted with a guess equal to X(I) + ETA.
Default: ETA = .01.

NROOT — The number of zeros to be found by ZREAL. (Input)
Default: NROOT = 1.

ITMAX — The maximum allowable number of iterations per zero. (Input)
Default: ITMAX = 100.

XGUESS — A vector of length NROOT. (Input)
XGUESS contains the initial guesses for the zeros.
Default: XGUESS = 0.0.

INFO — An integer vector of length NROOT. (Output)
INFO(J) contains the number of iterations used in finding the J-th zero when convergence was achieved. If convergence was not obtained in ITMAX iterations, INFO(J) will be greater than ITMAX.

FORTRAN 90 Interface

Generic: CALL ZREAL (F, X [, …])

Specific: The specific interface names are S_ZREAL and D_ZREAL.

FORTRAN 77 Interface

Single: CALL ZREAL (F, ERRABS, ERREL, EPS, ETA, NROOT, ITMAX, XGUESS, X, INFO)

Double: The double precision name is DZREAL.

Description

Routine ZREAL computes *n* real zeros of a real function *f*. Given a user-supplied function *f*(*x*) and an *n*-vector of initial guesses x_1, x_2,…, x_n, the routine uses Müller's method to locate *n* real zeros of *f*, that is, *n* real values of *x* for which *f*(*x*) = 0. The routine has two convergence criteria: the first requires that

$$\left| f\left(x_i^m\right) \right|$$

be less than ERRABS; the second requires that the relative change of any two successive approximations to an x_i be less than ERRREL. Here,

$$x_i^m$$

is the *m*-th approximation to x_i. Let ERRABS be ε_1, and ERRREL be ε_2.The criteria may be stated mathematically as follows:

Criterion 1:

$$\left| f\left(x_i^m\right) \right| < \varepsilon_1$$

Criterion 2:

$$\left| \frac{x_i^{m+1} - x_i^m}{x_i^m} \right| < \varepsilon_2$$

"Convergence" is the satisfaction of either criterion.

Comments

1. Informational error

Type	Code	Description
3	1	Failure to converge within ITMAX iterations for at least one of the NROOT roots.

2. Routine ZREAL always returns the last approximation for zero J in X(J). If the convergence criterion is satisfied, then INFO(J) is less than or equal to ITMAX. If the convergence criterion is not satisfied, then INFO(J) is set to ITMAX + 1.
3. The routine ZREAL assumes that there exist NROOT distinct real zeros for the function F and that they can be reached from the initial guesses supplied. The routine is designed so that convergence to any single zero cannot be obtained from two different initial guesses.
4. Scaling the X vector in the function F may be required, if any of the zeros are known to be less than one.

Example

This example finds the real zeros of the second-degree polynomial

$$f(x) = x^2 + 2x - 6$$

with the initial guess (4.6, –193.3).

```
      USE ZREAL_INT
      USE WRRRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    NROOT
      REAL       EPS, ERRABS, ERRREL
      PARAMETER  (NROOT=2)
!
      INTEGER    INFO(NROOT)
      REAL       F, X(NROOT), XGUESS(NROOT)
      EXTERNAL   F
!                                 Set values of initial guess
!                                 XGUESS = (  4.6 -193.3)
!
      DATA XGUESS/4.6, -193.3/
```

```
!
      EPS    = 1.0E-5
      ERRABS = 1.0E-5
      ERRREL = 1.0E-5

!                                 Find the zeros
      CALL ZREAL (F, X, errabs=errabs, errrel=errrel, eps=eps, &
                 nroot=nroot, xguess=xguess)
!
      CALL WRRRN ('The zeros are', X, 1, NROOT, 1)
!
      END
!
      REAL FUNCTION F (X)
      REAL       X
!
      F = X*X + 2.0*X - 6.0
      RETURN
      END
```

Output

```
The zeros are
    1       2
1.646  -3.646
```

NEQNF

Solves a system of nonlinear equations using a modified Powell hybrid algorithm and a finite-difference approximation to the Jacobian.

Required Arguments

FCN — User-supplied SUBROUTINE to evaluate the system of equations to be solved. The usage is CALL FCN (X, F, N) , where

X – The point at which the functions are evaluated. (Input)
X should not be changed by FCN.

F – The computed function values at the point X. (Output)

N – Length of X and F. (Input)

FCN must be declared EXTERNAL in the calling program.

X — A vector of length N. (Output)
X contains the best estimate of the root found by NEQNF.

Optional Arguments

ERRREL — Stopping criterion. (Input)
The root is accepted if the relative error between two successive approximations to this root is less than ERRREL.
Default: ERRREL = 1.e-4 for single precision and 1.d-8 for double precision.

N — The number of equations to be solved and the number of unknowns. (Input)
Default: N = size (X,1).

ITMAX — The maximum allowable number of iterations. (Input)
The maximum number of calls to FCN is ITMAX * (N + 1). Suggested value ITMAX = 200.
Default: ITMAX = 200.

XGUESS — A vector of length N. (Input)
XGUESS contains the initial estimate of the root.
Default: XGUESS = 0.0.

FNORM — A scalar that has the value $F(1)^2 + \ldots + F(N)^2$ at the point X. (Output)

FORTRAN 90 Interface

Generic: CALL NEQNF (FCN, X [, …])

Specific: The specific interface names are S_NEQNF and D_NEQNF.

FORTRAN 77 Interface

Single: CALL NEQNF (FCN, ERRREL, N, ITMAX, XGUESS, X, FNORM)

Double: The double precision name is DNEQNF.

Description

Routine NEQNF is based on the MINPACK subroutine HYBRD1, which uses a modification of M.J.D. Powell's hybrid algorithm. This algorithm is a variation of Newton's method, which uses a finite-difference approximation to the Jacobian and takes precautions to avoid large step sizes or increasing residuals. For further description, see More et al. (1980).

Since a finite-difference method is used to estimate the Jacobian, for single precision calculation, the Jacobian may be so incorrect that the algorithm terminates far from a root. In such cases, high precision arithmetic is recommended. Also, whenever the exact Jacobian can be easily provided, IMSL routine NEQNJ should be used instead.

Comments

1. Workspace may be explicitly provided, if desired, by use of N2QNF/DN2QNF. The reference is:

```
CALL N2QNF (FCN, ERRREL, N, ITMAX, XGUESS, X, FNORM, FVEC,
   FJAC, R, QTF, WK)
```

   The additional arguments are as follows:

   FVEC — A vector of length N. FVEC contains the functions evaluated at the point X.

   FJAC — An N by N matrix. FJAC contains the orthogonal matrix Q produced by the QR factorization of the final approximate Jacobian.

   R — A vector of length N * (N + 1)/2. R contains the upper triangular matrix produced by the QR factorization of the final approximate Jacobian. R is stored row-wise.

   QTF — A vector of length N. QTF contains the vector TRANS(Q) * FVEC.

   WK — A work vector of length 5 * N.

2. Informational errors

Type	Code	Description
4	1	The number of calls to FCN has exceeded ITMAX * (N + 1). A new initial guess may be tried.
4	2	ERRREL is too small. No further improvement in the approximate solution is possible.
4	3	The iteration has not made good progress. A new initial guess may be tried.

Example

The following 3 × 3 system of nonlinear equations

$$f_1(x) = x_1 + e^{x_1 - 1} + (x_2 + x_3)^2 - 27 = 0$$
$$f_2(x) = e^{x_2 - 2} / x_1 + x_3^2 - 10 = 0$$
$$f_3(x) = x_3 + \sin(x_2 - 2) + x_2^2 - 7 = 0$$

is solved with the initial guess (4.0, 4.0, 4.0).

```
      USE NEQNF_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    N
      PARAMETER  (N=3)
!
      INTEGER    K, NOUT
      REAL       FNORM, X(N), XGUESS(N)
      EXTERNAL   FCN
!                                 Set values of initial guess
!                                 XGUESS = (  4.0  4.0  4.0 )
!
      DATA XGUESS/4.0, 4.0, 4.0/
!
!
      CALL UMACH (2, NOUT)
!                                 Find the solution
      CALL NEQNF (FCN, X, xguess=xguess, fnorm=fnorm)
!                                 Output
      WRITE (NOUT,99999) (X(K),K=1,N), FNORM
99999 FORMAT ('  The solution to the system is', /, '  X = (', 3F5.1, &
            ')', /, '  with FNORM =', F5.4, //)
!
      END
!                                 User-defined subroutine
      SUBROUTINE FCN (X, F, N)
      INTEGER    N
      REAL       X(N), F(N)
!
      REAL       EXP, SIN
      INTRINSIC  EXP, SIN
!
```

```
      F(1) = X(1) + EXP(X(1)-1.0) + (X(2)+X(3))*(X(2)+X(3)) - 27.0
      F(2) = EXP(X(2)-2.0)/X(1) + X(3)*X(3) - 10.0
      F(3) = X(3) + SIN(X(2)-2.0) + X(2)*X(2) - 7.0
      RETURN
      END
```

Output

```
The solution to the system is
X = (  1.0  2.0  3.0)
with FNORM =.0000
```

NEQNJ

Solves a system of nonlinear equations using a modified Powell hybrid algorithm with a user-supplied Jacobian.

Required Arguments

FCN — User-supplied `SUBROUTINE` to evaluate the system of equations to be solved. The usage is `CALL FCN (X, F, N)`, where

`X` – The point at which the functions are evaluated. (Input)
`X` should not be changed by `FCN`.

`F` – The computed function values at the point `X`. (Output)

`N` – Length of `X`, `F`. (Input)

`FCN` must be declared `EXTERNAL` in the calling program.

LSJAC — User-supplied `SUBROUTINE` to evaluate the Jacobian at a point `X`. The usage is `CALL LSJAC (N, X, FJAC)`, where

`N` – Length of `X`. (Input)

`X` – The point at which the function is evaluated. (Input)
`X` should not be changed by `LSJAC`.

`FJAC` — The computed `N` by `N` Jacobian at the point `X`. (Output)

`LSJAC` must be declared `EXTERNAL` in the calling program.

X — A vector of length `N`. (Output)
`X` Contains the best estimate of the root found by `NEQNJ`.

Optional Arguments

ERRREL — Stopping criterion. (Input)
The root is accepted if the relative error between two successive approximations to this root is less than `ERRREL`.
Default: `ERRREL` = 1.e-4 for single precision and 1.d-8 for double precision.

N — The number of equations to be solved and the number of unknowns. (Input)
Default: `N` = size (`X`,1).

ITMAX — The maximum allowable number of iterations. (Input)
Suggested value = 200.
Default: `ITMAX` = 200.

XGUESS — A vector of length N. (Input)
XGUESS contains the initial estimate of the root.
Default: XGUESS = 0.0.

FNORM — A scalar that has the value $F(1)^2 + \ldots + F(N)^2$ at the point X. (Output)

FORTRAN 90 Interface

Generic: CALL NEQNJ (FCN, LSJAC, X [, …])

Specific: The specific interface names are S_NEQNJ and D_NEQNJ.

FORTRAN 77 Interface

Single: CALL NEQNJ (FCN, LSJAC, ERRREL, N, ITMAX, XGUESS, X, FNORM)

Double: The double precision name is DNEQNJ.

Description

Routine NEQNJ is based on the MINPACK subroutine HYBRDJ, which uses a modification of M.J.D. Powell's hybrid algorithm. This algorithm is a variation of Newton's method, which takes precautions to avoid large step sizes or increasing residuals. For further description, see More et al. (1980).

Comments

1. Workspace may be explicitly provided, if desired, by use of N2QNJ/DN2QNJ. The reference is:

```
CALL N2QNJ (FCN, LSJAC, ERRREL, N, ITMAX, XGUESS, X, FNORM,
   FVEC, FJAC, R, QTF, WK)
```

   The additional arguments are as follows:

   FVEC — A vector of length N. FVEC contains the functions evaluated at the point X.

   FJAC — An N by N matrix. FJAC contains the orthogonal matrix Q produced by the QR factorization of the final approximate Jacobian.

   R — A vector of length N * (N + 1)/2. R contains the upper triangular matrix produced by the QR factorization of the final approximate Jacobian. R is stored row-wise.

   QTF — A vector of length N. QTF contains the vector TRANS(Q) * FVEC.

   WK — A work vector of length 5 * N.

2. Informational errors

Type	Code	Description
4	1	The number of calls to FCN has exceeded ITMAX. A new initial guess may be tried.
4	2	ERRREL is too small. No further improvement in the approximate solution is possible.
4	3	The iteration has not made good progress. A new initial guess may be tried.

Example

The following 3 × 3 system of nonlinear equations

$$f_1(x) = x_1 + e^{x_1 - 1} + (x_2 + x_3)^2 - 27 = 0$$

$$f_2(x) = e^{x_2 - 2} / x_1 + x_3^2 - 10 = 0$$

$$f_3(x) = x_3 + \sin(x_2 - 2) + x_2^2 - 7 = 0$$

is solved with the initial guess (4.0, 4.0, 4.0).

```
      USE NEQNJ_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    N
      PARAMETER  (N=3)
!
      INTEGER    K, NOUT
      REAL       FNORM, X(N), XGUESS(N)
      EXTERNAL   FCN, LSJAC
!                                 Set values of initial guess
!                                 XGUESS = (  4.0  4.0  4.0  )
!
      DATA XGUESS/4.0, 4.0, 4.0/
!
!
      CALL UMACH (2, NOUT)
!                                 Find the solution
      CALL NEQNJ (FCN, LSJAC, X, XGUESS=XGUESS, FNORM=FNORM)
!                                 Output
      WRITE (NOUT,99999) (X(K),K=1,N), FNORM
99999 FORMAT ('  The roots found are', /, '  X = (', 3F5.1, &
            ')', /, '  with FNORM = ',F5.4, //)
!
      END
!                                 User-supplied subroutine
      SUBROUTINE FCN (X, F, N)
      INTEGER    N
      REAL       X(N), F(N)
!
      REAL       EXP, SIN
      INTRINSIC  EXP, SIN
!
```

```
      F(1) = X(1) + EXP(X(1)-1.0) + (X(2)+X(3))*(X(2)+X(3)) - 27.0
      F(2) = EXP(X(2)-2.0)/X(1) + X(3)*X(3) - 10.0
      F(3) = X(3) + SIN(X(2)-2.0) + X(2)*X(2) - 7.0
      RETURN
      END
!                                  User-supplied subroutine to
!                                  compute Jacobian
      SUBROUTINE LSJAC (N, X, FJAC)
      INTEGER    N
      REAL       X(N), FJAC(N,N)
!
      REAL       COS, EXP
      INTRINSIC  COS, EXP
!
      FJAC(1,1) = 1.0 + EXP(X(1)-1.0)
      FJAC(1,2) = 2.0*(X(2)+X(3))
      FJAC(1,3) = 2.0*(X(2)+X(3))
      FJAC(2,1) = -EXP(X(2)-2.0)*(1.0/X(1)**2)
      FJAC(2,2) = EXP(X(2)-2.0)*(1.0/X(1))
      FJAC(2,3) = 2.0*X(3)
      FJAC(3,1) = 0.0
      FJAC(3,2) = COS(X(2)-2.0) + 2.0*X(2)
      FJAC(3,3) = 1.0
      RETURN
      END
```

Output

```
 The roots found are
 X = (  1.0  2.0  3.0)
 with FNORM =.0000
```

NEQBF

more...

Solves a system of nonlinear equations using factored secant update with a finite-difference approximation to the Jacobian.

Required Arguments

FCN — User-supplied SUBROUTINE to evaluate the system of equations to be solved. The usage is CALL FCN (N, X, F), where

N – Length of X and F. (Input)

X – The point at which the functions are evaluated. (Input)
X should not be changed by FCN.

F – The computed function values at the point X. (Output)

FCN must be declared EXTERNAL in the calling program.

X — Vector of length N containing the approximate solution. (Output)

Optional Arguments

N — Dimension of the problem. (Input)
Default: N = size (X,1).

XGUESS — Vector of length N containing initial guess of the root. (Input)
Default: XGUESS = 0.0.

XSCALE — Vector of length N containing the diagonal scaling matrix for the variables. (Input)
XSCALE is used mainly in scaling the distance between two points. In the absence of other information, set all entries to 1.0. If internal scaling is desired for XSCALE, set IPARAM (6) to 1.
Default: XSCALE = 1.0.

FSCALE — Vector of length `N` containing the diagonal scaling matrix for the functions. (Input)
`FSCALE` is used mainly in scaling the function residuals. In the absence of other information, set all entries to 1.0.
Default: `FSCALE` = 1.0.

IPARAM — Parameter vector of length 6. (Input/Output)
Set `IPARAM(1)` to zero for default values of `IPARAM` and `RPARAM`. See Comment 4.
Default: `IPARAM` = 0.

RPARAM — Parameter vector of length 5. (Input/Output)
See Comment 4.

FVEC — Vector of length `N` containing the values of the functions at the approximate solution. (Output)

FORTRAN 90 Interface

Generic: `CALL NEQBF (FCN, X [, …])`

Specific: The specific interface names are `S_NEQBF` and `D_NEQBF`.

FORTRAN 77 Interface

Single: `CALL NEQBF (FCN, N, XGUESS, XSCALE, FSCALE, IPARAM, RPARAM, X, FVEC)`

Double: The double precision name is `DNEQBF`.

Description

Routine `NEQBF` uses a secant algorithm to solve a system of nonlinear equations, i.e.,

$$F(x) = 0$$

where $F : \mathbf{R}^n \rightarrow \mathbf{R}^n$, and $x \in \mathbf{R}^n$.

From a current point, the algorithm uses a double dogleg method to solve the following subproblem approximately:

$$\min_{s \in \mathrm{R}^n} \left\| F(x_c) + J(x_c)s \right\|_2$$

$$\text{subject to } \|s\|_2 \le \delta_c$$

to get a direction s_c, where $F(x_c)$ and $J(x_c)$ are the function values and the approximate Jacobian respectively evaluated at the current point x_c. Then, the function values at the point $x_n = x_c + s_c$ are evaluated and used to decide whether the new point x_n should be accepted.

When the point x_n is rejected, this routine reduces the trust region δ_c and goes back to solve the subproblem again. This procedure is repeated until a better point is found.

The algorithm terminates if the new point satisfies the stopping criterion. Otherwise, δ_c is adjusted, and the approximate Jacobian is updated by Broyden's formula,

$$J_n = J_c + \frac{\left(y - J_c s_c\right) s_c^T}{s_c^T s_c}$$

where $J_n = J(x_n)$, $J_c = J(x_c)$, and $y = F(x_n) - F(x_c)$. The algorithm then continues using the new point as the current point, i.e. $x_c \leftarrow x_n$.

For more details, see Dennis and Schnabel (1983, Chapter 8).

Since a finite-difference method is used to estimate the initial Jacobian, for single precision calculation, the Jacobian may be so incorrect that the algorithm terminates far from a root. In such cases, high precision arithmetic is recommended. Also, whenever the exact Jacobian can be easily provided, IMSL routine NEQBJ should be used instead.

Comments

1. Workspace may be explicitly provided, if desired, by use of N2QBF/DN2QBF. The reference is:

   CALL N2QBF (FCN, N, XGUESS, XSCALE, FSCALE, IPARAM, RPARAM, X, FVEC, WK, LWK)

   The additional arguments are as follows:

   WK — A work vector of length LWK. On output WK contains the following information:

   The third N locations contain the last step taken.

   The fourth N locations contain the last Newton step.

   The final N^2 locations contain an estimate of the Jacobian at the solution.

   LWK — Length of WK, which must be at least $2 * N^2 + 11 * N$. (Input)

2. Informational errors

Type	Code	Description
3	1	The last global step failed to decrease the 2-norm of F(X) sufficiently; either the current point is close to a root of F(X) and no more accuracy is possible, or the secant approximation to the Jacobian is inaccurate, or the step tolerance is too large.
3	3	The scaled distance between the last two steps is less than the step tolerance; the current point is probably an approximate root of F(X) (unless STEPTL is too large).

Type	Code	Description
3	4	Maximum number of iterations exceeded.
3	5	Maximum number of function evaluations exceeded.
3	7	Five consecutive steps of length STEPMX have been taken; either the 2-norm of F(X) asymptotes from above to a finite value in some direction or the maximum allowable step size STEPMX is too small.

3. The stopping criterion for NEQBF occurs when the scaled norm of the functions is less than the scaled function tolerance (RPARAM(1)).

4. If the default parameters are desired for NEQBF, then set IPARAM(1) to zero and call routine NEQBF. Otherwise, if any nondefault parameters are desired for IPARAM or RPARAM, then the following steps should be taken before calling NEQBF:

   CALL N4QBJ (IPARAM, RPARAM)

   Set nondefault values for desired IPARAM, RPARAM elements.

Note that the call to N4QBJ will set IPARAM and RPARAM to their default values, so only nondefault values need to be set above.

The following is a list of the parameters and the default values:

IPARAM — Integer vector of length 6.

IPARAM(1) = Initialization flag.

IPARAM(2) = Number of good digits in the function.
Default: Machine dependent.

IPARAM(3) = Maximum number of iterations.
Default: 100.

IPARAM(4) = Maximum number of function evaluations.
Default: 400.

IPARAM(5) = Maximum number of Jacobian evaluations.
Default: not used in NEQBF.

IPARAM(6) = Internal variable scaling flag.
If IPARAM(6) = 1, then the values of XSCALE are set internally.
Default: 0.

RPARAM — Real vector of length 5.

RPARAM(1) = Scaled function tolerance.
The scaled norm of the functions is computed as

$$\max_i (| f_i | * fs_i)$$

where f_i is the i-th component of the function vector F, and fs_i is the i-th component of FSCALE.
Default:

$$\sqrt{\varepsilon}$$

where **ε** is the machine precision.

RPARAM(2) = Scaled step tolerance. (STEPTL)
The scaled norm of the step between two points x and y is computed as

$$\max_i \left\{ \frac{| x_i - y_i |}{\max\left(| x_i | ,1 / s_i \right)} \right\}$$

where s_i is the i-th component of XSCALE.

Default: $\varepsilon^{2/3}$, where **ε** is the machine precision.

RPARAM(3) = False convergence tolerance.
Default: not used in NEQBF.

RPARAM(4) = Maximum allowable step size. (STEPMX)
Default:1000 * max(ε_1, ε_2), where

$$\varepsilon_1 = \sqrt{\sum_{i=1}^{n} \left(s_i t_i \right)^2}$$

$\varepsilon_2 = ||s|_2$, s = XSCALE, and t = XGUESS.

RPARAM(5) = Size of initial trust region.
Default: based on the initial scaled Cauchy step.

If double precision is desired, then DN4QBJ is called and RPARAM is declared double precision.

5. Users wishing to override the default print/stop attributes associated with error messages issued by this routine are referred to “Error Handling” in the Introduction.

Example

The following 3 × 3 system of nonlinear equations:

$$f_1(x) = x_1 + e^{x_1 - 1} + (x_2 + x_3)^2 - 27 = 0$$

$$f_2(x) = e^{x_2 - 2} / x_1 + x_3^2 - 10 = 0$$

$$f_3(x) = x_3 + \sin(x_2 - 2) + x_2^2 - 7 = 0$$

is solved with the initial guess (4.0, 4.0, 4.0).

```
      USE NEQBF_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    N
      PARAMETER  (N=3)
!
      INTEGER    K, NOUT
      REAL       X(N), XGUESS(N)
      EXTERNAL   FCN
!                                 Set values of initial guess
!                                 XGUESS = (  4.0  4.0  4.0 )
!
      DATA XGUESS/3*4.0/
!
!                                 Find the solution
      CALL NEQBF (FCN, X, XGUESS=XGUESS)
!                                 Output
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) (X(K),K=1,N)
99999 FORMAT ('  The solution to the system is', /, '  X = (', 3F8.3, &
            ')')
!
      END
!                                 User-defined subroutine
      SUBROUTINE FCN (N, X, F)
      INTEGER    N
      REAL       X(N), F(N)
!
      REAL       EXP, SIN
      INTRINSIC  EXP, SIN
!
      F(1) = X(1) + EXP(X(1)-1.0) + (X(2)+X(3))*(X(2)+X(3)) - 27.0
      F(2) = EXP(X(2)-2.0)/X(1) + X(3)*X(3) - 10.0
      F(3) = X(3) + SIN(X(2)-2.0) + X(2)*X(2) - 7.0
      RETURN
      END
```

Output

```
The solution to the system is
X = (   1.000   2.000   3.000)
```

NEQBJ

more...

Solves a system of nonlinear equations using factored secant update with a user-supplied Jacobian.

Required Arguments

FCN — User-supplied `SUBROUTINE` to evaluate the system of equations to be solved. The usage is `CALL FCN` (`N`, `X`, `F`), where

`N` — Length of `X` and `F`. (Input)

`X` — The point at which the functions are evaluated. (Input)
`X` should not be changed by `FCN`.

`F` — The computed function values at the point `X`. (Output)

`FCN` must be declared `EXTERNAL` in the calling program.

JAC — User-supplied `SUBROUTINE` to evaluate the Jacobian at a point `X`. The usage is `CALL JAC` (`N`, `X`, `FJAC`, `LDFJAC)`, where

`N` — Length of `X`. (Input)

`X` — Vector of length `N` at which point the Jacobian is evaluated. (Input)
`X` should not be changed by `JAC`.

`FJAC` – The computed `N` by `N` Jacobian at the point `X`. (Output)

`LDFJAC` — Leading dimension of `FJAC`. (Input)

`JAC` must be declared `EXTERNAL` in the calling program.

X — Vector of length `N` containing the approximate solution. (Output)

Optional Arguments

N — Dimension of the problem. (Input)
Default: `N` = size (`X`,1).

XGUESS — Vector of length `N` containing initial guess of the root. (Input)
Default: `XGUESS` = 0.0.

XSCALE — Vector of length `N` containing the diagonal scaling matrix for the variables. (Input)
`XSCALE` is used mainly in scaling the distance between two points. In the absence of other information, set all entries to 1.0. If internal scaling is desired for `XSCALE`, set `IPARAM`(6) to 1.
Default: `XSCALE` = 1.0.

FSCALE — Vector of length `N` containing the diagonal scaling matrix for the functions. (Input)
`FSCALE` is used mainly in scaling the function residuals. In the absence of other information, set all entries to 1.0.
Default: `FSCALE` = 1.0.

IPARAM — Parameter vector of length 6. (Input/Output)
Set `IPARAM` (1) to zero for default values of `IPARAM` and `RPARAM`.
See Comment 4.
Default: `IPARAM` = 0.

RPARAM — Parameter vector of length 5. (Input/Output)
See Comment 4.

FVEC — Vector of length `N` containing the values of the functions at the approximate solution. (Output)

FORTRAN 90 Interface

Generic: `CALL NEQBJ (FCN, JAC, X [, …])`

Specific: The specific interface names are `S_NEQBJ` and `D_NEQBJ`.

FORTRAN 77 Interface

Single: `CALL NEQBJ (FCN, JAC, N, XGUESS, XSCALE, FSCALE, IPARAM, RPARAM, X, FVEC)`

Double: The double precision name is `DNEQBJ`.

Description

Routine `NEQBJ` uses a secant algorithm to solve a system of nonlinear equations, i. e.,

$$F(x) = 0$$

where $F : \mathbf{R}^n \to \mathbf{R}^n$, and $x \in \mathbf{R}^n$.

From a current point, the algorithm uses a double dogleg method to solve the following subproblem approximately:

$$\min_{s \in R^n} \left\| F\left(x_c\right) + J\left(x_c\right)s \right\|_2$$

$$\text{subject to } \|s\|_2 \le \delta_c$$

to get a direction s_c, where $F(x_c)$ and $J(x_c)$ are the function values and the approximate Jacobian respectively evaluated at the current point x_c. Then, the function values at the point $x_n = x_c + s_c$ are evaluated and used to decide whether the new point x_n should be accepted.

When the point x_n is rejected, this routine reduces the trust region δ_c and goes back to solve the subproblem again. This procedure is repeated until a better point is found.

The algorithm terminates if the new point satisfies the stopping criterion. Otherwise, δ_c is adjusted, and the approximate Jacobian is updated by Broyden's formula,

$$J_n = J_c + \frac{\left(y - J_c s_c\right) s_c^T}{s_c^T s_c}$$

where $J_n = J(x_n)$, $J_c = J(x_c)$, and $y = F(x_n) - F(x_c)$. The algorithm then continues using the new point as the current point, i.e. $x_c \leftarrow x_n$.

For more details, see Dennis and Schnabel (1983, Chapter 8).

Comments

1. Workspace may be explicitly provided, if desired, by use of `N2QBJ/DN2QBJ`. The reference is:

   `CALL N2QBJ (FCN, JAC, N, XGUESS, XSCALE, FSCALE, IPARAM, RPARAM, X, FVEC, WK, LWK)`

   The additional arguments are as follows:

   WK — A work vector of length `LWK`. On output `WK` contains the following information: The third `N` locations contain the last step taken. The fourth N locations contain the last Newton step. The final N^2 locations contain an estimate of the Jacobian at the solution.

   LWK — Length of `WK`, which must be at least $2 * N^2 + 11 * N$. (Input)

2. Informational errors

Type	Code	Description
3	1	The last global step failed to decrease the 2-norm of F(X) sufficiently; either the current point is close to a root of F(X) and no more accuracy is possible, or the secant approximation to the Jacobian is inaccurate, or the step tolerance is too large.
3	3	The scaled distance between the last two steps is less than the step tolerance; the current point is probably an approximate root of F(X) (unless STEPTL is too large).
3	4	Maximum number of iterations exceeded.
3	5	Maximum number of function evaluations exceeded.
3	7	Five consecutive steps of length STEPMX have been taken; either the 2-norm of F(X) asymptotes from above to a finite value in some direction or the maximum allowable stepsize STEPMX is too small.

3. The stopping criterion for NEQBJ occurs when the scaled norm of the functions is less than the scaled function tolerance (RPARAM(1)).

4. If the default parameters are desired for NEQBJ, then set IPARAM(1) to zero and call routine NEQBJ. Otherwise, if any nondefault parameters are desired for IPARAM or RPARAM, then the following steps should be taken before calling NEQBJ:

   CALL N4QBJ (IPARAM, RPARAM)

   Set nondefault values for desired IPARAM, RPARAM elements.

Note that the call to N4QBJ will set IPARAM and RPARAM to their default values, so only nondefault values need to be set above.

The following is a list of the parameters and the default values:

IPARAM — Integer vector of length 6.

IPARAM(1) = Initialization flag.

IPARAM(2) = Number of good digits in the function.
Default: Machine dependent.

IPARAM(3) = Maximum number of iterations.
Default: 100.

IPARAM(4) = Maximum number of function evaluations.
Default: 400.

IPARAM(5) = Maximum number of Jacobian evaluations.
Default: not used in NEQBJ.

IPARAM(6) = Internal variable scaling flag.
If IPARAM(6) = 1, then the values of XSCALE are set internally.
Default: 0.

RPARAM — Real vector of length 5.

RPARAM(1) = Scaled function tolerance.
The scaled norm of the functions is computed as

$$\max_i \left(| f_i | * fs_i \right)$$

where f_i is the i-th component of the function vector F, and fs_i is the i-th component of FSCALE.
Default:

$$\sqrt{\varepsilon}$$

where **ε** is the machine precision.

RPARAM(2) = Scaled step tolerance. (STEPTL)
The scaled norm of the step between two points x and y is computed as

$$\max_i \left\{ \frac{| x_i - y_i |}{\max\left(| x_i | , 1 / s_i \right)} \right\}$$

where s_i is the i-th component of XSCALE.

Default: $\varepsilon^{2/3}$, where **ε** is the machine precision.

RPARAM(3) = False convergence tolerance.
Default: not used in NEQBJ.

RPARAM(4) = Maximum allowable step size. (STEPMX)
Default:1000 * max(ε_1, ε_2), where

$$\varepsilon_1 = \sqrt{\sum_{i=1}^{n} \left(s_i t_i \right)^2}$$

$\varepsilon_2 = \|s\|_2$, s = XSCALE, and t = XGUESS.

RPARAM(5) = Size of initial trust region.
Default: based on the initial scaled Cauchy step.

If double precision is desired, then DN4QBJ is called and RPARAM is declared double precision.

5. Users wishing to override the default print/stop attributes associated with error messages issued by this routine are referred to “Error Handling” in the Introduction.

Example

The following 3 × 3 system of nonlinear equations

$$f_1(x) = x_1 + e^{x_1 - 1} + (x_2 + x_3)^2 - 27 = 0$$

$$f_2(x) = e^{x_2 - 2} / x_1 + x_3^2 - 10 = 0$$

$$f_3(x) = x_3 + \sin(x_2 - 2) + x_2^2 - 7 = 0$$

is solved with the initial guess (4.0, 4.0, 4.0).

```
      USE NEQBJ_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                  Declare variables
      INTEGER    N
      PARAMETER  (N=3)
!
      INTEGER    K, NOUT
      REAL       X(N), XGUESS(N)
      EXTERNAL   FCN, JAC
!                                  Set values of initial guess
!                                  XGUESS = (  4.0  4.0  4.0 )
!
      DATA XGUESS/3*4.0/
!                                  Find the solution
      CALL NEQBJ (FCN, JAC, X, XGUESS=XGUESS)
!                                  Output
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) (X(K),K=1,N)
99999 FORMAT ('  The solution to the system is', /, '  X = (', 3F8.3, &
            ')')
!
      END
!                                  User-defined subroutine
      SUBROUTINE FCN (N, X, F)
      INTEGER    N
      REAL       X(N), F(N)
!
      REAL       EXP, SIN
      INTRINSIC  EXP, SIN
!
      F(1) = X(1) + EXP(X(1)-1.0) + (X(2)+X(3))*(X(2)+X(3)) - 27.0
      F(2) = EXP(X(2)-2.0)/X(1) + X(3)*X(3) - 10.0
      F(3) = X(3) + SIN(X(2)-2.0) + X(2)*X(2) - 7.0
      RETURN
      END
!                                  User-supplied subroutine to
!                                  compute Jacobian
      SUBROUTINE JAC (N, X, FJAC, LDFJAC)
      INTEGER    N, LDFJAC
      REAL       X(N), FJAC(LDFJAC,N)
!
      REAL       COS, EXP
      INTRINSIC  COS, EXP
!
      FJAC(1,1) = 1.0 + EXP(X(1)-1.0)
      FJAC(1,2) = 2.0*(X(2)+X(3))
      FJAC(1,3) = 2.0*(X(2)+X(3))
      FJAC(2,1) = -EXP(X(2)-2.0)*(1.0/X(1)**2)
      FJAC(2,2) = EXP(X(2)-2.0)*(1.0/X(1))
      FJAC(2,3) = 2.0*X(3)
      FJAC(3,1) = 0.0
      FJAC(3,2) = COS(X(2)-2.0) + 2.0*X(2)
```

```
      FJAC(3,3) = 1.0
      RETURN
      END
```

Output

```
The solution to the system is
X = (   1.000   2.000   3.000)
```

Optimization

Routines

Usage Notes

Unconstrained Minimization

The unconstrained minimization problem can be stated as follows:

$$\min_{x \in \mathbf{R}^n} f(x)$$

where $f : \mathbf{R}^n \rightarrow \mathbf{R}$ is at least continuous. The routines for unconstrained minimization are grouped into three categories: univariate functions (UV***), multivariate functions (UM***), and nonlinear least squares (UNLS*).

For the univariate function routines, it is assumed that the function is unimodal within the specified interval. Otherwise, only a local minimum can be expected. For further discussion on unimodality, see Brent (1973).

A quasi-Newton method is used for the multivariate function routines UMINF and UMING, whereas UMIDH and UMIAH use a modified Newton algorithm. The routines UMCGF and UMCGG make use of a conjugate gradient approach, and UMPOL uses a polytope method. For more details on these algorithms, see the documentation for the corresponding routines.

The nonlinear least squares routines use a modified Levenberg-Marquardt algorithm. If the nonlinear least squares problem is a nonlinear data-fitting problem, then software that is designed to deliver better statistical output may be useful; see IMSL (1991).

These routines are designed to find only a local minimum point. However, a function may have many local minima. It is often possible to obtain a better local solution by trying different initial points and intervals.

High precision arithmetic is recommended for the routines that use only function values. Also it is advised that the derivative-checking routines CH*** be used to ensure the accuracy of the user-supplied derivative evaluation subroutines.

Minimization with Simple Bounds

The minimization with simple bounds problem can be stated as follows:

$$\min_{x \in \mathrm{R}^n} f(x)$$

$$\text{subject to} \quad l_i \le x_i \le u_i, \quad \mathit{for}\ i = 1, 2, \ \ldots, n$$

where $f : \mathbf{R}^n \rightarrow \mathbf{R}$, and all the variables are not necessarily bounded.

The routines BCO** use the same algorithms as the routines UMI**, and the routines BCLS* are the corresponding routines of UNLS*. The only difference is that an active set strategy is used to ensure that each variable stays within its bounds. The routine BCPOL uses a function comparison method similar to the one used by UMPOL. Convergence for these polytope methods is not guaranteed; therefore, these routines should be used as a last alternative.

Linearly Constrained Minimization

The linearly constrained minimization problem can be stated as follows:

$$\min_{x \in \mathbf{R}^n} f(x)$$

$$\text{subject to } Ax = b$$

where $f : \mathbf{R}^n \rightarrow \mathbf{R}$, A is an $m \times n$ coefficient matrix, and b is a vector of length m. If $f(x)$ is linear, then the problem is a linear programming problem; if $f(x)$ is quadratic, the problem is a quadratic programming problem.

The routine DLPRS uses an active set strategy to solve small- to medium-sized linear programming problems. No sparsity is assumed since the coefficients are stored in full matrix form. SLPRS uses the revised simplex method to solve large linear programming problems, which have sparse constraints matrices. TRAN solves a transportation problem, which is a very sparse linear programming application.

QPROG is designed to solve convex quadratic programming problems using a dual quadratic programming algorithm. If the given Hessian is not positive definite, then QPROG modifies it to be positive definite. In this case, output should be interpreted with care.

The routines LCONF and LCONG use an iterative method to solve the linearly constrained problem with a general objective function. For a detailed description of the algorithm, see *Powell (1988, 1989)*.

Routine LIN_CON_TRUST_REGION, which is based on M.J.D. Powell's LINCOA algorithm (see *Powell (2014)*), is a derivative-free optimization method that uses an interpolation-based trust-region approach to minimize nonlinear objective functions subject to linear constraints. The routine can be used for problems in which derivatives of the function to be optimized are unavailable, expensive to compute, or unreliable. Usually, LIN_CON_TRUST_REGION is applied only to small-sized problems with no more than a few hundred variables.

Nonlinearly Constrained Minimization

The nonlinearly constrained minimization problem can be stated as follows:

$$\min_{x \in \mathrm{R}^n} f(x)$$

$$\text{subject to} \quad g_i(x) = 0, \qquad \mathit{for}\ i = 1, 2, \ \dots, m_1$$
$$g_i(x) \geq 0, \qquad \mathit{for}\ i = m_1 + 1, \ \dots, m$$

where f : $\mathbf{R}^n \rightarrow \mathbf{R}$ and g_i : $\mathbf{R}^n \rightarrow \mathbf{R}$, for i = 1, 2, …, m

The routines NNLPF and NNLPG use a sequential equality constrained quadratic programming method. A more complete discussion of this algorithm can be found in the documentation.

Selection of Routines

The following general guidelines are provided to aid in the selection of the appropriate routine.

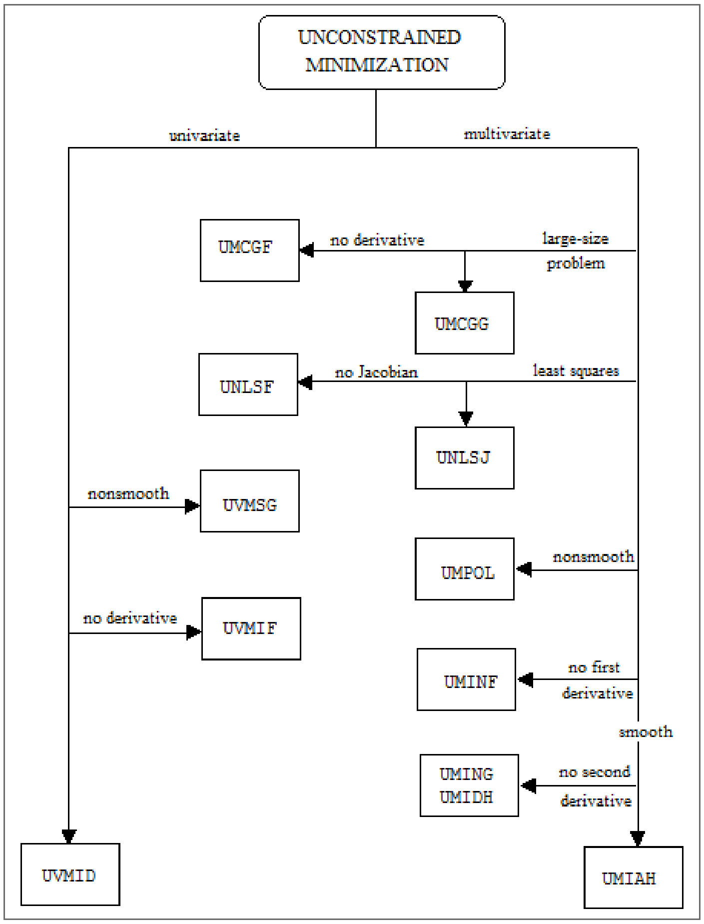
Unconstrained Minimization

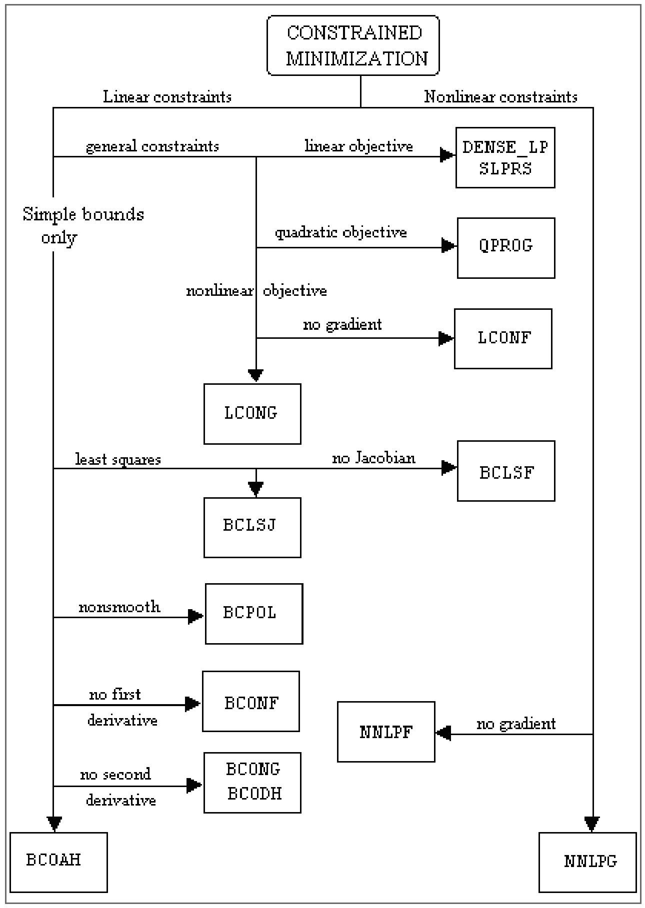
1. For the univariate case, use UVMID when the gradient is available, and use UVMIF when it is not. If discontinuities exist, then use UVMGS.
2. For the multivariate case, use UMCG* when storage is a problem, and use UMPOL when the function is nonsmooth. Otherwise, use UMI** depending on the availability of the gradient and the Hessian.
3. For least squares problems, use UNLSJ when the Jacobian is available, and use UNLSF when it is not.

Minimization with Simple Bounds

1. Use BCONF when only function values are available. When first derivatives are available, use either BCONG or BCODH. If first and second derivatives are available, then use BCOAH.
2. For least squares, use BCLSF or BCLSJ depending on the availability of the Jacobian.
3. Use BCPOL for nonsmooth functions that could not be solved satisfactorily by the other routines.

The following charts provide a quick reference to routines in this chapter:


UNCONSTRAINED MINIMIZATION
univariate
multivariate
UMCGF
no derivative
large-size problem
UMCGG
UNLSF
no Jacobian
least squares
UNLSJ
nonsmooth
UVMSG
UMPOL
nonsmooth
no derivative
UVMIF
UMINF
no first derivative
smooth
UMING
UMIDH
no second derivative
UVMID
UMIAH



CONSTRAINED MINIMIZATION
Linear constraints
Nonlinear constraints
general constraints
linear objective
DENSE_LP
SLPRS
Simple bounds only
quadratic objective
QPROG
nonlinear objective
no gradient
LCONF
LCONG
least squares
no Jacobian
BCLSF
BCLSJ
nonsmooth
BCPOL
no first derivative
BCONF
NNLPF
no gradient
no second derivative
BCONG
BCODH
BCOAH
NNLPG

UVMIF

Finds the minimum point of a smooth function of a single variable using only function evaluations.

Required Arguments

F — User-supplied function to compute the value of the function to be minimized. The form is `F(X)`, where

X – The point at which the function is evaluated. (Input)
`X` should not be changed by `F`.

`F` – The computed function value at the point `X`. (Output)

`F` must be declared `EXTERNAL` in the calling program.

XGUESS — An initial guess of the minimum point of `F`. (Input)

BOUND — A positive number that limits the amount by which `X` may be changed from its initial value. (Input)

X — The point at which a minimum value of `F` is found. (Output)

Optional Arguments

STEP — An order of magnitude estimate of the required change in `X`. (Input)
Default: `STEP` = 1.0.

XACC — The required absolute accuracy in the final value of `X`. (Input)
On a normal return there are points on either side of `X` within a distance `XACC` at which `F` is no less than `F`(`X`).
Default: `XACC` = 1.e-4.

MAXFN — Maximum number of function evaluations allowed. (Input)
Default: `MAXFN` = 1000.

FORTRAN 90 Interface

Generic: `CALL UVMIF (F, XGUESS, BOUND, X [, …])`

Specific: The specific interface names are `S_UVMIF` and `D_UVMIF`.

FORTRAN 77 Interface

Single: CALL UVMIF (F, XGUESS, STEP, BOUND, XACC, MAXFN, X)

Double: The double precision name is DUVMIF.

Description

The routine UVMIF uses a safeguarded quadratic interpolation method to find a minimum point of a univariate function. Both the code and the underlying algorithm are based on the routine ZXLSF written by M.J.D. Powell at the University of Cambridge.

The routine UVMIF finds the least value of a univariate function, f, that is specified by the function subroutine F. Other required data include an initial estimate of the solution, XGUESS , and a positive number BOUND. Let x_0 = XGUESS and b = BOUND, then x is restricted to the interval $[x_0 - b, x_0 + b]$. Usually, the algorithm begins the search by moving from x_0 to $x = x_0 + s$, where s = STEP is also provided by the user and may be positive or negative. The first two function evaluations indicate the direction to the minimum point, and the search strides out along this direction until a bracket on a minimum point is found or until x reaches one of the bounds $x_0 \pm b$. During this stage, the step length increases by a factor of between two and nine per function evaluation; the factor depends on the position of the minimum point that is predicted by quadratic interpolation of the three most recent function values.

When an interval containing a solution has been found, we will have three points, x_1, x_2, and x_3, with $x_1 < x_2 < x_0$ and $f(x_2) \le f(x_1)$ and $f(x_2) \le f(x_3)$. There are three main ingredients in the technique for choosing the new x from these three points. They are (i) the estimate of the minimum point that is given by quadratic interpolation of the three function values, (ii) a tolerance parameter ε, that depends on the closeness of f to a quadratic, and (iii) whether x_2 is near the center of the range between x_1 and x_3 or is relatively close to an end of this range. In outline, the new value of x is as near as possible to the predicted minimum point, subject to being at least ε from x_2, and subject to being in the longer interval between x_1 and x_2 or x_2 and x_3 when x_2 is particularly close to x_1 or x_3. There is some elaboration, however, when the distance between these points is close to the required accuracy; when the distance is close to the machine precision; or when ε is relatively large.

The algorithm is intended to provide fast convergence when f has a positive and continuous second derivative at the minimum and to avoid gross inefficiencies in pathological cases, such as

$$f(x) = x + 1.001|x|$$

The algorithm can make ε large automatically in the pathological cases. In this case, it is usual for a new value of x to be at the midpoint of the longer interval that is adjacent to the least calculated function value. The midpoint strategy is used frequently when changes to f are dominated by computer rounding errors, which will almost certainly happen if the user requests an accuracy that is less than the square root of the machine precision. In such cases, the routine claims to have achieved the required accuracy if it knows that there is a local minimum point within distance δ of x, where δ = XACC, even though the rounding errors in f may cause the existence of other local minimum points nearby. This difficulty is inevitable in minimization routines that use only function values, so high precision arithmetic is recommended.

Comments

Informational errors

Type	Code	Description
3	1	Computer rounding errors prevent further refinement of X.
3	2	The final value of X is at a bound. The minimum is probably beyond the bound.
4	3	The number of function evaluations has exceeded MAXFN.

Example

A minimum point of $e^x - 5x$ is found.

```
      USE UVMIF_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                  Declare variables
      INTEGER    MAXFN, NOUT
      REAL       BOUND, F, FX, STEP, X, XACC, XGUESS
      EXTERNAL   F
!                                  Initialize variables
      XGUESS = 0.0
      XACC   = 0.001
      BOUND  = 100.0
      STEP   = 0.1
      MAXFN  = 50
!
!                                 Find minimum for F = EXP(X) - 5X
      CALL UVMIF (F, XGUESS, BOUND, X, STEP=STEP, XACC=XACC, MAXFN=MAXFN)
      FX = F(X)
!                                 Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) X, FX
!
99999 FORMAT ('   The minimum is at ', 7X, F7.3, //, '   The function ' &
            , 'value is ', F7.3)
!
      END
!                                 Real function: F = EXP(X) - 5.0*X
      REAL FUNCTION F (X)
      REAL       X
!
      REAL       EXP
      INTRINSIC  EXP
!
      F = EXP(X) - 5.0E0*X
!
```

```
      RETURN
      END
```

Output

```
The minimum is at          1.609

The function value is  -3.047
```

UVMID

Finds the minimum point of a smooth function of a single variable using both function evaluations and first derivative evaluations.

Required Arguments

F — User-supplied function to define the function to be minimized. The form is
F(X), where

X — The point at which the function is to be evaluated. (Input)

F — The computed value of the function at X. (Output)

F must be declared EXTERNAL in the calling program.

G — User-supplied function to compute the derivative of the function. The form is
G(X), where

X — The point at which the derivative is to be computed. (Input)

G — The computed value of the derivative at X. (Output)

G must be declared EXTERNAL in the calling program.

A — A is the lower endpoint of the interval in which the minimum point of F is to be located. (Input)

B — B is the upper endpoint of the interval in which the minimum point of F is to be located. (Input)

X — The point at which a minimum value of F is found. (Output)

Optional Arguments

XGUESS — An initial guess of the minimum point of F. (Input)
Default: XGUESS = (a + b) / 2.0.

ERRREL — The required relative accuracy in the final value of X. (Input)
This is the first stopping criterion. On a normal return, the solution X is in an interval that contains a local minimum and is less than or equal to MAX(1.0, ABS(X)) * ERRREL. When the given ERRREL is less than machine epsilon, SQRT(machine epsilon) is used as ERRREL.
Default: ERRREL = 1.e-4.

GTOL — The derivative tolerance used to decide if the current point is a local minimum. (Input)
This is the second stopping criterion. X is returned as a solution when GX is less than or equal to GTOL. GTOL should be nonnegative, otherwise zero would be used.
Default: GTOL = 1.e-4.

MAXFN — Maximum number of function evaluations allowed. (Input)
Default: MAXFN = 1000.

FX — The function value at point X. (Output)

GX — The derivative value at point X. (Output)

FORTRAN 90 Interface

Generic: CALL UVMID (F, G, A, B, X [, …])

Specific: The specific interface names are S_UVMID and D_UVMID.

FORTRAN 77 Interface

Single: CALL UVMID (F, G, XGUESS, ERRREL, GTOL, MAXFN, A, B, X, FX, GX)

Double: The double precision name is DUVMID.

Description

The routine UVMID uses a descent method with either the secant method or cubic interpolation to find a minimum point of a univariate function. It starts with an initial guess and two endpoints. If any of the three points is a local minimum point and has least function value, the routine terminates with a solution. Otherwise, the point with least function value will be used as the starting point.

From the starting point, say x_c, the function value $f_c = f(x_c)$, the derivative value $g_c = g(x_c)$, and a new point x_n defined by $x_n = x_c - g_c$ are computed. The function $f_n = f(x_n)$, and the derivative $g_n = g(x_n)$ are then evaluated. If either $f_n \geq f_c$ or g_n has the opposite sign of g_c, then there exists a minimum point between x_c and x_n; and an initial interval is obtained. Otherwise, since x_c is kept as the point that has lowest function value, an interchange between x_n and x_c is performed. The secant method is then used to get a new point

$$x_s = x_c - g_c\left(\frac{g_n - g_c}{x_n - x_c}\right)$$

Let $x_n \leftarrow x_s$ and repeat this process until an interval containing a minimum is found or one of the convergence criteria is satisfied. The convergence criteria are as follows:

Criterion 1:

$$|x_c - x_n| \le \varepsilon_c$$

Criterion 2:

$$|g_c| \le \varepsilon_g$$

where $\varepsilon_c = \max\{1.0, |x_c|\}\varepsilon$, ε is a relative error tolerance and ε_g is a gradient tolerance.

When convergence is not achieved, a cubic interpolation is performed to obtain a new point. Function and derivative are then evaluated at that point; and accordingly, a smaller interval that contains a minimum point is chosen. A safeguarded method is used to ensure that the interval reduces by at least a fraction of the previous interval. Another cubic interpolation is then performed, and this procedure is repeated until one of the stopping criteria is met.

Comments

Informational errors

Type	Code	Description
3	1	The final value of X is at the lower bound. The minimum is probably beyond the bound.
3	2	The final value of X is at the upper bound. The minimum is probably beyond the bound.
4	3	The maximum number of function evaluations has been exceeded.

Example

A minimum point of $e^x - 5x$ is found.

```
      USE UVMID_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    MAXFN, NOUT
      REAL       A, B, ERRREL, F, FX, G, GTOL, GX, X, XGUESS, FTOL
      EXTERNAL   F, G
!                                 Initialize variables
      XGUESS = 0.0
!                                Set ERRREL to zero in order
!                                to use SQRT(machine epsilon)
!                                as relative error
      ERRREL = 0.0
      GTOL   = 0.0
      A      = -10.0
      B      = 10.0
      MAXFN  = 50
!
```

```
!                                  Find minimum for F = EXP(X) - 5X
      CALL UVMID (F, G, A, B, X, XGUESS=XGUESS, ERRREL=ERRREL,  &
                 GTOL=FTOL, MAXFN=MAXFN, FX=FX, GX=GX)
!                                  Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) X, FX, GX
!
99999 FORMAT ('   The minimum is at ', 7X, F7.3, //, '   The function ' &
            , 'value is ', F7.3, //, '   The derivative is ', F7.3)
!
      END
!                                  Real function: F = EXP(X) - 5.0*X
      REAL FUNCTION F (X)
      REAL       X
!
      REAL       EXP
      INTRINSIC  EXP
!
      F = EXP(X) - 5.0E0*X
!
      RETURN
      END
!
      REAL FUNCTION G (X)
      REAL       X
!
      REAL       EXP
      INTRINSIC  EXP
!
      G = EXP(X) - 5.0E0
      RETURN
      END
```

Output

```
The minimum is at       1.609

The function value is  -3.047

The derivative is  -0.001
```

UVMGS

Finds the minimum point of a nonsmooth function of a single variable.

Required Arguments

F — User-supplied function to compute the value of the function to be minimized. The form is `F(X)`, where

`X` – The point at which the function is evaluated. (Input)
`X` should not be changed by `F`.

F – The computed function value at the point `X`. (Output)

`F` must be declared `EXTERNAL` in the calling program.

A — On input, `A` is the lower endpoint of the interval in which the minimum of `F` is to be located. On output, `A` is the lower endpoint of the interval in which the minimum of `F` is located. (Input/Output)

B — On input, `B` is the upper endpoint of the interval in which the maximum of `F` is to be located. On output, `B` is the upper endpoint of the interval in which the minimum of `F` is located. (Input/Output)

XMIN — The approximate minimum point of the function `F` on the original interval (`A`, `B`). (Output)

Optional Arguments

TOL — The allowable length of the final subinterval containing the minimum point. (Input)
Default: `TOL` = 1.e-4.

FORTRAN 90 Interface

Generic: `CALL UVMGS (F, A, B, XMIN [, …])`

Specific: The specific interface names are `S_UVMGS` and `D_UVMGS`.

FORTRAN 77 Interface

Single: `CALL UVMGS (F, A, B, TOL, XMIN)`

Double: The double precision name is `DUVMGS`.

Description

The routine `UVMGS` uses the *golden section search* technique to compute to the desired accuracy the independent variable value that minimizes a unimodal function of one independent variable, where a known finite interval contains the minimum.

Let τ = `TOL`. The number of iterations required to compute the minimizing value to accuracy τ is the greatest integer less than or equal to

$$\frac{\ln\left(\tau / \left(b-a\right)\right)}{\ln\left(1-c\right)} + 1$$

where a and b define the interval and

$$c = \left(3-\sqrt{5}\right)/2$$

The first two test points are v_1 and v_2 that are defined as

$$v_1 = a + c(b - a), \text{ and } v_2 = b - c(b - a)$$

If $f(v_1) < f(v_2)$, then the minimizing value is in the interval (a, v_2). In this case, $b \leftarrow v_2$, $v_2 \leftarrow v_1$, and $v_1 \leftarrow a + c(b - a)$. If $f(v_1) \geq f(v_2)$, the minimizing value is in (v_1, b). In this case, $a \leftarrow v_1$, $v_1 \leftarrow v_2$, and $v_2 \leftarrow b - c(b - a)$.

The algorithm continues in an analogous manner where only one new test point is computed at each step. This process continues until the desired accuracy τ is achieved. `XMIN` is set to the point producing the minimum value for the current iteration.

Mathematically, the algorithm always produces the minimizing value to the desired accuracy; however, numerical problems may be encountered. If f is too flat in part of the region of interest, the function may appear to be constant to the computer in that region. Error code 2 indicates that this problem has occurred. The user may rectify the problem by relaxing the requirement on τ, modifying (scaling, etc.) the form of f or executing the program in a higher precision.

Comments

1. Informational errors

Type	**Code**	**Description**
3	1	TOL is too small to be satisfied.
4	2	Due to rounding errors F does not appear to be unimodal.

2. On exit from UVMGS without any error messages, the following conditions hold:
   (B-A) ≤ TOL.
   A ≤ XMIN and XMIN ≤ B
   F(XMIN) ≤ F(A) and F(XMIN) ≤ F(B)

3. On exit from UVMGS with error code 2, the following conditions hold:
   A ≤ XMIN and XMIN ≤ B
   F(XMIN) ≥ F(A) and F(XMIN) ≥ F(B) (only one equality can hold).
   Further analysis of the function F is necessary in order to determine whether it is not unimodal in the mathematical sense or whether it appears to be not unimodal to the routine due to rounding errors in which case the A, B, and XMIN returned may be acceptable.

Example

A minimum point of $3x^2 - 2x + 4$ is found.

```
      USE UVMGS_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                  Specification of variables
      INTEGER    NOUT
      REAL       A, B, FCN, FMIN, TOL, XMIN
      EXTERNAL   FCN
!                                  Initialize variables
      A   = 0.0E0
      B   = 5.0E0
      TOL = 1.0E-3
!                                  Minimize FCN
      CALL UVMGS (FCN, A, B, XMIN, TOL=TOL)
      FMIN = FCN(XMIN)
!                                  Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) XMIN, FMIN, A, B
99999 FORMAT ('   The minimum is at ', F5.3, //, '   The ', &
            'function value is ', F5.3, //, '   The final ', &
            'interval is (', F6.4, ',', F6.4, ')', /)
!
      END
!
!                                  REAL FUNCTION: F = 3*X**2 - 2*X + 4
      REAL FUNCTION FCN (X)
      REAL       X
!
      FCN = 3.0E0*X*X - 2.0E0*X + 4.0E0
!
      RETURN
      END
```

Output

```
The minimum is at 0.333
```

```
The function value is 3.667

The final interval is (0.3331,0.3340)
```

UMINF

Minimizes a function of N variables using a quasi-Newton method and a finite-difference gradient.

Required Arguments

FCN — User-supplied subroutine to evaluate the function to be minimized. The usage is CALL FCN (N, X, F) , where

N – Length of X. (Input)

X – The point at which the function is evaluated. (Input) X should not be changed by FCN.

F – The computed function value at the point X. (Output)

FCN must be declared EXTERNAL in the calling program.

X — Vector of length N containing the computed solution. (Output)

Optional Arguments

N — Dimension of the problem. (Input)
Default: N = SIZE (X,1).

XGUESS — Vector of length N containing an initial guess of the computed solution. (Input)
Default: XGUESS = 0.0.

XSCALE — Vector of length N containing the diagonal scaling matrix for the variables. (Input)
XSCALE is used mainly in scaling the gradient and the distance between two points. In the absence of other information, set all entries to 1.0.
Default: XSCALE = 1.0.

FSCALE — Scalar containing the function scaling. (Input)
FSCALE is used mainly in scaling the gradient. In the absence of other information, set FSCALE to 1.0.
Default: FSCALE = 1.0.

IPARAM — Parameter vector of length 7. (Input/Output)
Set IPARAM(1) to zero for default values of IPARAM and RPARAM. See Comment 4.
Default: IPARAM = 0.

RPARAM — Parameter vector of length 7.(Input/Output)
See Comment 4.

FVALUE — Scalar containing the value of the function at the computed solution. (Output)

FORTRAN 90 Interface

Generic: `CALL UMINF (FCN, X [, …])`

Specific: The specific interface names are `S_UMINF` and `D_UMINF`.

FORTRAN 77 Interface

Single: `CALL UMINF (FCN, N, XGUESS, XSCALE, FSCALE, IPARAM, RPARAM, X, FVALUE)`

Double: The double precision name is `DUMINF`.

Description

The routine `UMINF` uses a quasi-Newton method to find the minimum of a function $f(x)$ of n variables. Only function values are required. The problem is stated as follows:

$$\min_{x \in \mathrm{R}^n} f(x)$$

Given a starting point x_c, the search direction is computed according to the formula

$$d = -B^{-1} g_c$$

where B is a positive definite approximation of the Hessian and g_c is the gradient evaluated at x_c. A line search is then used to find a new point

$$x_n = x_c + \lambda d, \qquad \lambda > 0$$

such that

$$f(x_n) \le f(x_c) + \alpha g^T d, \alpha \in (0, 0.5)$$

Finally, the optimality condition $\|g(x)\| = \varepsilon$ is checked where ε is a gradient tolerance.

When optimality is not achieved, B is updated according to the `BFGS` formula

$$B \leftarrow B - \frac{Bss^T B}{s^T Bs} + \frac{yy^T}{y^T s}$$

where $s = x_n - x_c$ and $y = g_n - g_c$. Another search direction is then computed to begin the next iteration. For more details, see Dennis and Schnabel (1983, Appendix A).

Since a finite-difference method is used to estimate the gradient, for some single precision calculations, an inaccurate estimate of the gradient may cause the algorithm to terminate at a noncritical point. In such cases, high precision arithmetic is recommended. Also, whenever the exact gradient can be easily provided, IMSL routine UMING should be used instead.

Comments

1. Workspace may be explicitly provided, if desired, by use of U2INF/DU2INF. The reference is:

   CALL U2INF (FCN, N, XGUESS, XSCALE, FSCALE, IPARAM, RPARAM, X, FVALUE, WK)

   The additional argument is:

   WK — Work vector of length N(N + 8). WK contains the following information on output: The second N locations contain the last step taken. The third N locations contain the last Newton step. The fourth N locations contain an estimate of the gradient at the solution. The final N^2 locations contain the Cholesky factorization of a BFGS approximation to the Hessian at the solution.

2. Informational errors

Type	Code	Description
4	2	The iterates appear to be converging to a noncritical point.
4	3	Maximum number of iterations exceeded.
4	4	Maximum number of function evaluations exceeded.
4	5	Maximum number of gradient evaluations exceeded.
4	6	Five consecutive steps have been taken with the maximum step length.
2	7	Scaled step tolerance satisfied; the current point may be an approximate local solution, or the algorithm is making very slow progress and is not near a solution, or STEPTL is too big.
3	8	The last global step failed to locate a lower point than the current X value.

3. The first stopping criterion for UMINF occurs when the infinity norm of the scaled gradient is less than the given gradient tolerance (RPARAM(1)). The second stopping criterion for UMINF occurs when the scaled distance between the last two steps is less than the step tolerance (RPARAM(2)).

4. If the default parameters are desired for UMINF, then set IPARAM(1) to zero and call the routine UMINF. Otherwise, if any nondefault parameters are desired for IPARAM or RPARAM, then the following steps should be taken before calling UMINF:

   CALL U4INF (IPARAM, RPARAM)

   Set nondefault values for desired IPARAM, RPARAM elements.

   Note that the call to U4INF will set IPARAM and RPARAM to their default values so only nondefault values need to be set above.

   The following is a list of the parameters and the default values:

   IPARAM — Integer vector of length 7.

   IPARAM(1) = Initialization flag.

   IPARAM(2) = Number of good digits in the function
   Default: Machine dependent.

   IPARAM(3) = Maximum number of iterations.
   Default: 100.

   IPARAM(4) = Maximum number of function evaluations.
   Default: 400.

   IPARAM(5) = Maximum number of gradient evaluations.
   Default: 400.

   IPARAM(6) = Hessian initialization parameter.
   If IPARAM(6) = 0, the Hessian is initialized to the identity matrix; otherwise, it is initialized to a diagonal matrix containing

$$\max\left(|f(t)|, f_s\right) * s_i^2$$

   on the diagonal where t = XGUESS, f_s = FSCALE, and s = XSCALE.
   Default: 0.

   IPARAM(7) = Maximum number of Hessian evaluations.
   Default: Not used in UMINF.

   RPARAM — Real vector of length 7.

   RPARAM(1) = Scaled gradient tolerance.
   The i-th component of the scaled gradient at x is calculated as

$$\frac{|g_i| * \max\left(|x_i|, 1/s_i\right)}{\max\left(|f(x)|, f_s\right)}$$

   where $g = \nabla f(x)$, s = XSCALE, and f_s = FSCALE.
   Default:

$$\sqrt{\varepsilon}, \sqrt[3]{\varepsilon}$$

   in double where ε is the machine precision.

RPARAM(2) = Scaled step tolerance. (STEPTL)

The *i*-th component of the scaled step between two points *x* and *y* is computed as

$$\frac{|x_i - y_i|}{\max\left(|x_i|, 1/s_i\right)}$$

where *s* = XSCALE.

Default: $\varepsilon^{2/3}$ where ε is the machine precision.

RPARAM(3) = Relative function tolerance.

Default: Not used in UMINF.

RPARAM(4) = Absolute function tolerance

Default: Not used in UMINF.

RPARAM(5) = False convergence tolerance.

Default: Not used in UMINF.

RPARAM(6) = Maximum allowable step size.

Default: 1000 max(ε_1, ε_2) where

$$\varepsilon_1 = \sqrt{\sum_{i=1}^{n} \left(s_i t_i\right)^2},\ \varepsilon_2 = \|s\|_2,\ s = \text{XSCALE, and } t = \text{XGUESS}$$

RPARAM(7) = Size of initial trust region radius.

Default: Not used in UMINF.

If double precision is required, then DU4INF is called, and RPARAM is declared double precision.

5. Users wishing to override the default print/stop attributes associated with error messages issued by this routine are referred to “Error Handling” in the Introduction.

Example

The function

$$f(x) = 100\left(x_2 - x_1^2\right)^2 + \left(1 - x_1\right)^2$$

is minimized.

```
      USE UMINF_INT
      USE U4INF_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    N
      PARAMETER  (N=2)
!
      INTEGER    IPARAM(7), L, NOUT
      REAL       F, RPARAM(7), X(N), XGUESS(N), &
                XSCALE(N)
      EXTERNAL   ROSBRK
```

```
!
      DATA XGUESS/-1.2E0, 1.0E0/
!
!                                   Relax gradient tolerance stopping
!                                   criterion
      CALL U4INF (IPARAM, RPARAM)
      RPARAM(1) = 10.0E0*RPARAM(1)
!                                   Minimize Rosenbrock function using
!                                   initial guesses of -1.2 and 1.0
      CALL UMINF (ROSBRK, X, XGUESS=XGUESS, IPARAM=IPARAM, RPARAM=RPARAM, &
            FVALUE=F)
!                                   Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) X, F, (IPARAM(L),L=3,5)
!
99999 FORMAT ('  The solution is ', 6X, 2F8.3, //, '  The function ', &
            'value is ', F8.3, //, '  The number of iterations is ', &
            10X, I3, /, '  The number of function evaluations is ', &
            I3, /, '  The number of gradient evaluations is ', I3)
!
      END
!
      SUBROUTINE ROSBRK (N, X, F)
      INTEGER    N
      REAL       X(N), F
!
      F = 1.0E2*(X(2)-X(1)*X(1))**2 + (1.0E0-X(1))**2
!
      RETURN
      END
```

Output

```
The solution is          1.000   1.000

The function value is    0.000

The number of iterations is            15
The number of function evaluations is  40
The number of gradient evaluations is  19
```

UMING

Minimizes a function of N variables using a quasi-Newton method and a user-supplied gradient.

Required Arguments

FCN — User-supplied subroutine to evaluate the function to be minimized. The usage is
CALL FCN (N, X, F) , where

N – Length of X. (Input)

X – Vector of length N at which point the function is evaluated. (Input)
X should not be changed by FCN.

F – The computed function value at the point X. (Output)

FCN must be declared EXTERNAL in the calling program.

GRAD — User-supplied subroutine to compute the gradient at the point X. The usage is
CALL GRAD (N, X, G) , where

N – Length of X and G. (Input)

X – Vector of length N at which point the function is evaluated. (Input)
X should not be changed by GRAD .

G – The gradient evaluated at the point X. (Output)

GRAD must be declared EXTERNAL in the calling program.

X — Vector of length N containing the computed solution. (Output)

Optional Arguments

N — Dimension of the problem. (Input)
Default: N = SIZE (X,1).

XGUESS — Vector of length N containing the initial guess of the minimum. (Input)
Default: XGUESS = 0.0.

XSCALE — Vector of length N containing the diagonal scaling matrix for the variables. (Input)
XSCALE is used mainly in scaling the gradient and the distance between two points. In the absence of other information, set all entries to 1.0.
Default: XSCALE = 1.0.

FSCALE — Scalar containing the function scaling. (Input)

FSCALE is used mainly in scaling the gradient. In the absence of other information, set FSCALE to 1.0.

Default: FSCALE = 1.0.

IPARAM — Parameter vector of length 7. (Input/Output)

Set IPARAM(1) to zero for default values of IPARAM and RPARAM. See Comment 4.

Default: IPARAM = 0.

RPARAM — Parameter vector of length 7. (Input/Output)

See Comment 4.

FVALUE — Scalar containing the value of the function at the computed solution. (Output)

FORTRAN 90 Interface

Generic: CALL UMING (FCN, GRAD, X [, …])

Specific: The specific interface names are S_UMING and D_UMING.

FORTRAN 77 Interface

Single: CALL UMING (FCN, GRAD, N, XGUESS, XSCALE, FSCALE, IPARAM, RPARAM, X, FVALUE)

Double: The double precision name is DUMING.

Description

The routine UMING uses a quasi-Newton method to find the minimum of a function *f*(*x*) of *n* variables. Function values and first derivatives are required. The problem is stated as follows:

$$\min_{x \in \mathbf{R}^n} f(x)$$

Given a starting point x_c, the search direction is computed according to the formula

$$d = -B^{-1} g_c$$

where *B* is a positive definite approximation of the Hessian and g_c is the gradient evaluated at x_c. A line search is then used to find a new point

$$x_n = x_c + \lambda d, \qquad \lambda > 0$$

such that

$$f(x_n) \le f(x_c) + \alpha g^T d,\ \alpha \in (0, 0.5)$$

Finally, the optimality condition $\|g(x)\| = \varepsilon$ is checked where ε is a gradient tolerance.

When optimality is not achieved, B is updated according to the BFGS formula

$$B \leftarrow B - \frac{Bss^T B}{s^T Bs} + \frac{yy^T}{y^T s}$$

where $s = x_n - x_c$ and $y = g_n - g_c$. Another search direction is then computed to begin the next iteration. For more details, see Dennis and Schnabel (1983, Appendix A).

Comments

1. Workspace may be explicitly provided, if desired, by use of U2ING/DU2ING. The reference is:

   ```
   CALL U2ING (FCN, GRAD, N, XGUESS, XSCALE, FSCALE, IPARAM,
      RPARAM, X, FVALUE, WK)
   ```

   The additional argument is

   WK — Work vector of length `N * (N + 8)`. WK contains the following information on output: The second N locations contain the last step taken. The third N locations contain the last Newton step. The fourth N locations contain an estimate of the gradient at the solution. The final N^2 locations contain the Cholesky factorization of a BFGS approximation to the Hessian at the solution.

2. Informational errors

Type	**Code**	**Description**
4	2	The iterates appear to be converging to a noncritical point.
4	3	Maximum number of iterations exceeded.
4	4	Maximum number of function evaluations exceeded.
4	5	Maximum number of gradient evaluations exceeded.
4	6	Five consecutive steps have been taken with the maximum step length.
2	7	Scaled step tolerance satisfied; the current point may be an approximate local solution, or the algorithm is making very slow progress and is not near a solution, or STEPTL is too big.
3	8	The last global step failed to locate a lower point than the current X value.

3. The first stopping criterion for UMING occurs when the infinity norm of the scaled gradient is less than the given gradient tolerance (RPARAM(1)). The second stopping criterion for UMING occurs when the scaled distance between the last two steps is less than the step tolerance (RPARAM(2)).

4. If the default parameters are desired for UMING, then set IPARAM(1) to zero and call routine UMING. Otherwise, if any nondefault parameters are desired for IPARAM or RPARAM, then the following steps should be taken before calling UMING:

   CALL U4INF (IPARAM, RPARAM)

   Set nondefault values for desired IPARAM, RPARAM elements.

Note that the call to U4INF will set IPARAM and RPARAM to their default values so only nondefault values need to be set above.

The following is a list of the parameters and the default values:

IPARAM — Integer vector of length 7.

IPARAM(1) = Initialization flag.

IPARAM(2) = Number of good digits in the function.
Default: Machine dependent.

IPARAM(3) = Maximum number of iterations.
Default: 100.

IPARAM(4) = Maximum number of function evaluations.
Default: 400.

IPARAM(5) = Maximum number of gradient evaluations.
Default: 400.

IPARAM(6) = Hessian initialization parameter
If IPARAM(6) = 0, the Hessian is initialized to the identity matrix; otherwise, it is initialized to a diagonal matrix containing

$$\max\left(\mid f\left(t\right) \mid , f_s \right) * s_i^2$$

on the diagonal where t = XGUESS, f_s = FSCALE, and s = XSCALE.
Default: 0.

IPARAM(7) = Maximum number of Hessian evaluations.
Default: Not used in UMING.

RPARAM — Real vector of length 7.

RPARAM(1) = Scaled gradient tolerance.
The i-th component of the scaled gradient at x is calculated as

$$\frac{|g_i| * \max\left(|x_i|, 1/s_i\right)}{\max\left(|f\left(x\right)|, f_s\right)}$$

where $g = \nabla f(x)$, s = XSCALE, and f_s = FSCALE.
Default:

$$\sqrt{\varepsilon}, \sqrt[3]{\varepsilon}$$

in double where **ε** is the machine precision.

RPARAM(2) = Scaled step tolerance. (STEPTL)
The *i*-th component of the scaled step between two points *x* and *y* is computed as

$$\frac{|x_i - y_i|}{\max\left(|x_i|, 1/s_i\right)}$$

where *s* = XSCALE.
Default: $\varepsilon^{2/3}$ where **ε** is the machine precision.

RPARAM(3) = Relative function tolerance.
Default: Not used in UMING.

RPARAM(4) = Absolute function tolerance.
Default: Not used in UMING.

RPARAM(5) = False convergence tolerance.
Default: Not used in UMING.

RPARAM(6) = Maximum allowable step size.
Default: 1000 max(ε_1, ε_2) where

$$\varepsilon_1 = \sqrt{\sum_{i=1}^{n}\left(s_i t_i\right)^2}$$

$\varepsilon_2 = \|s\|_2$, *s* = XSCALE, and *t* = XGUESS.

RPARAM(7) = Size of initial trust region radius.
Default: Not used in UMING.

If double precision is required, then DU4INF is called, and RPARAM is declared double precision.

5. Users wishing to override the default print/stop attributes associated with error messages issued by this routine are referred to “Error Handling” in the Introduction.

Example

The function

$$f(x) = 100\left(x_2 - x_1^2\right)^2 + \left(1 - x_1\right)^2$$

is minimized. Default values for parameters are used.

```
      USE UMING_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    N
```

```
      PARAMETER  (N=2)
!
      INTEGER    IPARAM(7), L, NOUT
      REAL       F, X(N), XGUESS(N)
      EXTERNAL   ROSBRK, ROSGRD
!
      DATA XGUESS/-1.2E0, 1.0E0/
!
      IPARAM(1) = 0
!                                  Minimize Rosenbrock function using
!                                  initial guesses of -1.2 and 1.0
      CALL UMING (ROSBRK, ROSGRD, X, XGUESS=XGUESS, IPARAM=IPARAM, FVALUE=F)
!                                  Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) X, F, (IPARAM(L),L=3,5)
!
99999 FORMAT ('  The solution is ', 6X, 2F8.3, //, '  The function ', &
            'value is ', F8.3, //, '  The number of iterations is ', &
            10X, I3, /, '  The number of function evaluations is ', &
            I3, /, '  The number of gradient evaluations is ', I3)
!
      END
!
      SUBROUTINE ROSBRK (N, X, F)
      INTEGER    N
      REAL       X(N), F
!
      F = 1.0E2*(X(2)-X(1)*X(1))**2 + (1.0E0-X(1))**2
!
      RETURN
      END
!
      SUBROUTINE ROSGRD (N, X, G)
      INTEGER    N
      REAL       X(N), G(N)
!
      G(1) = -4.0E2*(X(2)-X(1)*X(1))*X(1) - 2.0E0*(1.0E0-X(1))
      G(2) = 2.0E2*(X(2)-X(1)*X(1))
!
      RETURN
      END
```

Output

```
The solution is          1.000   1.000

The function value is    0.000

The number of iterations is             18
The number of function evaluations is   31
The number of gradient evaluations is   22
```

UMIDH

Minimizes a function of N variables using a modified Newton method and a finite-difference Hessian.

Required Arguments

FCN — User-supplied subroutine to evaluate the function to be minimized. The usage is
CALL FCN (N, X, F), where

N – Length of X. (Input)

X – Vector of length N at which point the function is evaluated. (Input)
X should not be changed by FCN.

F – The computed function value at the point X. (Output)

FCN must be declared EXTERNAL in the calling program.

GRAD — User-supplied subroutine to compute the gradient at the point X. The usage is
CALL GRAD (N, X, G), where

N – Length of X and G. (Input)

X – The point at which the gradient is evaluated. (Input)
X should not be changed by GRAD.

G – The gradient evaluated at the point X. (Output)

GRAD must be declared EXTERNAL in the calling program.

X — Vector of length N containing the computed solution. (Output)

Optional Arguments

N — Dimension of the problem. (Input)
Default: N = SIZE (X,1).

XGUESS — Vector of length N containing initial guess. (Input)
Default: XGUESS = 0.0.

XSCALE — Vector of length N containing the diagonal scaling matrix for the variables. (Input)
XSCALE is used mainly in scaling the gradient and the distance between two points. In the absence of other information, set all entries to 1.0.
Default: XSCALE = 1.0.

FSCALE — Scalar containing the function scaling. (Input)
FSCALE is used mainly in scaling the gradient. In the absence of other information, set FSCALE to 1.0.
Default: FSCALE = 1.0.

IPARAM — Parameter vector of length 7. (Input/Output)
Set IPARAM(1) to zero for default values of IPARAM and RPARAM. See Comment 4.
Default: IPARAM = 0.

RPARAM — Parameter vector of length 7. (Input/Output)
See Comment 4.

FVALUE — Scalar containing the value of the function at the computed solution. (Output)

FORTRAN 90 Interface

Generic: CALL UMIDH (FCN, GRAD, X [, …])

Specific: The specific interface names are S_UMIDH and D_UMIDH.

FORTRAN 77 Interface

Single: CALL UMIDH (FCN, GRAD, N, XGUESS, XSCALE, FSCALE, IPARAM, RPARAM, X, FVALUE)

Double: The double precision name is DUMIDH.

Description

The routine UMIDH uses a modified Newton method to find the minimum of a function $f(x)$ of n variables. First derivatives must be provided by the user. The algorithm computes an optimal locally constrained step (Gay 1981) with a trust region restriction on the step. It handles the case that the Hessian is indefinite and provides a way to deal with negative curvature. For more details, see Dennis and Schnabel (1983, Appendix A) and Gay (1983).

Since a finite-difference method is used to estimate the Hessian for some single precision calculations, an inaccurate estimate of the Hessian may cause the algorithm to terminate at a noncritical point. In such cases, high precision arithmetic is recommended. Also, whenever the exact Hessian can be easily provided, IMSL routine UMIAH should be used instead.

Comments

1. Workspace may be explicitly provided, if desired, by use of U2IDH/DU2IDH. The reference is:

```
CALL U2IDH (FCN, GRAD, N, XGUESS, XSCALE, FSCALE, IPARAM,
   RPARAM, X, FVALUE, WK)
```

The additional argument is:

WK — Work vector of length N * (N + 9). WK contains the following information on output: The second N locations contain the last step taken. The third N locations contain the last Newton step. The fourth N locations contain an estimate of the gradient at the solution. The final N^2 locations contain the Hessian at the approximate solution.

2. Informational errors

Type	Code	Description
3	1	Both the actual and predicted relative reductions in the function are less than or equal to the relative function convergence tolerance.
4	2	The iterates appear to be converging to a noncritical point.
4	3	Maximum number of iterations exceeded.
4	4	Maximum number of function evaluations exceeded.
4	5	Maximum number of gradient evaluations exceeded.
4	6	Five consecutive steps have been taken with the maximum step length.
2	7	Scaled step tolerance satisfied; the current point may be an approximate local solution, or the algorithm is making very slow progress and is not near a solution, or STEPTL is too big.
4	7	Maximum number of Hessian evaluations exceeded.
3	8	The last global step failed to locate a lower point than the current X value.

3. The first stopping criterion for UMIDH occurs when the norm of the gradient is less than the given gradient tolerance (RPARAM(1)). The second stopping criterion for UMIDH occurs when the scaled distance between the last two steps is less than the step tolerance (RPARAM(2)).

4. If the default parameters are desired for UMIDH, then set IPARAM(1) to zero and call routine UMIDH. Otherwise, if any nondefault parameters are desired for IPARAM or RPARAM, then the following steps should be taken before calling UMIDH:

CALL U4INF (IPARAM, RPARAM)

Set nondefault values for desired IPARAM, RPARAM elements.

Note that the call to U4INF will set IPARAM and RPARAM to their default values so only nondefault values need to be set above.

The following is a list of the parameters and the default values:

IPARAM — Integer vector of length 7.

IPARAM(1) = Initialization flag.

IPARAM(2) = Number of good digits in the function.
Default: Machine dependent.

IPARAM(3) = Maximum number of iterations.
Default: 100.

IPARAM(4) = Maximum number of function evaluations.
Default: 400.

IPARAM(5) = Maximum number of gradient evaluations.
Default: 400.

IPARAM(6) = Hessian initialization parameter
Default: Not used in UMIDH.

IPARAM(7) = Maximum number of Hessian evaluations.
Default:100

RPARAM — Real vector of length 7.

RPARAM(1) = Scaled gradient tolerance.
The *i*-th component of the scaled gradient at *x* is calculated as

$$\frac{|g_i| * \max\left(|x_i|, 1/s_i\right)}{\max\left(|f(x)|, f_s\right)}$$

where $g = \nabla f(x)$, s = XSCALE, and f_s = FSCALE.
Default:

$$\sqrt{\varepsilon}, \sqrt[3]{\varepsilon}$$

in double where **ε** is the machine precision.

RPARAM(2) = Scaled step tolerance. (STEPTL)
The *i*-th component of the scaled step between two points *x* and *y* is computed as

$$\frac{|x_i - y_i|}{\max\left(|x_i|, 1/s_i\right)}$$

where s = XSCALE.
Default: $\varepsilon^{2/3}$ where **ε** is the machine precision.

RPARAM(3) = Relative function tolerance.
Default: $\max(10^{-10}, \varepsilon^{2/3})$, $\max(10^{-20}, \varepsilon^{2/3})$ in double where **ε** is the machine precision.

RPARAM(4) = Absolute function tolerance.
Default: Not used in UMIDH.

RPARAM(5) = False convergence tolerance.
Default: 100**ε** where **ε** is the machine precision.

RPARAM(6) = Maximum allowable step size.
Default: 1000 $\max(\varepsilon_1, \varepsilon_2)$ where

$$\varepsilon_1 = \sqrt{\sum_{i=1}^{n} (s_i t_i)^2}$$

$\varepsilon_2 = \|s\|_2$, s = XSCALE, and t = XGUESS.

RPARAM(7) = Size of initial trust region radius.
Default: Based on initial scaled Cauchy step.

If double precision is required, then DU4INF is called, and RPARAM is declared double precision.

5. Users wishing to override the default print/stop attributes associated with error messages issued by this routine are referred to “Error Handling” in the Introduction.

Example

The function

$$f(x) = 100\left(x_2 - x_1^2\right)^2 + \left(1 - x_1\right)^2$$

is minimized. Default values for parameters are used.

```
      USE UMIDH_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    N
      PARAMETER  (N=2)
!
      INTEGER    IPARAM(7), L, NOUT
      REAL       F, X(N), XGUESS(N)
      EXTERNAL   ROSBRK, ROSGRD
!
      DATA XGUESS/-1.2E0, 1.0E0/
!
      IPARAM(1) = 0
!                                  Minimize Rosenbrock function using
!                                  initial guesses of -1.2 and 1.0
      CALL UMIDH (ROSBRK, ROSGRD, X, XGUESS=XGUESS, IPARAM=IPARAM, FVALUE=F)
!                                  Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) X, F, (IPARAM(L),L=3,5), IPARAM(7)
!
99999 FORMAT ('  The solution is ', 6X, 2F8.3, //, '  The function ', &
            'value is ', F8.3, //, '  The number of iterations is ', &
            10X, I3, /, '  The number of function evaluations is ', &
            I3, /, '  The number of gradient evaluations is ', I3, /, &
            '  The number of Hessian evaluations is  ', I3)
!
      END
!
      SUBROUTINE ROSBRK (N, X, F)
      INTEGER    N
      REAL       X(N), F
!
      F = 1.0E2*(X(2)-X(1)*X(1))**2 + (1.0E0-X(1))**2
!
      RETURN
```

```
      END
!
      SUBROUTINE ROSGRD (N, X, G)
      INTEGER    N
      REAL       X(N), G(N)
!
      G(1) = -4.0E2*(X(2)-X(1)*X(1))*X(1) - 2.0E0*(1.0E0-X(1))
      G(2) = 2.0E2*(X(2)-X(1)*X(1))
!
      RETURN
      END
```

Output

```
 The solution is          1.000   1.000

 The function value is    0.000

 The number of iterations is            21
 The number of function evaluations is  30
 The number of gradient evaluations is  22
 The number of Hessian evaluations is   21
```

UMIAH

Minimizes a function of N variables using a modified Newton method and a user-supplied Hessian.

Required Arguments

FCN — User-supplied subroutine to evaluate the function to be minimized. The usage is
CALL FCN (N, X, F), where

N – Length of X. (Input)

X – Vector of length N at which point the function is evaluated. (Input)
X should not be changed by FCN.

F – The computed function value at the point X. (Output)

FCN must be declared EXTERNAL in the calling program.

GRAD — User-supplied subroutine to compute the gradient at the point X. The usage is
CALL GRAD (N, X, G), where

N – Length of X and G. (Input)

X – Vector of length N at which point the gradient is evaluated. (Input)
X should not be changed by GRAD.

G – The gradient evaluated at the point X. (Output)

GRAD must be declared EXTERNAL in the calling program.

HESS — User-supplied subroutine to compute the Hessian at the point X. The usage is
CALL HESS (N, X, H, LDH), where

N – Length of X. (Input)

X – Vector of length N at which point the Hessian is evaluated. (Input)
X should not be changed by HESS.

H – The Hessian evaluated at the point X. (Output)

LDH – Leading dimension of H exactly as specified in the dimension statement of the calling program. (Input)

HESS must be declared EXTERNAL in the calling program.

X — Vector of length N containing the computed solution. (Output)

Optional Arguments

N — Dimension of the problem. (Input)
Default: N = SIZE (X,1).

XGUESS — Vector of length N containing initial guess. (Input)
Default: XGUESS = 0.0.

XSCALE — Vector of length N containing the diagonal scaling matrix for the variables. (Input)
XSCALE is used mainly in scaling the gradient and the distance between two points. In the absence of other information, set all entries to 1.0.
Default: XSCALE = 1.0.

FSCALE — Scalar containing the function scaling. (Input)
FSCALE is used mainly in scaling the gradient. In the absence of other information, set FSCALE to 1.0.
Default: FSCALE = 1.0.

IPARAM — Parameter vector of length 7. (Input/Output)
Set IPARAM(1) to zero for default values of IPARAM and RPARAM. See Comment 4.
Default: IPARAM = 0.

RPARAM — Parameter vector of length 7. (Input/Output)
See Comment 4.

FVALUE — Scalar containing the value of the function at the computed solution. (Output)

FORTRAN 90 Interface

Generic: CALL UMIAH (FCN, GRAD, HESS, X, [, …])

Specific: The specific interface names are S_UMIAH and D_UMIAH.

FORTRAN 77 Interface

Single: CALL UMIAH (FCN, GRAD, HESS, N, XGUESS, XSCALE, FSCALE, IPARAM, RPARAM, X, FVALUE)

Double: The double precision name is DUMIAH.

Description

The routine UMIAH uses a modified Newton method to find the minimum of a function $f(x)$ of n variables. First and second derivatives must be provided by the user. The algorithm computes an optimal locally constrained step (Gay 1981) with a trust region restriction on the step. This algorithm handles the case where the Hessian is indefinite and provides a way to deal with negative curvature. For more details, see Dennis and Schnabel (1983, Appendix A) and Gay (1983).

Comments

1. Workspace may be explicitly provided, if desired, by use of U2IAH/DU2IAH. The reference is:

```
CALL U2IAH (FCN, GRAD, HESS, N, XGUESS, XSCALE, FSCALE,
   IPARAM, RPARAM, X, FVALUE, WK)
```

   The additional argument is:

   WK — Work vector of length N * (N + 9). WK contains the following information on output: The second N locations contain the last step taken. The third N locations contain the last Newton step. The fourth N locations contain an estimate of the gradient at the solution. The final N^2 locations contain the Hessian at the approximate solution.

2. Informational errors

Type	Code	Description
3	1	Both the actual and predicted relative reductions in the function are less than or equal to the relative function convergence tolerance.
4	2	The iterates appear to be converging to a noncritical point.
4	3	Maximum number of iterations exceeded.
4	4	Maximum number of function evaluations exceeded.
4	5	Maximum number of gradient evaluations exceeded.
4	6	Five consecutive steps have been taken with the maximum step length.
2	7	Scaled step tolerance satisfied; the current point may be an approximate local solution, or the algorithm is making very slow progress and is not near a solution, or STEPTL is too big.
4	7	Maximum number of Hessian evaluations exceeded.
3	8	The last global step failed to locate a lower point than the current X value.

3. The first stopping criterion for UMIAH occurs when the norm of the gradient is less than the given gradient tolerance (RPARAM(1)). The second stopping criterion for UMIAH occurs when the scaled distance between the last two steps is less than the step tolerance (RPARAM(2)).

4. If the default parameters are desired for `UMIAH`, then set `IPARAM`(1) to zero and call the routine `UMIAH`. Otherwise, if any nondefault parameters are desired for `IPARAM` or `RPARAM`, then the following steps should be taken before calling `UMIAH`:

   `CALL U4INF (IPARAM, RPARAM)`

   Set nondefault values for desired `IPARAM`, `RPARAM` elements.

Note that the call to `U4INF` will set `IPARAM` and `RPARAM` to their default values so only nondefault values need to be set above.

The following is a list of the parameters and the default values:

IPARAM — Integer vector of length 7.

`IPARAM`(1) = Initialization flag.

`IPARAM`(2) = Number of good digits in the function.
Default: Machine dependent.

`IPARAM`(3) = Maximum number of iterations.
Default: 100.

`IPARAM`(4) = Maximum number of function evaluations.
Default: 400.

`IPARAM`(5) = Maximum number of gradient evaluations.
Default: 400.

`IPARAM`(6) = Hessian initialization parameter
Default: Not used in `UMIAH`.

`IPARAM`(7) = Maximum number of Hessian evaluations.
Default: 100.

RPARAM — Real vector of length 7.

`RPARAM`(1) = Scaled gradient tolerance.
The *i*-th component of the scaled gradient at *x* is calculated as

$$\frac{|g_i| * \max\left(|x_i|, 1/s_i\right)}{\max\left(|f(x)|, f_s\right)}$$

where $g = \nabla f(x)$, s = `XSCALE`, and f_s = `FSCALE`.
Default:

$$\sqrt{\varepsilon}, \sqrt[3]{\varepsilon}$$

in double where **ε** is the machine precision.

`RPARAM`(2) = Scaled step tolerance. (`STEPTL`)
The *i*-th component of the scaled step between two points *x* and *y* is computed as

$$\frac{|x_i - y_i|}{\max\left(|x_i|, 1/s_i\right)}$$

where s = XSCALE.

Default: $\varepsilon^{2/3}$ where ε is the machine precision.

RPARAM(3) = Relative function tolerance.

Default: max(10^{-10}, $\varepsilon^{2/3}$), max(10^{-20}, $\varepsilon^{2/3}$) in double where ε is the machine precision.

RPARAM(4) = Absolute function tolerance.

Default: Not used in UMIAH.

RPARAM(5) = False convergence tolerance.

Default: 100ε where ε is the machine precision.

RPARAM(6) = Maximum allowable step size.

Default: 1000 max(ε_1, ε_2) where

$$\varepsilon_1 = \sqrt{\sum_{i=1}^{n} \left(s_i t_i\right)^2}$$

$\varepsilon_2 = \|s\|_2$, s = XSCALE, and t = XGUESS.

RPARAM(7) = Size of initial trust region radius.

Default: based on the initial scaled Cauchy step.

If double precision is required, then DU4INF is called, and RPARAM is declared double precision.

5. Users wishing to override the default print/stop attributes associated with error messages issued by this routine are referred to "Error Handling" in the Introduction.

Example

The function

$$f(x) = 100\left(x_2 - x_1^2\right)^2 + \left(1 - x_1\right)^2$$

is minimized. Default values for parameters are used.

```
      USE UMIAH_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    N
      PARAMETER  (N=2)
!
      INTEGER    IPARAM(7), L, NOUT
      REAL       F, FSCALE, RPARAM(7), X(N), &
                XGUESS(N), XSCALE(N)
      EXTERNAL   ROSBRK, ROSGRD, ROSHES
!
```

```
      DATA XGUESS/-1.2E0, 1.0E0/, XSCALE/1.0E0, 1.0E0/, FSCALE/1.0E0/
!
      IPARAM(1) = 0
!                                Minimize Rosenbrock function using
!                                initial guesses of -1.2 and 1.0
      CALL UMIAH (ROSBRK, ROSGRD, ROSHES, X, XGUESS=XGUESS, IPARAM=IPARAM, &
         FVALUE=F)
!                                Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) X, F, (IPARAM(L),L=3,5), IPARAM(7)
!
99999 FORMAT ('  The solution is ', 6X, 2F8.3, //, '  The function ', &
            'value is ', F8.3, //, '  The number of iterations is ', &
            10X, I3, /, '  The number of function evaluations is ', &
            I3, /, '  The number of gradient evaluations is ', I3, /, &
            '  The number of Hessian evaluations is  ', I3)
!
      END
!
      SUBROUTINE ROSBRK (N, X, F)
      INTEGER    N
      REAL       X(N), F
!
      F = 1.0E2*(X(2)-X(1)*X(1))**2 + (1.0E0-X(1))**2
!
      RETURN
      END
!
      SUBROUTINE ROSGRD (N, X, G)
      INTEGER    N
      REAL       X(N), G(N)
!
      G(1) = -4.0E2*(X(2)-X(1)*X(1))*X(1) - 2.0E0*(1.0E0-X(1))
      G(2) = 2.0E2*(X(2)-X(1)*X(1))
!
      RETURN
      END
!
      SUBROUTINE ROSHES (N, X, H, LDH)
      INTEGER    N, LDH
      REAL       X(N), H(LDH,N)
!
      H(1,1) = -4.0E2*X(2) + 1.2E3*X(1)*X(1) + 2.0E0
      H(2,1) = -4.0E2*X(1)
      H(1,2) = H(2,1)
      H(2,2) = 2.0E2
!
      RETURN
      END
```

Output

```
The solution is          1.000   1.000

The function value is    0.000

The number of iterations is             21
The number of function evaluations is   31
The number of gradient evaluations is   22
The number of Hessian evaluations is    21
```

UMCGF

Minimizes a function of `N` variables using a conjugate gradient algorithm and a finite-difference gradient.

Required Arguments

FCN — User-supplied subroutine to evaluate the function to be minimized. The usage is `CALL FCN (N, X, F)`, where

`N` – Length of `X`. (Input)

`X` – The point at which the function is evaluated. (Input) `X` should not be changed by `FCN`.

`F` – The computed function value at the point `X`. (Output)

`FCN` must be declared `EXTERNAL` in the calling program.

DFPRED — A rough estimate of the expected reduction in the function. (Input)
`DFPRED` is used to determine the size of the initial change to `X`.

X — Vector of length `N` containing the computed solution. (Output)

Optional Arguments

N — Dimension of the problem. (Input)
Default: `N` = `SIZE` (X,1).

XGUESS — Vector of length `N` containing the initial guess of the minimum. (Input)
Default: `XGUESS` = 0.0.

XSCALE — Vector of length `N` containing the diagonal scaling matrix for the variables. (Input)
Default: `XSCALE` = 1.0.

GRADTL — Convergence criterion. (Input)
The calculation ends when the sum of squares of the components of `G` is less than `GRADTL`.
Default: `GRADTL` = 1.e-4.

MAXFN — Maximum number of function evaluations. (Input)
If `MAXFN` is set to zero, then no restriction on the number of function evaluations is set.
Default: `MAXFN` = 0.

G — Vector of length `N` containing the components of the gradient at the final parameter estimates. (Output)

FVALUE — Scalar containing the value of the function at the computed solution. (Output)

FORTRAN 90 Interface

Generic: CALL UMCGF (FCN, DFPRED, X [, …])

Specific: The specific interface names are S_UMCGF and D_UMCGF.

FORTRAN 77 Interface

Single: CALL UMCGF (FCN, N, XGUESS, XSCALE, GRADTL, MAXFN, DFPRED, X, G, FVALUE)

Double: The double precision name is DUMCGF.

Description

The routine UMCGF uses a conjugate gradient method to find the minimum of a function $f(x)$ of n variables. Only function values are required.

The routine is based on the version of the conjugate gradient algorithm described in Powell (1977). The main advantage of the conjugate gradient technique is that it provides a fast rate of convergence without the storage of any matrices. Therefore, it is particularly suitable for unconstrained minimization calculations where the number of variables is so large that matrices of dimension n cannot be stored in the main memory of the computer. For smaller problems, however, a routine such as routine UMINF, is usually more efficient because each iteration makes use of additional information from previous iterations.

Since a finite-difference method is used to estimate the gradient for some single precision calculations, an inaccurate estimate of the gradient may cause the algorithm to terminate at a noncritical point. In such cases, high precision arithmetic is recommended. Also, whenever the exact gradient can be easily provided, routine UMCGG should be used instead.

Comments

1. Workspace may be explicitly provided, if desired, by use of U2CGF/DU2CGF. The reference is:

```
CALL U2CGF (FCN, N, XGUESS, XSCALE, GRADTL, MAXFN, DFPRED,
   X, G, FVALUE, S, RSS, RSG, GINIT, XOPT, GOPT)
```

The additional arguments are as follows:

S — Vector of length N used for the search direction in each iteration.

RSS — Vector of length N containing conjugacy information.

RSG — Vector of length N containing conjugacy information.

GINIT — Vector of length N containing the gradient values at the start of an iteration.

XOPT — Vector of length `N` containing the parameter values that yield the least calculated value for `FVALUE`.

GOPT — Vector of length `N` containing the gradient values that yield the least calculated value for `FVALUE`.

2. Informational errors

Type	Code	Description
4	1	The line search of an integration was abandoned. This error may be caused by an error in gradient.
4	2	The calculation cannot continue because the search is uphill.
4	3	The iteration was terminated because `MAXFN` was exceeded.
3	4	The calculation was terminated because two consecutive iterations failed to reduce the function.

3. Because of the close relation between the conjugate-gradient method and the method of steepest descent, it is very helpful to choose the scale of the variables in a way that balances the magnitudes of the components of a typical gradient vector. It can be particularly inefficient if a few components of the gradient are much larger than the rest.

4. If the value of the parameter `GRADTL` in the argument list of the routine is set to zero, then the subroutine will continue its calculation until it stops reducing the objective function. In this case, the usual behavior is that changes in the objective function become dominated by computer rounding errors before precision is lost in the gradient vector. Therefore, because the point of view has been taken that the user requires the least possible value of the function, a value of the objective function that is small due to computer rounding errors can prevent further progress. Hence, the precision in the final values of the variables may be only about half the number of significant digits in the computer arithmetic, but the least value of `FVALUE` is usually found to be quite accurate.

Example

The function

$$f(x) = 100\left(x_2 - x_1^2\right)^2 + \left(1 - x_1\right)^2$$

is minimized and the solution is printed.

```
      USE UMCGF_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                  Declaration of variables
      INTEGER    N
      PARAMETER  (N=2)
!
```

```
      INTEGER    I, MAXFN, NOUT
      REAL       DFPRED, FVALUE, G(N), GRADTL, X(N), XGUESS(N)
      EXTERNAL   ROSBRK
!
      DATA XGUESS/-1.2E0, 1.0E0/
!
      DFPRED = 0.2
      GRADTL = 1.0E-6
      MAXFN  = 100
!                                 Minimize the Rosenbrock function
      CALL UMCGF (ROSBRK, DFPRED, X, xguess=xguess, gradtl=gradtl, &
                 g=g, fvalue=fvalue)
!                                 Print the results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) (X(I),I=1,N), FVALUE, (G(I),I=1,N)
99999 FORMAT ('  The solution is ', 2F8.3, //, '  The function ', &
            'evaluated at the solution is ', F8.3, //, '  The ', &
            'gradient is ', 2F8.3, /)
!
      END
!
      SUBROUTINE ROSBRK (N, X, F)
      INTEGER    N
      REAL       X(N), F
!
      F = 1.0E2*(X(2)-X(1)*X(1))**2 + (1.0E0-X(1))**2
      RETURN
      END
```

Output

```
The solution is    0.999   0.998

The function evaluated at the solution is    0.000

The gradient is   -0.001   0.000
```

UMCGG

Minimizes a function of N variables using a conjugate gradient algorithm and a user-supplied gradient.

Required Arguments

FCN — User-supplied subroutine to evaluate the function to be minimized. The usage is
CALL FCN (N, X, F), where

N – Length of X. (Input)

X – The point at which the function is evaluated. (Input)
X should not be changed by FCN.

F – The computed function value at the point X. (Output)

FCN must be declared EXTERNAL in the calling program.

GRAD — User-supplied subroutine to compute the gradient at the point X. The usage is
CALL GRAD (N, X, G), where

N – Length of X and G. (Input)

X – The point at which the gradient is evaluated. (Input)
X should not be changed by GRAD.

G – The gradient evaluated at the point X. (Output)

GRAD must be declared EXTERNAL in the calling program.

DFPRED — A rough estimate of the expected reduction in the function. (Input)
DFPRED is used to determine the size of the initial change to X.

X — Vector of length N containing the computed solution. (Output)

Optional Arguments

N — Dimension of the problem. (Input)
Default: N = SIZE (X,1).

XGUESS — Vector of length N containing the initial guess of the minimum. (Input)
Default: XGUESS = 0.0.

GRADTL — Convergence criterion. (Input)
The calculation ends when the sum of squares of the components of G is less than GRADTL.
Default: GRADTL = 1.e-4.

MAXFN — Maximum number of function evaluations. (Input)
Default: MAXFN = 100.

G — Vector of length N containing the components of the gradient at the final parameter estimates. (Output)

FVALUE — Scalar containing the value of the function at the computed solution. (Output)

FORTRAN 90 Interface

Generic: CALL UMCGG (FCN, GRAD, DFPRED, X [, …])

Specific: The specific interface names are S_UMCGG and D_UMCGG.

FORTRAN 77 Interface

Single: CALL UMCGG (FCN, GRAD, N, XGUESS, GRADTL, MAXFN, DFPRED, X, G, FVALUE)

Double: The double precision name is DUMCGG.

Description

The routine UMCGG uses a conjugate gradient method to find the minimum of a function $f(x)$ of n variables. Function values and first derivatives are required.

The routine is based on the version of the conjugate gradient algorithm described in Powell (1977). The main advantage of the conjugate gradient technique is that it provides a fast rate of convergence without the storage of any matrices. Therefore, it is particularly suitable for unconstrained minimization calculations where the number of variables is so large that matrices of dimension n cannot be stored in the main memory of the computer. For smaller problems, however, a subroutine such as IMSL routine UMING, is usually more efficient because each iteration makes use of additional information from previous iterations.

Comments

1. Workspace may be explicitly provided, if desired, by use of U2CGG/DU2CGG. The reference is:

```
CALL U2CGG (FCN, GRAD, N, XGUESS, GRADTL, MAXFN, DFPRED, X,
   G, FVALUE, S, RSS, RSG, GINIT, XOPT, GOPT)
```

The additional arguments are as follows:

S — Vector of length N used for the search direction in each iteration.

RSS — Vector of length N containing conjugacy information.

RSG — Vector of length N containing conjugacy information.

GINIT — Vector of length N containing the gradient values at the start on an iteration.

XOPT — Vector of length N containing the parameter values which yield the least calculated value for FVALUE.

GOPT — Vector of length N containing the gradient values which yield the least calculated value for FVALUE.

2. Informational errors

Type	Code	Description
4	1	The line search of an integration was abandoned. This error may be caused by an error in gradient.
4	2	The calculation cannot continue because the search is uphill.
4	3	The iteration was terminated because MAXFN was exceeded.
3	4	The calculation was terminated because two consecutive iterations failed to reduce the function.

3. The routine includes no thorough checks on the part of the user program that calculates the derivatives of the objective function. Therefore, because derivative calculation is a frequent source of error, the user should verify independently the correctness of the derivatives that are given to the routine.

4. Because of the close relation between the conjugate-gradient method and the method of steepest descent, it is very helpful to choose the scale of the variables in a way that balances the magnitudes of the components of a typical gradient vector. It can be particularly inefficient if a few components of the gradient are much larger than the rest.

5. If the value of the parameter GRADTL in the argument list of the routine is set to zero, then the subroutine will continue its calculation until it stops reducing the objective function. In this case, the usual behavior is that changes in the objective function become dominated by computer rounding errors before precision is lost in the gradient vector. Therefore, because the point of view has been taken that the user requires the least possible value of the function, a value of the objective function that is small due to computer rounding errors can prevent further progress. Hence, the precision in the final values of the variables may be only about half the number of significant digits in the computer arithmetic, but the least value of FVALUE is usually found to be quite accurate.

Example

The function

$$f(x) = 100\left(x_2 - x_1^2\right)^2 + \left(1 - x_1\right)^2$$

is minimized and the solution is printed.

```
      USE UMCGG_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                  Declaration of variables
      INTEGER    N
      PARAMETER  (N=2)
!
      INTEGER    I, NOUT
      REAL       DFPRED, FVALUE, G(N), GRADTL, X(N), &
                XGUESS(N)
      EXTERNAL   ROSBRK, ROSGRD
!
      DATA XGUESS/-1.2E0, 1.0E0/
!
      DFPRED = 0.2
      GRADTL = 1.0E-7
!                                  Minimize the Rosenbrock function
      CALL UMCGG (ROSBRK, ROSGRD, DFPRED, X, xguess=xguess, &
                 gradtl=gradtl, g=g, fvalue=fvalue)
!                                  Print the results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) (X(I),I=1,N), FVALUE, (G(I),I=1,N)
99999 FORMAT ('  The solution is ', 2F8.3, //, '  The function ', &
            'evaluated at the solution is ', F8.3, //, '  The ', &
            'gradient is ', 2F8.3, /)
!
      END
!
      SUBROUTINE ROSBRK (N, X, F)
      INTEGER    N
      REAL       X(N), F
!
      F = 1.0E2*(X(2)-X(1)*X(1))**2 + (1.0E0-X(1))**2
      RETURN
      END
!
      SUBROUTINE ROSGRD (N, X, G)
      INTEGER    N
      REAL       X(N), G(N)
!
      G(1) = -4.0E2*(X(2)-X(1)*X(1))*X(1) - 2.0E0*(1.0E0-X(1))
      G(2) = 2.0E2*(X(2)-X(1)*X(1))
!
      RETURN
      END
```

Output

```
  The solution is    1.000   1.000

  The function evaluated at the solution is    0.000

  The gradient is    0.000  -0.000
```

UMPOL

Minimizes a function of N variables using a direct search polytope algorithm.

Required Arguments

FCN — User-supplied subroutine to evaluate the function to be minimized. The usage is
CALL FCN (N, X, F), where

N – Length of X. (Input)

X – Vector of length N at which point the function is evaluated. (Input)
X should not be changed by FCN.

F – The computed function value at the point X. (Output)

FCN must be declared EXTERNAL in the calling program.

X — Real vector of length N containing the best estimate of the minimum found. (Output)

Optional Arguments

N — Dimension of the problem. (Input)
Default: N = SIZE (X,1).

XGUESS — Real vector of length N which contains an initial guess to the minimum. (Input)
Default: XGUESS = 0.0.

S — On input, real scalar containing the length of each side of the initial simplex. (Input/Output)
If no reasonable information about S is known, S could be set to a number less than or equal to zero and UMPOL will generate the starting simplex from the initial guess with a random number generator. On output, the average distance from the vertices to the centroid that is taken to be the solution; see Comment 4.
Default: S = 0.0.

FTOL — First convergence criterion. (Input)
The algorithm stops when a relative error in the function values is less than FTOL, i.e. when (F(worst) − F(best)) < FTOL * (1 + ABS(F(best))) where F(worst) and F(best) are the function values of the current worst and best points, respectively. Second convergence criterion. The algorithm stops when the standard deviation of the function values at the N + 1 current points is less than FTOL. If the subroutine terminates prematurely, try again with a smaller value for FTOL.
Default: FTOL = 1.e-7.

MAXFCN — On input, maximum allowed number of function evaluations. (Input/ Output)
On output, actual number of function evaluations needed.
Default: `MAXFCN` = 200.

FVALUE — Function value at the computed solution. (Output)

FORTRAN 90 Interface

Generic: `CALL UMPOL (FCN, X [, …])`

Specific: The specific interface names are `S_UMPOL` and `D_UMPOL`.

FORTRAN 77 Interface

Single: `CALL UMPOL (FCN, N, XGUESS, S, FTOL, MAXFCN, X, FVALUE)`

Double: The double precision name is `DUMPOL`.

Description

The routine `UMPOL` uses the polytope algorithm to find a minimum point of a function $f(x)$ of n variables. The polytope method is based on function comparison; no smoothness is assumed. It starts with $n + 1$ points x_1, x_2, …, x_{n+1}. At each iteration, a new point is generated to replace the worst point x_j, which has the largest function value among these $n + 1$ points. The new point is constructed by the following formula:

$$x_k = c + \alpha(c - x_j)$$

where

$$c = \frac{1}{n}\sum_{i \neq j} x_i$$

and $\alpha(\alpha > 0)$ is the *reflection coefficient*.

When x_k is a best point, that is $f(x_k) \le f(x_i)$ for $i = 1, …, n + 1$, an expansion point is computed $x_e = c + \beta(x_k - c)$ where $\beta(\beta > 1)$ is called the *expansion coefficient*. If the new point is a worst point, then the polytope would be contracted to get a better new point. If the contraction step is unsuccessful, the polytope is shrunk by moving the vertices halfway toward current best point. This procedure is repeated until one of the following stopping criteria is satisfied:

Criterion 1:

$$f_{best} - f_{worst} \le \varepsilon_f(1. + |f_{best}|)$$

Criterion 2:

$$\sum_{i=1}^{n+1}\left(f_i - \frac{\sum_{j=1}^{n+1} f_j}{n+1}\right)^2 \le \varepsilon_f$$

where $f_i = f(x_i)$, $f_j = f(x_j)$, and ε_f is a given tolerance. For a complete description, see Nelder and Mead (1965) or Gill et al. (1981).

Comments

1. Workspace may be explicitly provided, if desired, by use of U2POL/DU2POL. The reference is:

   CALL U2POL (FCN, N, XGUESS, S, FTOL, MAXFCN, X, FVALUE, WK)

   The additional argument is:

   WK — Real work vector of length N**2 + 5 * N + 1.

2. Informational error

Type	Code	Description
4	1	Maximum number of function evaluations exceeded.

3. Since UMPOL uses only function value information at each step to determine a new approximate minimum, it could be quite inefficient on smooth problems compared to other methods such as those implemented in routine UMINF that takes into account derivative information at each iteration. Hence, routine UMPOL should only be used as a last resort. Briefly, a set of N + 1 points in an N-dimensional space is called a simplex. The minimization process iterates by replacing the point with the largest function value by a new point with a smaller function value. The iteration continues until all the points cluster sufficiently close to a minimum.

4. The value returned in ***S*** is useful for assessing the flatness of the function near the computed minimum. The larger its value for a given value of FTOL, the flatter the function tends to be in the neighborhood of the returned point.

Example

The function

$$f(x) = 100\left(x_2 - x_1^2\right)^2 + \left(1 - x_1\right)^2$$

is minimized and the solution is printed.

```
      USE UMPOL_INT
      USE UMACH_INT
```

```
      IMPLICIT   NONE
!                                  Variable declarations
      INTEGER    N
      PARAMETER  (N=2)
!
      INTEGER    K, NOUT
      REAL       FTOL, FVALUE, S, X(N), XGUESS(N)
      EXTERNAL   FCN
!
!                                  Initializations
!                                  XGUESS = ( -1.2, 1.0)
!
      DATA XGUESS/-1.2, 1.0/
!
      FTOL   = 1.0E-10
      S      = 1.0
!
      CALL UMPOL (FCN, X, xguess=xguess, s=s, ftol=ftol,&
                  fvalue=fvalue)
!
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) (X(K),K=1,N), FVALUE
99999 FORMAT ('  The best estimate for the minimum value of the', /, &
            '  function is X = (', 2(2X,F4.2), ')', /, '  with ', &
            'function value FVALUE = ', E12.6)
!
      END
!                                  External function to be minimized
      SUBROUTINE FCN (N, X, F)
      INTEGER    N
      REAL       X(N), F
!
      F = 100.0*(X(1)*X(1)-X(2))**2 + (1.0-X(1))**2
      RETURN
      END
```

Output

```
    The best estimate for the minimum value of the
    function is X = (  1.00  1.00)
    with function value FVALUE = 0.502496E-10
```

UNLSF

more...

Solves a nonlinear least-squares problem using a modified Levenberg-Marquardt algorithm and a finite-difference Jacobian.

Required Arguments

FCN — User-supplied subroutine to evaluate the function that defines the least-squares problem. The usage is
CALL FCN (M, N, X, F), where

M – Length of F. (Input)

N – Length of X. (Input)

X – Vector of length N at which point the function is evaluated. (Input)
X should not be changed by FCN.

F – Vector of length M containing the function values at X. (Output)

FCN must be declared EXTERNAL in the calling program.

M — Number of functions. (Input)

X — Vector of length N containing the approximate solution. (Output)

Optional Arguments

N — Number of variables. N must be less than or equal to M. (Input)
Default: N = SIZE (X,1).

XGUESS — Vector of length N containing the initial guess. (Input)
Default: XGUESS = 0.0.

XSCALE — Vector of length `N` containing the diagonal scaling matrix for the variables. (Input)
`XSCALE` is used mainly in scaling the gradient and the distance between two points. By default, the values for `XSCALE` are set internally. See `IPARAM`(6) in Comment 4.
Default: `XSCALE` = 1.0.

FSCALE — Vector of length `M` containing the diagonal scaling matrix for the functions. (Input)
`FSCALE` is used mainly in scaling the gradient. In the absence of other information, set all entries to 1.0.
Default: `FSCALE` = 1.0.

IPARAM — Parameter vector of length 6. (Input/Output)
Set `IPARAM`(1) to zero for default values of `IPARAM` and `RPARAM`. See Comment 4.
Default: `IPARAM` = 0.

RPARAM — Parameter vector of length 7. (Input/Output)
See Comment 4.

FVEC — Vector of length `M` containing the residuals at the approximate solution. (Output)

FJAC — `M` by `N` matrix containing a finite difference approximate Jacobian at the approximate solution. (Output)

LDFJAC — Leading dimension of `FJAC` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDFJAC` = `SIZE` (`FJAC`,1).

FORTRAN 90 Interface

Generic: `CALL UNLSF` (`FCN`, `M`, `X` [, …])

Specific: The specific interface names are `S_UNLSF` and `D_UNLSF`.

FORTRAN 77 Interface

Single: `CALL UNLSF` (`FCN`, `M`, `N`, `XGUESS`, `XSCALE`, `FSCALE`, `IPARAM`, `RPARAM`, `X`, `FVEC`, `FJAC`, `LDFJAC`)

Double: The double precision name is `DUNLSF`.

Description

The routine `UNLSF` is based on the MINPACK routine `LMDIF` by Moré et al. (1980). It uses a modified Levenberg-Marquardt method to solve nonlinear least squares problems. The problem is stated as follows:

$$\min_{x \in \mathbb{R}^n} \frac{1}{2} F(x)^T F(x) = \frac{1}{2} \sum_{i=1}^{m} f_i(x)^2$$

where $m \geq n$, $F : \mathbf{R}^n \to \mathbf{R}^m$, and $f_i(x)$ is the i-th component function of $F(x)$. From a current point, the algorithm uses the trust region approach:

$$\min_{x_n \in \mathbb{R}^n} \left\| F(x_c) + J(x_c)(x_n - x_c) \right\|_2$$

$$\text{subject to } \|x_n - x_c\|_2 \leq \delta_c$$

to get a new point x_n, which is computed as

$$x_n = x_c - \left(J(x_c)^T J(x_c) + \mu_c I \right)^{-1} J(x_c)^T F(x_c)$$

where $\mu_c = 0$ if $\delta_c \geq \|(J(x_c)^T J(x_c))^{-1} J(x_c)^T F(x_c)\|_2$ and $\mu_c > 0$ otherwise. $F(x_c)$ and $J(x_c)$ are the function values and the Jacobian evaluated at the current point x_c. This procedure is repeated until the stopping criteria are satisfied. For more details, see Levenberg (1944), Marquardt (1963), or Dennis and Schnabel (1983, Chapter 10).

Since a finite-difference method is used to estimate the Jacobian for some single precision calculations, an inaccurate estimate of the Jacobian may cause the algorithm to terminate at a noncritical point. In such cases, high precision arithmetic is recommended. Also, whenever the exact Jacobian can be easily provided, routine `UNLSJ` should be used instead.

Comments

1. Workspace may be explicitly provided, if desired, by use of `U2LSF/DU2LSF`. The reference is:

```
CALL U2LSF (FCN, M, N, XGUESS, XSCALE, FSCALE, IPARAM,
   RPARAM, X, FVEC, FJAC, LDFJAC, WK, IWK)
```

   The additional arguments are as follows:

   WK — Real work vector of length 9 * `N` + 3 * `M` – 1. `WK` contains the following information on output: The second `N` locations contain the last step taken. The third `N` locations contain the last Gauss-Newton step. The fourth `N` locations contain an estimate of the gradient at the solution.

   IWK — Integer work vector of length `N` containing the permutations used in the `QR` factorization of the Jacobian at the solution.

2. Informational errors

Type	Code	Description
3	1	Both the actual and predicted relative reductions in the function are less than or equal to the relative function convergence tolerance.
3	2	The iterates appear to be converging to a noncritical point.
4	3	Maximum number of iterations exceeded.
4	4	Maximum number of function evaluations exceeded.
3	6	Five consecutive steps have been taken with the maximum step length.
2	7	Scaled step tolerance satisfied; the current point may be an approximate local solution, or the algorithm is making very slow progress and is not near a solution, or STEPTL is too big.

3. The first stopping criterion for UNLSF occurs when the norm of the function is less than the absolute function tolerance (RPARAM(4)). The second stopping criterion occurs when the norm of the scaled gradient is less than the given gradient tolerance (RPARAM(1)). The third stopping criterion for UNLSF occurs when the scaled distance between the last two steps is less than the step tolerance (RPARAM(2)).

4. If the default parameters are desired for UNLSF, then set IPARAM(1) to zero and call the routine UNLSF. Otherwise, if any nondefault parameters are desired for IPARAM or RPARAM, then the following steps should be taken before calling UNLSF:

   CALL U4LSF (IPARAM, RPARAM)

   Set nondefault values for desired IPARAM, RPARAM elements.

Note that the call to U4LSF will set IPARAM and RPARAM to their default values so only nondefault values need to be set above.

The following is a list of the parameters and the default values:

IPARAM — Integer vector of length 6.

IPARAM(1) = Initialization flag.

IPARAM(2) = Number of good digits in the function.
Default: Machine dependent.

IPARAM(3) = Maximum number of iterations.
Default: 100.

IPARAM(4) = Maximum number of function evaluations.
Default: 400.

IPARAM(5) = Maximum number of Jacobian evaluations.
Default: Not used in UNLSF.

IPARAM(6) = Internal variable scaling flag.
If IPARAM(6) = 1, then the values for XSCALE are set internally.
Default: 1.

RPARAM — Real vector of length 7.

RPARAM(1) = Scaled gradient tolerance.

The *i*-th component of the scaled gradient at x is calculated as

$$\frac{|g_i| * \max\left(|x_i|, 1/s_i \right)}{\| F(x) \|_2^2}$$

where

$$g_i = \left(J(x)^T F(x) \right)_i * \left(f_s \right)_i^2$$

$J(x)$ is the Jacobian, s = XSCALE, and f_s = FSCALE.

Default:

$$\sqrt{\varepsilon}, \sqrt[3]{\varepsilon}$$

in double where **ε** is the machine precision.

RPARAM(2) = Scaled step tolerance. (STEPTL)

The *i*-th component of the scaled step between two points *x* and *y* is computed as

$$\frac{|x_i - y_i|}{\max\left(|x_i|, 1/s_i \right)}$$

where s = XSCALE.

Default: $\varepsilon^{2/3}$ where **ε** is the machine precision.

RPARAM(3) = Relative function tolerance.

Default: $\max(10^{-10}, \varepsilon^{2/3})$, $\max(10^{-20}, \varepsilon^{2/3})$ in double where **ε** is the machine precision.

RPARAM(4) = Absolute function tolerance.

Default: $\max(10^{-20}, \varepsilon^2)$, $\max(10^{-40}, \varepsilon^2)$ in double where **ε** is the machine precision.

RPARAM(5) = False convergence tolerance.

Default: 100**ε** where **ε** is the machine precision.

RPARAM(6) = Maximum allowable step size.

Default: $1000 \max(\varepsilon_1, \varepsilon_2)$ where

$$\varepsilon_1 = \sqrt{\sum_{i=1}^{n} \left(s_i t_i \right)^2}$$

$\varepsilon_2 = \|s\|_2$, s = XSCALE, and t = XGUESS.

RPARAM(7) = Size of initial trust region radius.

Default: based on the initial scaled Cauchy step.

If double precision is desired, then DU4LSF is called and RPARAM is declared double precision.

5. Users wishing to override the default print/stop attributes associated with error messages issued by this routine are referred to "*Error Handling*" in the Introduction.

Example

The nonlinear least squares problem

$$\min_{x \in \mathbb{R}^2} \frac{1}{2} \sum_{i=1}^{2} f_i(x)^2$$

where

$$f_1(x) = 10\left(x_2 - x_1^2\right) \text{ and } f_2(x) = \left(1 - x_1\right)$$

is solved. `RPARAM`(4) is changed to a non-default value.

```
      USE UMACH_INT
      USE U4LSF_INT
      USE UNLSF_INT

      IMPLICIT   NONE
!                                 Declaration of variables
      INTEGER    LDFJAC, M, N
      PARAMETER  (LDFJAC=2, M=2, N=2)
!
      INTEGER    IPARAM(6), NOUT
      REAL       FVEC(M), RPARAM(7),X(N), XGUESS(N)
      EXTERNAL   ROSBCK
!                                 Compute the least squares for the
!                                 Rosenbrock function.
      DATA XGUESS/-1.2E0, 1.0E0/
!
!                                 Relax the first stopping criterion by
!                                 calling U4LSF and scaling the
!                                 absolute function tolerance by 10.
      CALL U4LSF (IPARAM, RPARAM)
      RPARAM(4) = 10.0E0*RPARAM(4)
!
      CALL UNLSF (ROSBCK, M, X,xguess=xguess, iparam=iparam, rparam=rparam,&
       fvec=fvec)
!                                 Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) X, FVEC, IPARAM(3), IPARAM(4)
!
99999 FORMAT ('  The solution is ', 2F9.4, //, '  The function ', &
            'evaluated at the solution is ', /, 18X, 2F9.4, //, &
            '  The number of iterations is ', 10X, I3, /, '  The ', &
            'number of function evaluations is ', I3, /)
      END
!
      SUBROUTINE ROSBCK (M, N, X, F)
      INTEGER    M, N
      REAL       X(N), F(M)
!
      F(1) = 10.0E0*(X(2)-X(1)*X(1))
      F(2) = 1.0E0 - X(1)
```

```
      RETURN
      END
```

Output

```
The solution is    1.0000   1.0000

The function evaluated at the solution is
0.0000   0.0000

The number of iterations is            24
The number of function evaluations is  33
```

UNLSJ

more...

Solves a nonlinear least squares problem using a modified Levenberg-Marquardt algorithm and a user-supplied Jacobian.

Required Arguments

FCN — User-supplied subroutine to evaluate the function which defines the least-squares problem. The usage is
`CALL FCN (M, N, X, F)`, where

`M` – Length of F. (Input)

`N` – Length of X. (Input)

`X` – Vector of length N at which point the function is evaluated. (Input)
`X` should not be changed by `FCN`.

`F` – Vector of length M containing the function values at X. (Output)

`FCN` must be declared `EXTERNAL` in the calling program.

JAC — User-supplied subroutine to evaluate the Jacobian at a point `X`. The usage is
`CALL JAC (M, N, X, FJAC, LDFJAC)`, where

`M` – Length of F. (Input)

`N` – Length of X. (Input)

`X` – Vector of length N at which point the Jacobian is evaluated. (Input)
`X` should not be changed by JAC.

`FJAC` – The computed M by N Jacobian at the point X. (Output)

`LDFJAC` – Leading dimension of `FJAC`. (Input)

`JAC` must be declared `EXTERNAL` in the calling program.

M — Number of functions. (Input)

X — Vector of length `N` containing the approximate solution. (Output)

Optional Arguments

N — Number of variables. N must be less than or equal to M. (Input)
Default: N = SIZE (X,1).

XGUESS — Vector of length N containing the initial guess. (Input)
Default: XGUESS = 0.0.

XSCALE — Vector of length N containing the diagonal scaling matrix for the variables. (Input)
XSCALE is used mainly in scaling the gradient and the distance between two points. By default, the values for XSCALE are set internally. See IPARAM(6) in Comment 4.
Default: XSCALE = 1.0.

FSCALE — Vector of length M containing the diagonal scaling matrix for the functions. (Input)
FSCALE is used mainly in scaling the gradient. In the absence of other information, set all entries to 1.0.
Default: FSCALE = 1.0.

IPARAM — Parameter vector of length 6. (Input/Output)
Set IPARAM(1) to zero for default values of IPARAM and RPARAM. See Comment 4.
Default: IPARAM = 0.

RPARAM — Parameter vector of length 7. (Input/Output)
See Comment 4.

FVEC — Vector of length M containing the residuals at the approximate solution. (Output)

FJAC — M by N matrix containing a finite-difference approximate Jacobian at the approximate solution. (Output)

LDFJAC — Leading dimension of FJAC exactly as specified in the dimension statement of the calling program. (Input)
Default: LDFJAC = SIZE (FJAC,1).

FORTRAN 90 Interface

Generic: CALL UNLSJ (FCN, JAC, M, X [, …])

Specific: The specific interface names are S_UNLSJ and D_UNLSJ.

FORTRAN 77 Interface

Single: CALL UNLSJ (FCN, JAC, M, N, XGUESS, XSCALE, FSCALE, IPARAM, RPARAM, X, FVEC, FJAC, LDFJAC)

Double: The double precision name is DUNLSJ.

Description

The routine UNLSJ is based on the MINPACK routine LMDER by Moré et al. (1980). It uses a modified Levenberg-Marquardt method to solve nonlinear least squares problems. The problem is stated as follows:

$$\min_{x \in \mathbf{R}^n} \frac{1}{2} F(x)^T F(x) = \frac{1}{2} \sum_{i=1}^{m} f_i(x)^2$$

where $m \geq n$, $F : \mathbf{R}^n \rightarrow \mathbf{R}^m$, and $f_i(x)$ is the i-th component function of $F(x)$. From a current point, the algorithm uses the trust region approach:

$$\min_{x_n \in \mathbf{R}^n} \left\| F(x_c) + J(x_c)(x_n - x_c) \right\|_2$$

$$\text{subject to } \|x_n - x_c\|_2 \leq \delta_c$$

to get a new point x_n, which is computed as

$$x_n = x_c - \left(J(x_c)^T J(x_c) + \mu_c I \right)^{-1} J(x_c)^T F(x_c)$$

where

$$\mu_c = 0 \text{ if } \delta_c \geq \left\| \left(J(x_c)^T J(x_c) \right)^{-1} J(x_c)^T F(x_c) \right\|_2$$

and $\mu_c > 0$ otherwise. $F(x_c)$ and $J(x_c)$ are the function values and the Jacobian evaluated at the current point x_c. This procedure is repeated until the stopping criteria are satisfied. For more details, see Levenberg (1944), Marquardt(1963), or Dennis and Schnabel (1983, Chapter 10).

Comments

1. Workspace may be explicitly provided, if desired, by use of U2LSJ/DU2LSJ. The reference is:

```
CALL U2LSJ (FCN, JAC, M, N, XGUESS, XSCALE, FSCALE, IPARAM,
   RPARAM, X, FVEC, FJAC, LDFJAC, WK, IWK)
```

   The additional arguments are as follows:

   WK — Work vector of length 9 * N + 3 * M − 1. WK contains the following information on output: The second N locations contain the last step taken. The third N locations contain the last Gauss-Newton step. The fourth N locations contain an estimate of the gradient at the solution.

   IWK — Work vector of length N containing the permutations used in the QR factorization of the Jacobian at the solution.

2. Informational errors

Type	Code	Description
3	1	Both the actual and predicted relative reductions in the function are less than or equal to the relative function convergence tolerance.
3	2	The iterates appear to be converging to a noncritical point.
4	3	Maximum number of iterations exceeded.
4	4	Maximum number of function evaluations exceeded.
4	5	Maximum number of Jacobian evaluations exceeded.
3	6	Five consecutive steps have been taken with the maximum step length.
2	7	Scaled step tolerance satisfied; the current point may be an approximate local solution, or the algorithm is making very slow progress and is not near a solution, or STEPTL is too big.

3. The first stopping criterion for UNLSJ occurs when the norm of the function is less than the absolute function tolerance (RPARAM(4)). The second stopping criterion occurs when the norm of the scaled gradient is less than the given gradient tolerance (RPARAM(1)). The third stopping criterion for UNLSJ occurs when the scaled distance between the last two steps is less than the step tolerance (RPARAM(2)).

4. If the default parameters are desired for UNLSJ, then set IPARAM(1) to zero and call the routine UNLSJ. Otherwise, if any nondefault parameters are desired for IPARAM or RPARAM, then the following steps should be taken before calling UNLSJ:

   CALL U4LSF (IPARAM, RPARAM)

   Set nondefault values for desired IPARAM, RPARAM elements.

Note that the call to U4LSF will set IPARAM and RPARAM to their default values, so only nondefault values need to be set above.

The following is a list of the parameters and the default values:

IPARAM — Integer vector of length 6.

IPARAM(1) = Initialization flag.

IPARAM(2) = Number of good digits in the function.
Default: Machine dependent.

IPARAM(3) = Maximum number of iterations.
Default: 100.

IPARAM(4) = Maximum number of function evaluations.
Default: 400.

IPARAM(5) = Maximum number of Jacobian evaluations.
Default: 100.

IPARAM(6) = Internal variable scaling flag.

If IPARAM(6) = 1, then the values for XSCALE are set internally.

Default: 1.

RPARAM — Real vector of length 7.

RPARAM(1) = Scaled gradient tolerance.

The *i*-th component of the scaled gradient at x is calculated as

$$\frac{|g_i| * \max\left(|x_i|, 1/s_i\right)}{\|F(x)\|_2^2}$$

where

$$g_i = \left(J(x)^T F(x)\right)_i * \left(f_s\right)_i^2$$

$J(x)$ is the Jacobian, s = XSCALE, and f_s = FSCALE.

Default:

$$\sqrt{\varepsilon}, \sqrt[3]{\varepsilon}$$

in double where **ε** is the machine precision.

RPARAM(2) = Scaled step tolerance. (STEPTL)

The *i*-th component of the scaled step between two points *x* and *y* is computed as

$$\frac{|x_i - y_i|}{\max\left(|x_i|, 1/s_i\right)}$$

where s = XSCALE.

Default: $\varepsilon^{2/3}$ where **ε** is the machine precision.

RPARAM(3) = Relative function tolerance.

Default: $\max(10^{-10}, \varepsilon^{2/3})$, $\max(10^{-20}, \varepsilon^{2/3})$ in double where **ε** is the machine precision.

RPARAM(4) = Absolute function tolerance.

Default: $\max(10^{-20}, \varepsilon^2)$, $\max(10^{-40}, \varepsilon^2)$ in double where **ε** is the machine precision.

RPARAM(5) = False convergence tolerance.

Default: 100ε where **ε** is the machine precision.

RPARAM(6) = Maximum allowable step size.

Default: $1000 \max(\varepsilon_1, \varepsilon_2)$ where

$$\varepsilon_1 = \sqrt{\sum_{i=1}^{n} \left(s_i t_i\right)^2}$$

$\varepsilon_2 = \|s\|_2$, s = XSCALE, and t = XGUESS.

RPARAM(7) = Size of initial trust region radius.
Default: based on the initial scaled Cauchy step.

If double precision is desired, then DU4LSF is called and RPARAM is declared double precision.

5. Users wishing to override the default print/stop attributes associated with error messages issued by this routine are referred to “Error Handling” in the Introduction.

Example

The nonlinear least-squares problem

$$\min_{x \in \mathbf{R}^n} \frac{1}{2} \sum_{i=1}^{2} f_i(x)^2$$

where

$$f_1(x) = 10\left(x_2 - x_1^2\right) \text{ and } f_2(x) = \left(1 - x_1\right)$$

is solved; default values for parameters are used.

```
      USE UNLSJ_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                  Declaration of variables
      INTEGER    LDFJAC, M, N
      PARAMETER  (LDFJAC=2, M=2, N=2)
!
      INTEGER    IPARAM(6), NOUT
      REAL       FVEC(M), X(N), XGUESS(N)
      EXTERNAL   ROSBCK, ROSJAC
!                                  Compute the least squares for the
!                                  Rosenbrock function.
      DATA XGUESS/-1.2E0, 1.0E0/
      IPARAM(1) = 0
!
      CALL UNLSJ (ROSBCK, ROSJAC, M, X, XGUESS=XGUESS, &
                 IPARAM=IPARAM, FVEC=FVEC)
!                                  Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) X, FVEC, IPARAM(3), IPARAM(4), IPARAM(5)
!
99999 FORMAT ('  The solution is ', 2F9.4, //, '  The function ', &
            'evaluated at the solution is ', /, 18X, 2F9.4, //, &
            '  The number of iterations is ', 10X, I3, /, '  The ', &
            'number of function evaluations is ', I3, /, '  The ', &
            'number of Jacobian evaluations is ', I3, /)
      END
!
      SUBROUTINE ROSBCK (M, N, X, F)
      INTEGER    M, N
      REAL       X(N), F(M)
!
      F(1) = 10.0E0*(X(2)-X(1)*X(1))
```

```
      F(2) = 1.0E0 - X(1)
      RETURN
      END
!
      SUBROUTINE ROSJAC (M, N, X, FJAC, LDFJAC)
      INTEGER    M, N, LDFJAC
      REAL       X(N), FJAC(LDFJAC,N)
!
      FJAC(1,1) = -20.0E0*X(1)
      FJAC(2,1) = -1.0E0
      FJAC(1,2) = 10.0E0
      FJAC(2,2) = 0.0E0
      RETURN
      END
```

Output

```
The solution is    1.0000   1.0000

The function evaluated at the solution is
0.0000   0.0000

The number of iterations is            23
The number of function evaluations is  32
The number of Jacobian evaluations is  24
```

BCONF

Minimizes a function of N variables subject to bounds on the variables using a quasi-Newton method and a finite-difference gradient.

Required Arguments

FCN — User-supplied subroutine to evaluate the function to be minimized. The usage is
CALL FCN (N, X, F), where

N – Length of X. (Input)

X – Vector of length N at which point the function is evaluated. (Input)
X should not be changed by FCN.

F – The computed function value at the point X. (Output)

FCN must be declared EXTERNAL in the calling program.

IBTYPE — Scalar indicating the types of bounds on variables. (Input)

IBTYPE	Action
0	User will supply all the bounds.
1	All variables are nonnegative.
2	All variables are nonpositive.
3	User supplies only the bounds on 1st variable, all other variables will have the same bounds.

XLB — Vector of length N containing the lower bounds on variables. (Input, if IBTYPE = 0; output, if IBTYPE = 1 or 2; input/output, if IBTYPE = 3)

XUB — Vector of length N containing the upper bounds on variables. (Input, if IBTYPE = 0; output, if IBTYPE = 1 or 2; input/output, if IBTYPE = 3)

X — Vector of length N containing the computed solution. (Output)

Optional Arguments

N — Dimension of the problem. (Input)
Default: N = SIZE (X,1).

XGUESS — Vector of length N containing an initial guess of the computed solution. (Input)
Default: XGUESS = 0.0.

XSCALE — Vector of length N containing the diagonal scaling matrix for the variables. (Input)
XSCALE is used mainly in scaling the gradient and the distance between two points. In the absence of other information, set all entries to 1.0.
Default: XSCALE = 1.0.

FSCALE — Scalar containing the function scaling. (Input)
FSCALE is used mainly in scaling the gradient. In the absence of other information, set FSCALE to 1.0.
Default: FSCALE = 1.0.

IPARAM — Parameter vector of length 7. (Input/Output)
Set IPARAM(1) to zero for default values of IPARAM and RPARAM. See Comment 4.
Default: IPARAM = 0.

RPARAM — Parameter vector of length 7. (Input/Output)
See Comment 4.

FVALUE — Scalar containing the value of the function at the computed solution. (Output)

FORTRAN 90 Interface

Generic:	CALL BCONF (FCN, IBTYPE, XLB, XUB, X [, …])
Specific:	The specific interface names are S_BCONF and D_BCONF.

FORTRAN 77 Interface

Single:	CALL BCONF (FCN, N, XGUESS, IBTYPE, XLB, XUB, XSCALE, FSCALE, IPARAM, RPARAM, X, FVALUE)
Double:	The double precision name is DBCONF.

Description

The routine BCONF uses a quasi-Newton method and an active set strategy to solve minimization problems subject to simple bounds on the variables. The problem is stated as follows:

$$\min_{x \in \mathbf{R}^n} f(x)$$

$$\text{subject to } l \leq x \leq u$$

From a given starting point x^c, an active set IA, which contains the indices of the variables at their bounds, is built. A variable is called a "free variable" if it is not in the active set. The routine then computes the search direction for the free variables according to the formula

$$d = -B^{-1} g^c$$

where B is a positive definite approximation of the Hessian and g^c is the gradient evaluated at x^c; both are computed with respect to the free variables. The search direction for the variables in IA is set to zero. A line search is used to find a new point x^n,

$$x^n = x^c + \lambda d, \qquad \lambda \in (0, 1]$$

such that

$$f(x^n) \le f(x^c) + \alpha g^T d, \qquad \alpha \in (0, 0.5)$$

Finally, the optimality conditions

$$\|g(x_i)\| \le \varepsilon, \; l_i < x_i < u_i$$

$$g(x_i) < 0, \; x_i = u_i$$

$$g(x_i) > 0, \; x_i = l_i$$

are checked, where ε is a gradient tolerance. When optimality is not achieved, B is updated according to the BFGS formula:

$$B \leftarrow B - \frac{Bss^T B}{s^T Bs} + \frac{yy^T}{y^T s}$$

where $s = x^n - x^c$ and $y = g^n - g^c$. Another search direction is then computed to begin the next iteration.

The active set is changed only when a free variable hits its bounds during an iteration or the optimality condition is met for the free variables but not for all variables in IA, the active set. In the latter case, a variable that violates the optimality condition will be dropped out of IA. For more details on the quasi-Newton method and line search, see Dennis and Schnabel (1983). For more detailed information on active set strategy, see Gill and Murray (1976).

Since a finite-difference method is used to estimate the gradient for some single precision calculations, an inaccurate estimate of the gradient may cause the algorithm to terminate at a noncritical point. In such cases, high precision arithmetic is recommended. Also, whenever the exact gradient can be easily provided, routine BCONG should be used instead.

Comments

1. Workspace may be explicitly provided, if desired, by use of B2ONF/DB2ONF. The reference is:

```
CALL B2ONF (FCN, N, XGUESS, IBTYPE, XLB, XUB, XSCALE,
   FSCALE, IPARAM, RPARAM, X, FVALUE, WK, IWK)
```

The additional arguments are as follows:

WK — Real work vector of length `N * (2 * N + 8)`. `WK` contains the following information on output: The second `N` locations contain the last step taken. The third `N` locations contain the last Newton step. The fourth `N` locations contain an estimate of the gradient at the solution. The final N^2 locations contain a `BFGS` approximation to the Hessian at the solution. Only the lower triangular portion of the matrix is stored in `WK`. The values returned in the upper triangle should be ignored.

IWK — Work vector of length `N` stored in column order.

2. Informational errors

Type	Code	Description
3	1	Both the actual and predicted relative reductions in the function are less than or equal to the relative function convergence tolerance.
4	2	The iterates appear to be converging to a noncritical point.
4	3	Maximum number of iterations exceeded.
4	4	Maximum number of function evaluations exceeded.
4	5	Maximum number of gradient evaluations exceeded.
4	6	Five consecutive steps have been taken with the maximum step length.
2	7	Scaled step tolerance satisfied; the current point may be an approximate local solution, or the algorithm is making very slow progress and is not near a solution, or `STEPTL` is too big.
3	8	The last global step failed to locate a lower point than the current `X` value.

3. The first stopping criterion for `BCONF` occurs when the norm of the gradient is less than the given gradient tolerance (`RPARAM`(1)). The second stopping criterion for `BCONF` occurs when the scaled distance between the last two steps is less than the step tolerance (`RPARAM`(2)).

4. If the default parameters are desired for `BCONF`, then set `IPARAM`(1) to zero and call the routine `BCONF`. Otherwise, if any nondefault parameters are desired for `IPARAM` or `RPARAM`, then the following steps should be taken before calling `BCONF`:

```
CALL U4INF (IPARAM, RPARAM)
```

Set nondefault values for desired `IPARAM`, `RPARAM` elements.

Note that the call to `U4INF` will set `IPARAM` and `RPARAM` to their default values so only nondefault values need to be set above.

The following is a list of the parameters and the default values:

IPARAM — Integer vector of length 7.

IPARAM(1) = Initialization flag.

IPARAM(2) = Number of good digits in the function.
Default: Machine dependent.

IPARAM(3) = Maximum number of iterations.
Default: 100.

IPARAM(4) = Maximum number of function evaluations.
Default: 400.

IPARAM(5) = Maximum number of gradient evaluations.
Default: 400.

IPARAM(6) = Hessian initialization parameter.
If IPARAM(6) = 0, the Hessian is initialized to the identity matrix; otherwise, it is initialized to a diagonal matrix containing

$$\max\left(|f(t)|, f_s\right) * s_i^2$$

on the diagonal where t = XGUESS, f_s = FSCALE, and s = XSCALE.
Default: 0.

IPARAM(7) = Maximum number of Hessian evaluations.
Default: Not used in BCONF.

RPARAM — Real vector of length 7.

RPARAM(1) = Scaled gradient tolerance.
The i-th component of the scaled gradient at x is calculated as

$$\frac{|g_i| * \max\left(|x_i|, 1/s_i\right)}{\max\left(|f(x)|, f_s\right)}$$

where $g = \nabla f(x)$, s = XSCALE, and f_s = FSCALE.
Default:

$$\sqrt{\varepsilon}, \sqrt[3]{\varepsilon}$$

in double where ε is the machine precision.

RPARAM(2) = Scaled step tolerance. (STEPTL)
The i-th component of the scaled step between two points x and y is computed as

$$\frac{|x_i - y_i|}{\max\left(|x_i|, 1/s_i\right)}$$

where s = XSCALE.
Default: $\varepsilon^{2/3}$ where ε is the machine precision.

RPARAM(3) = Relative function tolerance.
Default: Not used in BCONF.

`RPARAM(4)` = Absolute function tolerance.
Default: Not used in `BCONF`.

`RPARAM(5)` = False convergence tolerance.
Default: Not used in `BCONF`.

`RPARAM(6)` = Maximum allowable step size.
Default: 1000 max(ε_1, ε_2) where

$$\varepsilon_1 = \sqrt{\sum_{i=1}^{n} \left(s_i t_i\right)^2}$$

$\varepsilon_2 = \|s\|_2$, s = `XSCALE`, and t = `XGUESS`.

`RPARAM(7)` = Size of initial trust region radius.
Default: based on the initial scaled Cauchy step.

If double precision is required, then `DU4INF` is called and `RPARAM` is declared double precision.

5. Users wishing to override the default print/stop attributes associated with error messages issued by this routine are referred to “Error Handling” in the Introduction.

Example

The problem

$$\min f(x) = 100\left(x_2 - x_1^2\right)^2 + \left(1 - x_1\right)^2$$
$$\text{subject to} \quad -2 \le x_1 \le 0.5$$
$$-1 \le x_2 \le 2$$

is solved with an initial guess (−1.2, 1.0) and default values for parameters.

```
      USE BCONF_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    N
      PARAMETER  (N=2)
!
      INTEGER    IPARAM(7), ITP, L, NOUT
      REAL       F, FSCALE, RPARAM(7), X(N), XGUESS(N), &
                XLB(N), XSCALE(N), XUB(N)
      EXTERNAL   ROSBRK
!
      DATA XGUESS/-1.2E0, 1.0E0/
      DATA XLB/-2.0E0, -1.0E0/, XUB/0.5E0, 2.0E0/
!                                 All the bounds are provided
      ITP = 0
!                                 Default parameters are used
      IPARAM(1) = 0
!                                 Minimize Rosenbrock function using
!                                 initial guesses of -1.2 and 1.0
```

```
      CALL BCONF (ROSBRK, ITP, XLB, XUB, X, XGUESS=XGUESS,  &
                  iparam=iparam, FVALUE=F)
!                                  Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) X, F, (IPARAM(L),L=3,5)
!
99999 FORMAT ('  The solution is ', 6X, 2F8.3, //, '  The function ', &
            'value is ', F8.3, //, '  The number of iterations is ', &
            10X, I3, /, '  The number of function evaluations is ', &
            I3, /, '  The number of gradient evaluations is ', I3)
!
      END
!
      SUBROUTINE ROSBRK (N, X, F)
      INTEGER    N
      REAL       X(N), F
!
      F = 1.0E2*(X(2)-X(1)*X(1))**2 + (1.0E0-X(1))**2
!
      RETURN
      END
```

Output

```
The solution is          0.500   0.250

The function value is    0.250

The number of iterations is            24
The number of function evaluations is  34
The number of gradient evaluations is  26
```

BCONG

Minimizes a function of N variables subject to bounds on the variables using a quasi-Newton method and a user-supplied gradient.

Required Arguments

FCN — User-supplied subroutine to evaluate the function to be minimized. The usage is CALL FCN (N, X, F), where

N – Length of X. (Input)

X – Vector of length N at which point the function is evaluated. (Input) X should not be changed by FCN.

F – The computed function value at the point X. (Output)

FCN must be declared EXTERNAL in the calling program.

GRAD — User-supplied subroutine to compute the gradient at the point X. The usage is CALL GRAD (N, X, G), where

N – Length of X and G. (Input)

X – Vector of length N at which point the gradient is evaluated. (Input) X should not be changed by GRAD.

G – The gradient evaluated at the point X. (Output)

GRAD must be declared EXTERNAL in the calling program.

IBTYPE — Scalar indicating the types of bounds on variables. (Input)

IBTYPE	Action
1	User will supply all the bounds.
2	All variables are nonnegative.
3	All variables are nonpositive.
4	User supplies only the bounds on 1st variable, all other variables will have the same bounds.

XLB — Vector of length N containing the lower bounds on variables. (Input, if IBTYPE = 0; output, if IBTYPE = 1 or 2; input/output, if IBTYPE = 3)

XUB — Vector of length N containing the upper bounds on variables. (Input, if IBTYPE = 0; output, if IBTYPE = 1 or 2; input/output, if IBTYPE = 3)

X — Vector of length N containing the computed solution. (Output)

Optional Arguments

N — Dimension of the problem. (Input)
Default: N = SIZE (X,1).

XGUESS — Vector of length N containing the initial guess of the minimum. (Input)
Default: XGUESS = 0.0.

XSCALE — Vector of length N containing the diagonal scaling matrix for the variables. (Input)
XSCALE is used mainly in scaling the gradient and the distance between two points. In the absence of other information, set all entries to 1.0.
Default: XSCALE = 1.0.

FSCALE — Scalar containing the function scaling. (Input)
FSCALE is used mainly in scaling the gradient. In the absence of other information, set FSCALE to 1.0.
Default: FSCALE = 1.0.

IPARAM — Parameter vector of length 7. (Input/Output)
Set IPARAM(1) to zero for default values of IPARAM and RPARAM. See Comment 4.
Default: IPARAM = 0.

RPARAM — Parameter vector of length 7. (Input/Output)
See Comment 4.

FVALUE — Scalar containing the value of the function at the computed solution. (Output)

FORTRAN 90 Interface

Generic: CALL BCONG (FCN, GRAD, IBTYPE, XLB, XUB, X [, …])

Specific: The specific interface names are S_BCONG and D_BCONG.

FORTRAN 77 Interface

Single: CALL BCONG (FCN, GRAD, N, XGUESS, IBTYPE, XLB, XUB, XSCALE, FSCALE, IPARAM, RPARAM, X, FVALUE)

Double: The double precision name is DBCONG.

Description

The routine BCONG uses a quasi-Newton method and an active set strategy to solve minimization problems subject to simple bounds on the variables. The problem is stated as follows:

$$\min_{x \in \mathbf{R}^n} f(x)$$

$$\text{subject to } l \leq x \leq u$$

From a given starting point x^c, an active set IA, which contains the indices of the variables at their bounds, is built. A variable is called a “free variable” if it is not in the active set. The routine then computes the search direction for the free variables according to the formula

$$d = -B^{-1} g^c$$

where B is a positive definite approximation of the Hessian and g^c is the gradient evaluated at x^c; both are computed with respect to the free variables. The search direction for the variables in IA is set to zero. A line search is used to find a new point x^n ,

$$x^n = x^c + \lambda d, \qquad \lambda \in (0, 1]$$

such that

$$f(x^n) \leq f(x^c) + \alpha g^T d, \qquad \alpha \in (0, 0.5)$$

Finally, the optimality conditions

$$\|g(x_i)\| \leq \varepsilon, l_i < x_i < u_i$$

$$g(x_i) < 0, \ x_i = u_i$$

$$g(x_i) > 0, x_i = l_i$$

are checked, where ε is a gradient tolerance. When optimality is not achieved, B is updated according to the BFGS formula:

$$B \leftarrow B - \frac{Bss^T B}{s^T Bs} + \frac{yy^T}{y^T s}$$

where $s = x^n - x^c$ and $y = g^n - g^c$. Another search direction is then computed to begin the next iteration.

The active set is changed only when a free variable hits its bounds during an iteration or the optimality condition is met for the free variables but not for all variables in IA, the active set. In the latter case, a variable that violates the optimality condition will be dropped out of IA. For more details on the quasi-Newton method and line search, see Dennis and Schnabel (1983). For more detailed information on active set strategy, see Gill and Murray (1976).

Comments

1. Workspace may be explicitly provided, if desired, by use of B2ONG/DB2ONG. The reference is:

   CALL B2ONG (FCN, GRAD, N, XGUESS, IBTYPE, XLB, XUB, XSCALE, FSCALE, IPARAM, RPARAM, X, FVALUE, WK, IWK)

   The additional arguments are as follows:

   WK — Real work vector of length N * (2 * N + 8). WK contains the following information on output: The second N locations contain the last step taken. The third N locations contain the last Newton step. The fourth N locations contain an estimate of the gradient at the solution. The final N^2 locations contain a BFGS approximation to the Hessian at the solution. Only the lower triangular portion of the matrix is stored in WK. The values returned in the upper triangle should be ignored.

   IWK — Work vector of length N stored in column order.

2. Informational errors

Type	Code	Description
3	1	Both the actual and predicted relative reductions in the function are less than or equal to the relative function convergence tolerance.
4	2	The iterates appear to be converging to a noncritical point.
4	3	Maximum number of iterations exceeded.
4	4	Maximum number of function evaluations exceeded.
4	5	Maximum number of gradient evaluations exceeded.
4	6	Five consecutive steps have been taken with the maximum step length.
2	7	Scaled step tolerance satisfied; the current point may be an approximate local solution, or the algorithm is making very slow progress and is not near a solution, or STEPTL is too big.
3	8	The last global step failed to locate a lower point than the current X value.

3. The first stopping criterion for BCONG occurs when the norm of the gradient is less than the given gradient tolerance (RPARAM(1)). The second stopping criterion for BCONG occurs when the scaled distance between the last two steps is less than the step tolerance (RPARAM(2)).

4. If the default parameters are desired for BCONG, then set IPARAM(1) to zero and call the routine BCONG. Otherwise, if any nondefault parameters are desired for IPARAM or RPARAM, then the following steps should be taken before calling BCONG:

   CALL U4INF (IPARAM, RPARAM)

Set nondefault values for desired IPARAM, RPARAM elements.

Note that the call to U4INF will set IPARAM and RPARAM to their default values so only nondefault values need to be set above.

The following is a list of the parameters and the default values:

IPARAM — Integer vector of length 7.

IPARAM(1) = Initialization flag.

IPARAM(2) = Number of good digits in the function.
Default: Machine dependent.

IPARAM(3) = Maximum number of iterations.
Default: 100.

IPARAM(4) = Maximum number of function evaluations.
Default: 400.

IPARAM(5) = Maximum number of gradient evaluations.
Default: 400.

IPARAM(6) = Hessian initialization parameter.
If IPARAM (6) = 0, the Hessian is initialized to the identity matrix; otherwise, it is initialized to a diagonal matrix containing

$$\max\left(|f(t)|, f_s\right) * s_i^2$$

on the diagonal where t = XGUESS, f_s = FSCALE, and s = XSCALE.
Default: 0.

IPARAM(7) = Maximum number of Hessian evaluations.
Default: Not used in BCONG.

RPARAM — Real vector of length 7.

RPARAM(1) = Scaled gradient tolerance.
The *i*-th component of the scaled gradient at x is calculated as

$$\frac{|g_i| * \max\left(|x_i|, 1/s_i\right)}{\max\left(|f(x)|, f_s\right)}$$

where $g = \nabla f(x)$, s = XSCALE, and f_s = FSCALE.
Default:

$$\sqrt{\varepsilon}, \sqrt[3]{\varepsilon}$$

in double where ε is the machine precision.

RPARAM(2) = Scaled step tolerance. (STEPTL)
The *i*-th component of the scaled step between two points *x* and *y* is computed as

$$\frac{|x_i - y_i|}{\max\left(|x_i|, 1/s_i\right)}$$

where s = XSCALE.

Default: $\varepsilon^{2/3}$ where ε is the machine precision.

RPARAM(3) = Relative function tolerance.

Default: Not used in BCONG.

RPARAM(4) = Absolute function tolerance.

Default: Not used in BCONG.

RPARAM(5) = False convergence tolerance.

Default: Not used in BCONG.

RPARAM(6) = Maximum allowable step size.

Default: 1000 max(ε_1, ε_2) where

$$\varepsilon_1 = \sqrt{\sum_{i=1}^{n} \left(s_i t_i\right)^2}$$

$\varepsilon_2 = \|s\|_2$, s = XSCALE, and t = XGUESS.

RPARAM(7) = Size of initial trust region radius.

Default: based on the initial scaled Cauchy step.

If double precision is required, then DU4INF is called and RPARAM is declared double precision.

5. Users wishing to override the default print/stop attributes associated with error messages issued by this routine are referred to “Error Handling” in the Introduction.

Example

The problem

$$\min f(x) = 100\left(x_2 - x_1^2\right)^2 + \left(1 - x_1\right)^2$$
$$\text{subject to} \quad -2 \le x_1 \le 0.5$$
$$-1 \le x_2 \le 2$$

is solved with an initial guess (−1.2, 1.0), and default values for parameters.

```
      USE BCONG_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    N
      PARAMETER  (N=2)
!
      INTEGER    IPARAM(7), ITP, L, NOUT
      REAL       F, X(N), XGUESS(N), XLB(N), XUB(N)
```

```
      EXTERNAL   ROSBRK, ROSGRD
!
      DATA XGUESS/-1.2E0, 1.0E0/
      DATA XLB/-2.0E0, -1.0E0/, XUB/0.5E0, 2.0E0/
!                                 All the bounds are provided
      ITP = 0
!                                 Default parameters are used
      IPARAM(1) = 0
!                                 Minimize Rosenbrock function using
!                                 initial guesses of -1.2 and 1.0
      CALL BCONG (ROSBRK, ROSGRD, ITP, XLB, XUB, X, XGUESS=XGUESS, &
                 IPARAM=IPARAM, FVALUE=F)
!                                 Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) X, F, (IPARAM(L),L=3,5)
!
99999 FORMAT ('  The solution is ', 6X, 2F8.3, //, '  The function ', &
            'value is ', F8.3, //, '  The number of iterations is ', &
            10X, I3, /, '  The number of function evaluations is ', &
            I3, /, '  The number of gradient evaluations is ', I3)
!
      END
!
      SUBROUTINE ROSBRK (N, X, F)
      INTEGER    N
      REAL       X(N), F
!
      F = 1.0E2*(X(2)-X(1)*X(1))**2 + (1.0E0-X(1))**2
!
      RETURN
      END
!
      SUBROUTINE ROSGRD (N, X, G)
      INTEGER    N
      REAL       X(N), G(N)
!
      G(1) = -4.0E2*(X(2)-X(1)*X(1))*X(1) - 2.0E0*(1.0E0-X(1))
      G(2) = 2.0E2*(X(2)-X(1)*X(1))
!
      RETURN
      END
```

Output

```
The solution is          0.500   0.250

The function value is    0.250

The number of iterations is            22
The number of function evaluations is  32
The number of gradient evaluations is  23
```

BCODH

Minimizes a function of N variables subject to bounds on the variables using a modified Newton method and a finite-difference Hessian.

Required Arguments

FCN — User-supplied subroutine to evaluate the function to be minimized. The usage is CALL FCN (N, X, F), where

N – Length of X. (Input)

X – Vector of length N at which point the function is evaluated. (Input) X should not be changed by FCN.

F – The computed function value at the point X. (Output)

FCN must be declared EXTERNAL in the calling program.

GRAD — User-supplied subroutine to compute the gradient at the point X. The usage is CALL GRAD (N, X, G), where

N – Length of X and G. (Input)

X – Vector of length N at which point the gradient is evaluated. (Input) X should not be changed by GRAD.

G – The gradient evaluated at the point X. (Output)

GRAD must be declared EXTERNAL in the calling program.

IBTYPE — Scalar indicating the types of bounds on variables. (Input)

IBTYPE	Action
0	User will supply all the bounds.
1	All variables are nonnegative.
2	All variables are nonpositive.
3	User supplies only the bounds on 1st variable, all other variables will have the same bounds.

XLB — Vector of length N containing the lower bounds on the variables. (Input)

XUB — Vector of length N containing the upper bounds on the variables. (Input)

X — Vector of length N containing the computed solution. (Output)

Optional Arguments

N — Dimension of the problem. (Input)
Default: N = SIZE (X,1).

XGUESS — Vector of length N containing the initial guess of the minimum. (Input)
Default: XGUESS = 0.0.

XSCALE — Vector of length N containing the diagonal scaling matrix for the variables. (Input)
XSCALE is used mainly in scaling the gradient and the distance between two points. In the absence of other information, set all entries to 1.0.
Default: XSCALE = 1.0.

FSCALE — Scalar containing the function scaling. (Input)
FSCALE is used mainly in scaling the gradient. In the absence of other information, set FSCALE to 1.0.
Default: FSCALE = 1.0.

IPARAM — Parameter vector of length 7. (Input/Output)
Set IPARAM(1) to zero for default values of IPARAM and RPARAM. See Comment 4.
Default: IPARAM = 0.

RPARAM — Parameter vector of length 7. (Input/Output)
See Comment 4.

FVALUE — Scalar containing the value of the function at the computed solution. (Output)

FORTRAN 90 Interface

Generic: CALL BCODH (FCN, GRAD, IBTYPE, XLB, XUB, X [, …])

Specific: The specific interface names are S_BCODH and D_BCODH.

FORTRAN 77 Interface

Single: CALL BCODH (FCN, GRAD, N, XGUESS, IBTYPE, XLB, XUB, XSCALE, FSCALE, IPARAM, RPARAM, X, FVALUE)

Double: The double precision name is DBCODH.

Description

The routine BCODH uses a modified Newton method and an active set strategy to solve minimization problems subject to simple bounds on the variables. The problem is stated as

$$\min_{x \in \mathbf{R}^n} f(x)$$

$$\text{subject to } l \le x \le u$$

From a given starting point x^c, an active set IA, which contains the indices of the variables at their bounds, is built. A variable is called a “free variable” if it is not in the active set. The routine then computes the search direction for the free variables according to the formula

$$d = -H^{-1} g^c$$

where H is the Hessian and g^c is the gradient evaluated at x^c; both are computed with respect to the free variables. The search direction for the variables in IA is set to zero. A line search is used to find a new point x^n ,

$$x^n = x^c + \lambda d, \qquad \lambda \in (0, 1]$$

such that

$$f(x^n) \le f(x^c) + \alpha g^T d, \qquad \alpha \in (0, 0.5)$$

Finally, the optimality conditions

$$\|g(x_i)\| \le \varepsilon, l_i < x_i < u_i$$

$$g(x_i) < 0, \ x_i = u_i$$

$$g(x_i) > 0, x_i = l_i$$

are checked where ε is a gradient tolerance. When optimality is not achieved, another search direction is computed to begin the next iteration. This process is repeated until the optimality criterion is met.

The active set is changed only when a free variable hits its bounds during an iteration or the optimality condition is met for the free variables but not for all variables in IA, the active set. In the latter case, a variable that violates the optimality condition will be dropped out of IA. For more details on the modified Newton method and line search, see Dennis and Schnabel (1983). For more detailed information on active set strategy, see Gill and Murray (1976).

Since a finite-difference method is used to estimate the Hessian for some single precision calculations, an inaccurate estimate of the Hessian may cause the algorithm to terminate at a noncritical point. In such cases, high precision arithmetic is recommended. Also, whenever the exact Hessian can be easily provided, routine `BCOAH` should be used instead.

Comments

1. Workspace may be explicitly provided, if desired, by use of `B2ODH/DB2ODH`. The reference is:

```
CALL B2ODH (FCN, GRAD, N, XGUESS, IBTYPE, XLB, XUB, XSCALE,
   FSCALE, IPARAM, RPARAM, X, FVALUE, WK, IWK)
```

The additional arguments are as follows:

WK — Real work vector of length `N * (N + 8)`. `WK` contains the following information on output: The second `N` locations contain the last step taken. The third `N` locations contain the last Newton step. The fourth `N` locations contain an estimate of the gradient at the solution. The final N^2 locations contain the Hessian at the approximate solution.

IWK — Integer work vector of length `N`.

2. Informational errors

Type	Code	Description
3	1	Both the actual and predicted relative reductions in the function are less than or equal to the relative function convergence tolerance.
4	2	The iterates appear to be converging to a noncritical point.
4	3	Maximum number of iterations exceeded.
4	4	Maximum number of function evaluations exceeded.
4	5	Maximum number of gradient evaluations exceeded.
4	6	Five consecutive steps have been taken with the maximum step length.
2	7	Scaled step tolerance satisfied; the current point may be an approximate local solution, or the algorithm is making very slow progress and is not near a solution, or `STEPTL` is too big.
4	7	Maximum number of Hessian evaluations exceeded.

3. The first stopping criterion for `BCODH` occurs when the norm of the gradient is less than the given gradient tolerance (`RPARAM`(1)). The second stopping criterion for `BCODH` occurs when the scaled distance between the last two steps is less than the step tolerance (`RPARAM`(2)).

4. If the default parameters are desired for `BCODH`, then set `IPARAM`(1) to zero and call the routine `BCODH`. Otherwise, if any nondefault parameters are desired for `IPARAM` or `RPARAM`; then the following steps should be taken before calling `BCODH`:

   `CALL U4INF (IPARAM, RPARAM)`

   Set nondefault values for desired `IPARAM`, `RPARAM` elements.

> Note that the call to `U4INF` will set `IPARAM` and `RPARAM` to their default values so only nondefault values need to be set above.

The following is a list of the parameters and the default values:

IPARAM — Integer vector of length 7.

`IPARAM`(1) = Initialization flag.

`IPARAM`(2) = Number of good digits in the function.
Default: Machine dependent.

`IPARAM`(3) = Maximum number of iterations.
Default: 100.

`IPARAM`(4) = Maximum number of function evaluations.
Default: 400.

`IPARAM`(5) = Maximum number of gradient evaluations.
Default: 400.

`IPARAM`(6) = Hessian initialization parameter.
Default: Not used in `BCODH`.

`IPARAM`(7) = Maximum number of Hessian evaluations.
Default: 100.

RPARAM — Real vector of length 7.

`RPARAM`(1) = Scaled gradient tolerance.
The *i*-th component of the scaled gradient at x is calculated as

$$\frac{|g_i| * \max\left(|x_i|, 1/s_i\right)}{\max\left(|f(x)|, f_s\right)}$$

where $g = \nabla f(x)$, s = `XSCALE`, and f_s = `FSCALE`.
Default:

$$\sqrt{\varepsilon}, \sqrt[3]{\varepsilon}$$

in double where **ε** is the machine precision.

`RPARAM`(2) = Scaled step tolerance. (`STEPTL`)
The *i*-th component of the scaled step between two points *x* and *y* is computed as

$$\frac{|x_i - y_i|}{\max\left(|x_i|, 1/s_i\right)}$$

where s = `XSCALE`.
Default: $\varepsilon^{2/3}$ where **ε** is the machine precision.

`RPARAM`(3) = Relative function tolerance.
Default: $\max(10^{-10}, \varepsilon^{2/3})$, $\max(10^{-20}, \varepsilon^{2/3})$ in double where **ε** is the machine precision.

`RPARAM`(4) = Absolute function tolerance.
Default: Not used in `BCODH`.

`RPARAM`(5) = False convergence tolerance.
Default: 100**ε** where **ε** is the machine precision.

`RPARAM`(6) = Maximum allowable step size.
Default: 1000 $\max(\varepsilon_1, \varepsilon_2)$ where

$$\varepsilon_1 = \sqrt{\sum_{i=1}^{n} \left(s_i t_i\right)^2}$$

$\varepsilon_2 = \|s\|_2$, s = XSCALE, and t = XGUESS.

RPARAM(7) = Size of initial trust region radius.
Default: based on the initial scaled Cauchy step.

If double precision is required, then DU4INF is called and RPARAM is declared double precision.

5. Users wishing to override the default print/stop attributes associated with error messages issued by this routine are referred to “Error Handling” in the Introduction.

Example

The problem

$$\min f(x) = 100\left(x_2 - x_1^2\right)^2 + \left(1 - x_1\right)^2$$
$$\text{subject to} \quad -2 \le x_1 \le 0.5$$
$$-1 \le x_2 \le 2$$

is solved with an initial guess (−1.2, 1.0), and default values for parameters.

```
      USE BCODH_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    N
      PARAMETER  (N=2)
!
      INTEGER    IP, IPARAM(7), L, NOUT
      REAL       F, X(N), XGUESS(N), XLB(N), XUB(N)
      EXTERNAL   ROSBRK, ROSGRD
!
      DATA XGUESS/-1.2E0, 1.0E0/
      DATA XLB/-2.0E0, -1.0E0/, XUB/0.5E0, 2.0E0/
!
      IPARAM(1) = 0
      IP        = 0
!                                 Minimize Rosenbrock function using
!                                 initial guesses of -1.2 and 1.0
      CALL BCODH (ROSBRK, ROSGRD, IP, XLB, XUB, X, XGUESS=XGUESS, &
                 IPARAM=IPARAM, FVALUE=F)
!                                 Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) X, F, (IPARAM(L),L=3,5)
!
99999 FORMAT ('  The solution is ', 6X, 2F8.3, //, '  The function ', &
            'value is ', F8.3, //, '  The number of iterations is ', &
            10X, I3, /, '  The number of function evaluations is ', &
            I3, /, '  The number of gradient evaluations is ', I3)
!
      END
!
```

```
      SUBROUTINE ROSBRK (N, X, F)
      INTEGER    N
      REAL       X(N), F
!
      F = 1.0E2*(X(2)-X(1)*X(1))**2 + (1.0E0-X(1))**2
!
      RETURN
      END
      SUBROUTINE ROSGRD (N, X, G)
      INTEGER    N
      REAL       X(N), G(N)
!
      G(1) = -4.0E2*(X(2)-X(1)*X(1))*X(1) - 2.0E0*(1.0E0-X(1))
      G(2) = 2.0E2*(X(2)-X(1)*X(1))
!
      RETURN
      END
```

Output

```
The solution is          0.500   0.250

The function value is    0.250

The number of iterations is             17
The number of function evaluations is   26
The number of gradient evaluations is   18
```

BCOAH

Minimizes a function of N variables subject to bounds on the variables using a modified Newton method and a user-supplied Hessian.

Required Arguments

FCN — User-supplied subroutine to evaluate the function to be minimized. The usage is
CALL FCN (N, X, F), where

N – Length of X. (Input)

X – Vector of length N at which point the function is evaluated. (Input)
X should not be changed by FCN.

F – The computed function value at the point X. (Output)

FCN must be declared EXTERNAL in the calling program.

GRAD — User-supplied subroutine to compute the gradient at the point X. The usage is
CALL GRAD (N, X, G), where

N – Length of X and G. (Input)

X – Vector of length N at which point the gradient is evaluated. (Input)
X should not be changed by GRAD.

G – The gradient evaluated at the point X. (Output)

GRAD must be declared EXTERNAL in the calling program.

HESS — User-supplied subroutine to compute the Hessian at the point X. The usage is
CALL HESS (N, X, H, LDH), where

N – Length of X. (Input)

X – Vector of length N at which point the Hessian is evaluated. (Input)
X should not be changed by HESS.

H – The Hessian evaluated at the point X. (Output)

LDH – Leading dimension of H exactly as specified in the dimension statement of the calling program. (Input)

HESS must be declared EXTERNAL in the calling program.

IBTYPE — Scalar indicating the types of bounds on variables. (Input)

IBTYPE	Action
1	User will supply all the bounds.
2	All variables are nonnegative.
3	User supplies only the bounds on 1st variable, all other variables will have the same bounds.

XLB — Vector of length N containing the lower bounds on the variables. (Input)

XUB — Vector of length N containing the upper bounds on the variables. (Input)

X — Vector of length N containing the computed solution. (Output)

Optional Arguments

N — Dimension of the problem. (Input)
Default: N = SIZE (X,1).

XGUESS — Vector of length N containing the initial guess. (Input)
Default: XGUESS = 0.0.

XSCALE — Vector of length N containing the diagonal scaling matrix for the variables. (Input)
XSCALE is used mainly in scaling the gradient and the distance between two points. In the absence of other information, set all entries to 1.0.
Default: XSCALE = 1.0.

FSCALE — Scalar containing the function scaling. (Input)
FSCALE is used mainly in scaling the gradient. In the absence of other information, set FSCALE to 1.0.
Default: FSCALE = 1.0.

IPARAM — Parameter vector of length 7. (Input/Output)
Set IPARAM(1) to zero for default values of IPARAM and RPARAM. See Comment 4.
Default: IPARAM = 0.

RPARAM — Parameter vector of length 7. (Input/Output)
See Comment 4.

FVALUE — Scalar containing the value of the function at the computed solution. (Output)

FORTRAN 90 Interface

Generic: `CALL BCOAH (FCN, GRAD, HESS, IBTYPE, XLB, XUB, X [, …])`

Specific: The specific interface names are `S_BCOAH` and `D_BCOAH`.

FORTRAN 77 Interface

Single: `CALL BCOAH (FCN, GRAD, HESS, N, XGUESS, IBTYPE, XLB, XUB, XSCALE, FSCALE, IPARAM, RPARAM, X, FVALUE)`

Double: The double precision name is `DBCOAH`.

Description

The routine `BCOAH` uses a modified Newton method and an active set strategy to solve minimization problems subject to simple bounds on the variables. The problem is stated as follows:

$$\min_{x \in \mathbf{R}^n} f(x)$$

$$\text{subject to } l \le x \le u$$

From a given starting point x^c, an active set IA, which contains the indices of the variables at their bounds, is built. A variable is called a “free variable” if it is not in the active set. The routine then computes the search direction for the free variables according to the formula

$$d = -H^{-1} g^c$$

where H is the Hessian and g^c is the gradient evaluated at x^c; both are computed with respect to the free variables. The search direction for the variables in IA is set to zero. A line search is used to find a new point x^n ,

$$x^n = x^c + \lambda d, \qquad \lambda \in (0, 1]$$

such that

$$f(x^n) \le f(x^c) + \alpha g^T d, \qquad \alpha \in (0, 0.5)$$

Finally, the optimality conditions

$$\|g(x_i)\| \le \varepsilon,\ l_i < x_i < u_i$$

$$g(x_i) < 0,\ x_i = u_i$$

$$g(x_i) > 0,\ x_i = l_i$$

are checked where ε is a gradient tolerance. When optimality is not achieved, another search direction is computed to begin the next iteration. This process is repeated until the optimality criterion is met.

The active set is changed only when a free variable hits its bounds during an iteration or the optimality condition is met for the free variables but not for all variables in IA, the active set. In the latter case, a variable that violates the optimality condition will be dropped out of IA. For more details on the modified Newton method and line search, see Dennis and Schnabel (1983). For more detailed information on active set strategy, see Gill and Murray (1976).

Comments

1. Workspace may be explicitly provided, if desired, by use of B2OAH/DB2OAH. The reference is:

   ```
   CALL B2OAH (FCN, GRAD, HESS, N, XGUESS, IBTYPE, XLB, XUB,
      XSCALE, FSCALE, IPARAM, RPARAM, X, FVALUE, WK, IWK)
   ```

   The additional arguments are as follows:

   WK — Work vector of length N * (N + 8). WK contains the following information on output: The second N locations contain the last step taken. The third N locations contain the last Newton step. The fourth N locations contain an estimate of the gradient at the solution. The final N^2 locations contain the Hessian at the approximate solution.

   IWK — Work vector of length N.

2. Informational errors

Type	Code	Description
3	1	Both the actual and predicted relative reductions in the function are less than or equal to the relative function convergence tolerance.
4	2	The iterates appear to be converging to a noncritical point.
4	3	Maximum number of iterations exceeded.
4	4	Maximum number of function evaluations exceeded.
4	5	Maximum number of gradient evaluations exceeded.
4	6	Five consecutive steps have been taken with the maximum step length.
2	7	Scaled step tolerance satisfied; the current point may be an approximate local solution, or the algorithm is making very slow progress and is not near a solution, or STEPTL is too big.
4	7	Maximum number of Hessian evaluations exceeded.
3	8	The last global step failed to locate a lower point than the current X value.

3. The first stopping criterion for BCOAH occurs when the norm of the gradient is less than the given gradient tolerance (RPARAM(1)). The second stopping criterion for BCOAH occurs when the scaled distance between the last two steps is less than the step tolerance (RPARAM(2)).

4. If the default parameters are desired for BCOAH, then set IPARAM(1) to zero and call the routine BCOAH. Otherwise, if any nondefault parameters are desired for IPARAM or RPARAM, then the following steps should be taken before calling BCOAH:

   CALL U4INF (IPARAM, RPARAM)

   Set nondefault values for desired IPARAM, RPARAM elements.

Note that the call to U4INF will set IPARAM and RPARAM to their default values so only nondefault values need to be set above.

The following is a list of the parameters and the default values:

IPARAM — Integer vector of length 7.

IPARAM(1) = Initialization flag.

IPARAM(2) = Number of good digits in the function.
Default: Machine dependent.

IPARAM(3) = Maximum number of iterations.
Default: 100.

IPARAM(4) = Maximum number of function evaluations.
Default: 400.

IPARAM(5) = Maximum number of gradient evaluations.
Default: 400.

IPARAM(6) = Hessian initialization parameter.
Default: Not used in BCOAH.

IPARAM(7) = Maximum number of Hessian evaluations.
Default: 100.

RPARAM — Real vector of length 7.

RPARAM(1) = Scaled gradient tolerance.
The *i*-th component of the scaled gradient at x is calculated as

$$\frac{|g_i| * \max\left(|x_i|, 1/s_i\right)}{\max\left(|f(x)|, f_s\right)}$$

where $g = \nabla f(x)$, s = XSCALE, and f_s = FSCALE.
Default:

$$\sqrt{\varepsilon}, \sqrt[3]{\varepsilon}$$

in double where **ε** is the machine precision.

RPARAM(2) = Scaled step tolerance. (STEPTL)
The *i*-th component of the scaled step between two points *x* and *y* is computed as

$$\frac{|x_i - y_i|}{\max\left(|x_i|, 1/s_i\right)}$$

where s = `XSCALE`.

Default: $\varepsilon^{2/3}$ where ε is the machine precision.

`RPARAM`(3) = Relative function tolerance.

Default: max(10^{-10}, $\varepsilon^{2/3}$), max (10^{-20}, $\varepsilon^{2/3}$) in double where ε is the machine precision.

`RPARAM`(4) = Absolute function tolerance.

Default: Not used in `BCOAH`.

`RPARAM`(5) = False convergence tolerance.

Default: 100ε where ε is the machine precision.

`RPARAM`(6) = Maximum allowable step size.

Default: 1000 max(ε_1, ε_2) where

$$\varepsilon_1 = \sqrt{\sum_{i=1}^{n}\left(s_i t_i\right)^2}$$

$\varepsilon_2 = \|s\|_2$, s = `XSCALE`, and t = `XGUESS`.

`RPARAM`(7) = Size of initial trust region radius.

Default: based on the initial scaled Cauchy step.

If double precision is required, then `DU4INF` is called and `RPARAM` is declared double precision.

5. Users wishing to override the default print/stop attributes associated with error messages issued by this routine are referred to “Error Handling” in the Introduction.

Example

The problem

$$\begin{aligned} \min f(x) &= 100\left(x_2 - x_1^2\right)^2 + \left(1 - x_1\right)^2 \\ \text{subject to } & -2 \le x_1 \le 0.5 \\ & -1 \le x_2 \le 2 \end{aligned}$$

is solved with an initial guess (−1.2, 1.0), and default values for parameters.

```
      USE BCOAH_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    N
      PARAMETER  (N=2)
!
```

```
      INTEGER    IP, IPARAM(7), L, NOUT
      REAL       F, X(N), XGUESS(N), XLB(N), XUB(N)
      EXTERNAL   ROSBRK, ROSGRD, ROSHES
!
      DATA XGUESS/-1.2E0, 1.0E0/
      DATA XLB/-2.0E0, -1.0E0/, XUB/0.5E0, 2.0E0/
!
      IPARAM(1) = 0
      IP        = 0
!                                 Minimize Rosenbrock function using
!                                 initial guesses of -1.2 and 1.0
      CALL BCOAH (ROSBRK, ROSGRD, ROSHES, IP, XLB, XUB, X, &
                 XGUESS=XGUESS,IPARAM=IPARAM, FVALUE=F)
!                                 Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) X, F, (IPARAM(L),L=3,5), IPARAM(7)
!
99999 FORMAT ('  The solution is ', 6X, 2F8.3, //, '  The function ', &
            'value is ', F8.3, //, '  The number of iterations is ', &
            10X, I3, /, '  The number of function evaluations is ', &
            I3, /, '  The number of gradient evaluations is ', I3, /, &
            '  The number of Hessian evaluations is  ', I3)
!
      END
!
      SUBROUTINE ROSBRK (N, X, F)
      INTEGER    N
      REAL       X(N), F
!
      F = 1.0E2*(X(2)-X(1)*X(1))**2 + (1.0E0-X(1))**2
!
      RETURN
      END
!
      SUBROUTINE ROSGRD (N, X, G)
      INTEGER    N
      REAL       X(N), G(N)
!
      G(1) = -4.0E2*(X(2)-X(1)*X(1))*X(1) - 2.0E0*(1.0E0-X(1))
      G(2) = 2.0E2*(X(2)-X(1)*X(1))
!
      RETURN
      END
!
      SUBROUTINE ROSHES (N, X, H, LDH)
      INTEGER    N, LDH
      REAL       X(N), H(LDH,N)
!
      H(1,1) = -4.0E2*X(2) + 1.2E3*X(1)*X(1) + 2.0E0
      H(2,1) = -4.0E2*X(1)
      H(1,2) = H(2,1)
      H(2,2) = 2.0E2
!
      RETURN
      END
```

Output

```
The solution is          0.500   0.250

The function value is    0.250

The number of iterations is            18
The number of function evaluations is  29
The number of gradient evaluations is  19
```

```
  The number of Hessian evaluations is   18
```

BCPOL

Minimizes a function of N variables subject to bounds on the variables using a direct search complex algorithm.

Required Arguments

FCN — User-supplied subroutine to evaluate the function to be minimized. The usage is CALL FCN (N, X, F), where

N – Length of X. (Input)

X – Vector of length N at which point the function is evaluated. (Input)
X should not be changed by FCN.

F – The computed function value at the point X. (Output)

FCN must be declared EXTERNAL in the calling program.

IBTYPE — Scalar indicating the types of bounds on variables. (Input)

IBTYPE	Action
0	User will supply all the bounds.
1	All variables are nonnegative.
2	All variables are nonpositive.
3	User supplies only the bounds on first variable. All other variables will have the same bounds.

XLB — Vector of length N containing the lower bounds on the variables. (Input, if IBTYPE = 0; output, if IBTYPE = 1 or 2; input/output, if IBTYPE = 3)

XUB — Vector of length N containing the upper bounds on the variables. (Input, if IBTYPE = 0; output, if IBTYPE = 1 or 2; input/output, if IBTYPE = 3)

X — Real vector of length N containing the best estimate of the minimum found. (Output)

Optional Arguments

N — The number of variables. (Input)
Default: N = SIZE (X,1).

XGUESS — Real vector of length N that contains an initial guess to the minimum. (Input)
Default: XGUESS = 0.0.

FTOL — The convergence tolerance. (Input)

First convergence criterion: The algorithm stops when the relative error in the function values is less than FTOL, i.e. when F(worst) − F(best) < FTOL * (1 + ABS(F(best))) where F(worst) and F(best) are the function values of the current worst and best point, respectively.

Second convergence criterion: The algorithm stops when the standard deviation of the function values at the 2 * N current points is less than FTOL. If the subroutine terminates prematurely, try again with a smaller value FTOL.
Default: FTOL = 1.0e-4 for single and 1.0d-8 for double precision.

MAXFCN — The number of function evaluations. (Input/Output)
On input, maximum allowed number of function evaluations. On output, actual number of function evaluations needed.
Default: MAXFCN = 300.

FVALUE — Function value at the computed solution. (Output)

XCPLX — Real N x 2*N matrix containing the 2 * N initial complex points. (Input)
If the XCPLX optional argument is used, then the initial guess must be specified in XCPLX(:,1) and there is no need to provide optional argument XGUESS. Thus, if both optional arguments XCPLX and XGUESS are supplied, XGUESS will be ignored.

REFLCOEF — Real scalar containing the reflection coefficient. (Input)
REFLCOEF must be greater than 0.
Default: REFLCOEF = 1.0.

EXPNCOEF — Real scalar containing the expansion coefficient. (Input)
EXPNCOEF must be greater than 1.
Default: EXPNCOEF = 2.0.

CNTRCOEF — Real scalar containing the contraction coefficient. (Input)
CNTRCOEF must be greater than 0 and less than 1.
Default: CNTRCOEF = 0.5.

FORTRAN 90 Interface

Generic: CALL BCPOL (FCN, IBTYPE, XLB, XUB, X [, …])

Specific: The specific interface names are S_BCPOL and D_BCPOL.

FORTRAN 77 Interface

Single: CALL BCPOL (FCN, N, XGUESS, IBTYPE, XLB, XUB, FTOL, MAXFCN, X, FVALUE)

Double: The double precision name is DBCPOL.

NOTE: To maintain backward compatibility, the argument list for the Fortran 77 interface does not include the optional arguments XCPLX, REFLCOEF, EXPNCOEF, or CNTRCOEF, and therefore cannot be used to specify these arguments.

Description

The routine BCPOL uses the complex method to find a minimum point of a function of *n* variables. The method is based on function comparison; no smoothness is assumed. It starts with an initial complex of 2*n* points x_1, x_2, …, x_{2n} which is either user-specified (using optional argument XCPLX, see above) or is otherwise, by default, randomly initialized. At each iteration, a new point is generated to replace the "worst" point x_j, which has the largest function value among these 2*n* points, as described below.

Each iteration begins by determining the best and two worst points in the present complex, and then constructing a new "reflection" point x_r by the formula

$$x_r = c + \alpha(c - x_j)$$

where

$$c = \frac{1}{2n-1} \sum_{i \neq j} x_i$$

is the *centroid* of the 2*n* - 1 best points and $\alpha(\alpha > 0)$ is the *reflection coefficient*. (See optional argument REFLCOEF above). Depending on how the new reflection point x_r compares with the existing complex points, the iteration proceeds as follows:

If x_r is neither better than the best point nor worse than the second worst point, then x_r replaces the worst point x_j and, if neither of the stopping criteria (see below) are satisfied, a new iteration begins.

If x_r is a best point, that is, if $f(x_r) \le f(x_i)$ for i = 1, …, 2*n*, an expansion point x_e is computed to see if an even better point can be obtained by moving further in the reflection direction:

$$x_e = c + \beta(x_r - c)$$

where $\beta(\beta > 1)$ is called the *expansion coefficient* (see optional argument EXPNCOEF above), and worst point x_j is replaced by the better of x_e and x_r and, if neither of the stopping criteria are satisfied, a new iteration begins.

If x_r and x_j are the two worst points, then the complex is contracted to try to get a better new contraction point x_c :

$$x_c = \begin{cases} c + \gamma(x_j - c) & \text{if } f(x_r) \ge f(x_j) \\ c + \gamma(x_r - c) & \text{if } f(x_j) > f(x_r) \end{cases}$$

where $\gamma(0 < \gamma < 1)$ is called the *contraction coefficient*. (See optional argument CNTRCOEF above.) If the contraction step is successful (i.e. if min($f(x_r)$, $f(x_j)$) > $f(x_c)$), then worst point x_j is replaced by x_c. If the contraction step is unsuccessful, then the complex is shrunk by moving the $2n - 1$ worst points halfway towards the current best point. Following the contraction step, if neither of the stopping criteria are satisfied, a new iteration begins.

Whenever the new point generated is beyond the bound, it will be set to the bound. If, at the end of an iteration, one of the following stopping criteria is satisfied, then the process ends with the best point returned as the optimum.

Criterion 1:

$$f_{worst} - f_{best} \le \varepsilon_f(1. + |f_{best}|)$$

Criterion 2:

$$\frac{1}{2n}\sum_{i=1}^{2n}\left(f_i - \frac{\sum_{j=1}^{2n} f_j}{2n}\right)^2 \le \varepsilon_f^2$$

where $f_i = f(x_i)$, $f_j = f(x_j)$, and ε_f is a given tolerance. For a complete description, see Nelder and Mead (1965) or Gill et al. (1981).

Comments

1. Workspace may be explicitly provided, if desired, by use of B2POL/DB2POL. The reference is:

```
CALL B2POL (FCN, N, XGUESS, IBTYPE, XLB, XUB, FTOL, MAXFCN,
   X, FVALUE, WK)
```

The additional argument is:

WK — Real work vector of length `2 * N**2 + 5 * N`

NOTE: To maintain backward compatibility, the argument list for B2POL/DB2POL does not include the optional arguments XCPLX, REFLCOEF, EXPNCOEF, or CNTRCOEF, and therefore cannot be used to specify these arguments.

2. Informational error

Type	Code	Description
3	1	The maximum number of function evaluations is exceeded.

3. Since BCPOL uses only function-value information at each step to determine a new approximate minimum, it could be quite inefficient on smooth problems compared to other methods such as those implemented in routine BCONF, which takes into account derivative information at each iteration. Hence, routine BCPOL should only be used as a last resort. Briefly, a set of 2 * N points in an N-dimensional space is called a complex. The minimization process iterates by replacing the point with the largest function value by a new point with a smaller function value. The iteration continues until all the points cluster sufficiently close to a minimum.

Example 1

The problem

$$\min f(x) = 100\left(x_2 - x_1^2\right)^2 + \left(1 - x_1\right)^2$$
$$\text{subject to} \quad -2 \le x_1 \le 0.5$$
$$-1 \le x_2 \le 2$$

is solved with an initial guess (1.2, 1.0), and the solution is printed.

```
      USE BCPOL_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                 Variable declarations
      INTEGER    N
      PARAMETER  (N=2)
!
      INTEGER    IBTYPE, K, NOUT
      REAL       FTOL, FVALUE, X(N), XGUESS(N), XLB(N), XUB(N)
      EXTERNAL   FCN
!
!                                 Initializations
!                                 XGUESS = (-1.2,  1.0)
!                                 XLB    = (-2.0, -1.0)
!                                 XUB    = ( 0.5,  2.0)
      DATA  XGUESS/-1.2, 1.0/, XLB/-2.0E0, -1.0E0/, XUB/0.5E0, 2.0E0/
!
      FTOL   = 1.0E-5
      IBTYPE = 0
!
      CALL BCPOL (FCN, IBTYPE, XLB, XUB, X, xguess=xguess, ftol=ftol, &
                 fvalue=fvalue)
!
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) (X(K),K=1,N), FVALUE
99999 FORMAT ('  The best estimate for the minimum value of the', /, &
```

```
              '  function is X = (', 2(2X,F4.2), ')', /, '  with ', &
              'function value FVALUE = ', E12.6)
!
      END
!                                   External function to be minimized
      SUBROUTINE FCN (N, X, F)
      INTEGER    N
      REAL       X(N), F
!
      F = 100.0*(X(2)-X(1)*X(1))**2 + (1.0-X(1))**2
      RETURN
      END
```

Output

```
The best estimate for the minimum value of the
function is X = (  0.50  0.25)
with function value FVALUE = 0.250002E+00
```

Example 2

This example is intended to illustrate the use of optional arguments available for BCPOL, and how their use can affect the number of function calls needed to complete the optimization process. The same problem as in Example 1 is approached in five ways, including the use of a function penalty in an attempt to constrain the solution space. In each case the number of function evaluations required is output.

Solution 1 uses XLB and XUB to impose bounds, as in Example 1. Solutions 2 through 5 use a function penalty to impose constraints, and to varying degrees make use of optional arguments XCPLX, REFLCOEF, EXPNCOEF, and CNTRCOEF.

Note, the actual number of function calls required to complete the minimization process may vary, depending on the computing platform and precision used.

```
!
!                                    BCPOL_EX_2.F90
      USE BCPOL_INT
      USE UMACH_INT
      IMPLICIT NONE
!
      integer :: IBTYPE, MAXFCN, N
      integer, parameter :: NNN=2
      real(kind(1d0)) :: FTOL
      integer :: K, NOUT
      real(kind(1d0)) :: FVALUE
      integer :: ICTYPE
      integer :: I, II, JJ, IARGTST
      real(kind(1d0)) :: X(NNN), XLB(NNN), XUB(NNN)
      real(kind(1d0)) :: XCPLX0(NNN,2*NNN), XCPLX(NNN,2*NNN)
      real(kind(1d0)) :: ALFA, BETA, DGAMMA
!
!                                    SPECIFICATIONS FOR SUBROUTINES
      external  FCN, FCN2
      real(kind(1d0)), dimension(2) ::  XGUESS = (/ -1.2d0, 1.0d0 /)
      real(kind(1d0)), dimension(2) ::  XCN = (/ -2.0d0, -1.0d0 /), XCX = (/0.5d0, 2.0d0/)
      call umach (2, nout)
!
```

```
      IBTYPE = 0
      FTOL = 1.0d-15
      N = 2
      MAXFCN = 500
!                                  Constraints imposed with Bounds
      XLB(1) = -2.0d0
      XLB(2) = -1.0d0
      XUB(1) = 0.5d0
      XUB(2) = 2.0d0
!
      WRITE (NOUT,'(/"  Solution 1:")')
      WRITE (NOUT,'(/"  Bounds: XLB = (-2.0, -1.0);  XUB = (0.5, 2.0)")')
      WRITE (NOUT,'( "  Constraints imposed with Bounds")')
      WRITE (NOUT,'( "  using no optional complex or step-size arguments:")')
!
      CALL BCPOL (FCN, IBTYPE, XLB, XUB, X, n=N, xguess=XGUESS, &
                  ftol=FTOL, maxfcn=MAXFCN, fvalue=FVALUE)
!
      WRITE (NOUT,99999) (X(K),K=1,N), FVALUE, MAXFCN
!
!                                  Lower and Upper Bounds:
!                                   -2. <= X(1) <= 2. ;  -2. <= X(2) <= 2.;
!                                  Constraints:
!                                   -2. <= X(1) <= 0.5;  -1. <= X(2) <= 2.;
!
!                                  Constraints imposed with function penalties
!                                  User-supplied initial complex XCPLX
!                                  chosen to be within constraint boundaries
      XLB(1) = -2.0d0
      XUB(1) = 2.0d0
      XLB(2) = -2.0d0
      XUB(2) = 2.0d0
!
      XCPLX0(1,1) = XGUESS(1)
      XCPLX0(2,1) = XGUESS(2)
      XCPLX0(1,2) = XCX(1)
      XCPLX0(2,2) = XCX(2)
      XCPLX0(1,3) = XCN(1)
      XCPLX0(2,3) = XCN(2)
      XCPLX0(1,4) = XCX(1)
      XCPLX0(2,4) = XCN(2)
!
      IBTYPE = 0
      ALFA = 1.0d0
!
      WRITE (NOUT,'(/"----------------------------------------------"/)')
      WRITE (NOUT,'("  Solutions 2 - 5:"/)')
      WRITE (NOUT,'("  Constraints: -2. <= x(1) <= 0.5; -1. <= x(2) <= 2.")')
      WRITE (NOUT,'("  Bounds: XLB = (-2.0, -2.0);  XUB = (2.0, 2.0)")')
      WRITE (NOUT,'("  Constraints imposed with function penalties")')
      WRITE (NOUT,'("  using optional complex and step-size arguments:")')
!
!-----------------------------------------------------------------------
!
      WRITE (NOUT,'(/"----------------------------------------------"/)')
      WRITE (NOUT,'( "  Solutions 2 - 3:"/)')
      WRITE (NOUT,'( "  User Specified Initial Complex:")')
      WRITE (NOUT,'(/"----------------------------------------------"/)')
      WRITE (NOUT,'( "  Solution 2: step-size coefficients with default values:"/)')
!
      DO JJ=1,2*N
         DO II=1,N
            XCPLX(II,JJ) = XCPLX0(II,JJ)
         END DO
      END DO
      MAXFCN = 10000
```

```
      BETA = 2.0D+01
      DGAMMA = 0.5D+00
!
      WRITE (NOUT,99998) ALFA, BETA, DGAMMA
!
      CALL BCPOL (FCN2, IBTYPE, XLB, XUB, X, &
                  xguess=XGUESS, ftol=FTOL, maxfcn=MAXFCN, &
                  fvalue=FVALUE, xcplx=XCPLX)
!
      WRITE (NOUT,99999) (X(K),K=1,N), FVALUE, MAXFCN
!
!-----------------------------------------------------------------------
!
      WRITE (NOUT, '(/"-----------------------------------------------"/)')
      WRITE (NOUT,'("  Solution 3: step-size coefficients with user-specified values:"/)')
!
      DO JJ=1,2*N
         DO II=1,N
            XCPLX(II,JJ) = XCPLX0(II,JJ)
         END DO
      END DO
      MAXFCN = 10000
!
      BETA = 0.31841776469083554D+01
      DGAMMA = 0.33464404002126491D+00
!
      WRITE (NOUT,99998) ALFA, BETA, DGAMMA
!
      CALL BCPOL (FCN2, IBTYPE, XLB, XUB, X, &
                  xguess=XGUESS, ftol=FTOL, maxfcn=MAXFCN, &
                  fvalue=FVALUE, xcplx=XCPLX, &
                  reflcoef=ALFA, expncoef=BETA, cntrcoef=DGAMMA)
!
      WRITE (NOUT,99999) (X(K),K=1,N), FVALUE, MAXFCN
!
!-----------------------------------------------------------------------
!
      WRITE (NOUT,'(/"-----------------------------------------------"/)')
      WRITE (NOUT,'( "  Solutions 4 - 5:"/)')
      WRITE (NOUT,'( "  Randomly Generated Initial Complex:")')
      WRITE (NOUT,'(/"-----------------------------------------------"/)')
      WRITE (NOUT,'( "  Solution 4: step-size coefficients with default values:"/)')
!
      MAXFCN = 10000
      BETA = 2.0D+01
      DGAMMA = 0.5D+00
!
      WRITE (NOUT,99998) ALFA, BETA, DGAMMA
!
      CALL BCPOL (FCN2, IBTYPE, XLB, XUB, X, &
                  xguess=XGUESS, ftol=FTOL, maxfcn=MAXFCN, &
                  fvalue=FVALUE)
!
      WRITE (NOUT,99999) (X(K),K=1,N), FVALUE, MAXFCN
!
!-----------------------------------------------------------------------
!
      WRITE (NOUT, '(/"-----------------------------------------------"/)')
      WRITE (NOUT,'("  Solution 5: step-size coefficients with user-specified values:"/)')
!
      MAXFCN = 10000
!
      BETA = 0.18204845270362373D+02
      DGAMMA = 0.31542073037934792D+00
!
      WRITE (NOUT,99998) ALFA, BETA, DGAMMA
```

```
!
      CALL BCPOL (FCN2, IBTYPE, XLB, XUB, X, &
                  xguess=XGUESS, ftol=FTOL, maxfcn=MAXFCN, &
                  fvalue=FVALUE, &
                  reflcoef=ALFA, expncoef=BETA, cntrcoef=DGAMMA)
!
      WRITE (NOUT,99999) (X(K),K=1,N), FVALUE, MAXFCN
!
!-----------------------------------------------------------------------
!
99998 FORMAT ('  REFLCOEF = ', D25.17 / &
              '  EXPNCOEF = ', D25.17 / &
              '  CNTRCOEF = ', D25.17 )
!
99999 FORMAT (/'  The best estimate for the minimum value of the' / &
              '  function is X = ( ', d14.7,' , ', d14.7, ' )' / &
              '  with function value FVALUE = ', d14.7 / &
              '  and # fcn calls MAXFCN = ', I7 )
      end
!
!-----------------------------------------------------------------------
!
      SUBROUTINE FCN (N, X, F)
         integer :: N
         real(kind(1d0)) :: X(N), F
!
         F = 100.0*(X(2)-X(1)*X(1))**2 + (1.0-X(1))**2
!
         RETURN
      END
!
!-----------------------------------------------------------------------
!
      SUBROUTINE FCN2 (N, X, F)
         integer :: N
         real(kind(1d0)) :: X(N), F
!
         IF ( ((-2.0 .LE. X(1)) .AND. (X(1) .LE. 0.5)) .AND. &
              ((-1.0 .LE. X(2)) .AND. (X(2) .LE. 2.0))) THEN
            F = 100.0*(X(2)-X(1)*X(1))**2 + (1.0-X(1))**2
         ELSE
            F = 1000.
         END IF
!
         RETURN
      END
```

Output

```
  Solution 1:

  Bounds: XLB = (-2.0, -1.0);  XUB = (0.5, 2.0)
  Constraints imposed with Bounds
  using no optional complex or step-size arguments:

  The best estimate for the minimum value of the
  function is X = (  0.5000000D+00 ,  0.2500000D+00 )
  with function value FVALUE =  0.2500000D+00
  and # fcn calls MAXFCN =     226

----------------------------------------------

  Solutions 2 - 5:
```

```
  Constraints: -2. <= x(1) <= 0.5; -1. <= x(2) <= 2.
  Bounds: XLB = (-2.0, -2.0);  XUB = (2.0, 2.0)
  Constraints imposed with function penalties
  using optional complex and step-size arguments:

----------------------------------------------

  Solutions 2 - 3:

  User Specified Initial Complex:

----------------------------------------------

  Solution 2: step-size coefficients with default values:

  REFLCOEF =   0.10000000000000000D+01
  EXPNCOEF =   0.20000000000000000D+02
  CNTRCOEF =   0.50000000000000000D+00

  The best estimate for the minimum value of the
  function is X = (  0.5000000D+00 ,  0.2500000D+00 )
  with function value FVALUE =  0.2500000D+00
  and # fcn calls MAXFCN =     379

----------------------------------------------

  Solution 3: step-size coefficients with user-specified values:

  REFLCOEF =   0.10000000000000000D+01
  EXPNCOEF =   0.31841776469083554D+01
  CNTRCOEF =   0.33464404002126491D+00

  The best estimate for the minimum value of the
  function is X = (  0.5000000D+00 ,  0.2500000D+00 )
  with function value FVALUE =  0.2500000D+00
  and # fcn calls MAXFCN =     323

----------------------------------------------

  Solutions 4 - 5:

  Randomly Generated Initial Complex:

----------------------------------------------

  Solution 4: step-size coefficients with default values:

  REFLCOEF =   0.10000000000000000D+01
  EXPNCOEF =   0.20000000000000000D+02
  CNTRCOEF =   0.50000000000000000D+00

  The best estimate for the minimum value of the
  function is X = (  0.5000000D+00 ,  0.2500000D+00 )
  with function value FVALUE =  0.2500000D+00
  and # fcn calls MAXFCN =     430

----------------------------------------------

  Solution 5: step-size coefficients with user-specified values:

  REFLCOEF =   0.10000000000000000D+01
  EXPNCOEF =   0.18204845270362373D+02
  CNTRCOEF =   0.31542073037934792D+00

  The best estimate for the minimum value of the
  function is X = (  0.5000000D+00 ,  0.2500000D+00 )
```

```
    with function value FVALUE =  0.2500000D+00
    and # fcn calls MAXFCN =     294
```

BCLSF

more...

Solves a nonlinear least squares problem subject to bounds on the variables using a modified Levenberg-Marquardt algorithm and a finite-difference Jacobian.

Required Arguments

FCN — User-supplied subroutine to evaluate the function to be minimized. The usage is CALL FCN (M, N, X, F), where

M – Length of F. (Input)

N – Length of X. (Input)

X – The point at which the function is evaluated. (Input)
X should not be changed by FCN.

F – The computed function at the point X. (Output)

FCN must be declared EXTERNAL in the calling program.

M — Number of functions. (Input)

IBTYPE — Scalar indicating the types of bounds on variables. (Input)

IBTYPE	Action
0	User will supply all the bounds.
1	All variables are nonnegative.
2	All variables are nonpositive.
3	User supplies only the bounds on 1st variable, all other variables will have the same bounds.

XLB — Vector of length N containing the lower bounds on variables. (Input, if IBTYPE = 0; output, if IBTYPE = 1 or 2; input/output, if IBTYPE = 3)

XUB — Vector of length N containing the upper bounds on variables. (Input, if IBTYPE = 0; output, if IBTYPE = 1 or 2; input/output, if IBTYPE = 3)

X — Vector of length N containing the approximate solution. (Output)

Optional Arguments

N — Number of variables. (Input)
N must be less than or equal to M.
Default: N = SIZE (X,1).

XGUESS — Vector of length N containing the initial guess. (Input)
Default: XGUESS = 0.0.

XSCALE — Vector of length N containing the diagonal scaling matrix for the variables. (Input)
XSCALE is used mainly in scaling the gradient and the distance between two points. By default, the values for XSCALE are set internally. See IPARAM(6) in Comment 4.

FSCALE — Vector of length M containing the diagonal scaling matrix for the functions. (Input)
FSCALE is used mainly in scaling the gradient. In the absence of other information, set all entries to 1.0.
Default: FSCALE = 1.0.

IPARAM — Parameter vector of length 6. (Input/Output)
Set IPARAM(1) to zero for default values of IPARAM and RPARAM. See Comment 4.
Default: IPARAM= 0.

RPARAM — Parameter vector of length 7. (Input/Output)
See Comment 4.

FVEC — Vector of length M containing the residuals at the approximate solution. (Output)

FJAC — M by N matrix containing a finite difference approximate Jacobian at the approximate solution. (Output)

LDFJAC — Leading dimension of FJAC exactly as specified in the dimension statement of the calling program. (Input)
Default: LDFJAC = SIZE (FJAC ,1).

FORTRAN 90 Interface

Generic: CALL BCLSF (FCN, M, IBTYPE, XLB, XUB, X [, …])

Specific: The specific interface names are S_BCLSF and D_BCLSF.

FORTRAN 77 Interface

Single: `CALL BCLSF (FCN, M, N, XGUESS, IBTYPE, XLB, XUB, XSCALE, FSCALE, IPARAM, RPARAM, X, FVEC, FJAC, LDFJAC)`

Double: The double precision name is `DBCLSF`.

Description

The routine `BCLSF` uses a modified Levenberg-Marquardt method and an active set strategy to solve nonlinear least squares problems subject to simple bounds on the variables. The problem is stated as follows:

$$\min_{x \in \mathbf{R}^n} \frac{1}{2} F(x)^T F(x) = \frac{1}{2} \sum_{i=1}^{m} f_i(x)^2$$

$$\text{subject to } l \le x \le u$$

where $m \ge n$, $F : \mathbf{R}^n \to \mathbf{R}^m$, and $f_i(x)$ is the i-th component function of $F(x)$. From a given starting point, an active set IA, which contains the indices of the variables at their bounds, is built. A variable is called a “free variable” if it is not in the active set. The routine then computes the search direction for the free variables according to the formula

$$d = -(J^T J + \mu I)^{-1} J^T F$$

where μ is the Levenberg-Marquardt parameter, $F = F(x)$, and J is the Jacobian with respect to the free variables. The search direction for the variables in IA is set to zero. The trust region approach discussed by Dennis and Schnabel (1983) is used to find the new point. Finally, the optimality conditions are checked. The conditions are

$$\|g(x_i)\| \le \varepsilon, \, l_i < x_i < u_i$$

$$g(x_i) < 0, \;\; x_i = u_i$$

$$g(x_i) > 0, \, x_i = l_i$$

where ε is a gradient tolerance. This process is repeated until the optimality criterion is achieved.

The active set is changed only when a free variable hits its bounds during an iteration or the optimality condition is met for the free variables but not for all variables in IA, the active set. In the latter case, a variable that violates the optimality condition will be dropped out of IA. For more detail on the Levenberg-Marquardt method, see Levenberg (1944), or Marquardt (1963). For more detailed information on active set strategy, see Gill and Murray (1976).

Since a finite-difference method is used to estimate the Jacobian for some single precision calculations, an inaccurate estimate of the Jacobian may cause the algorithm to terminate at a noncritical point. In such cases, high precision arithmetic is recommended. Also, whenever the exact Jacobian can be easily provided, routine BCLSJ should be used instead.

Comments

1. Workspace may be explicitly provided, if desired, by use of B2LSF/DB2LSF. The reference is:

```
CALL B2LSF (FCN, M, N, XGUESS, IBTYPE, XLB, XUB, XSCALE,
   FSCALE, IPARAM, RPARAM, X, FVEC, FJAC, LDFJAC, WK, IWK)
```

   The additional arguments are as follows:

   WK — Work vector of length 11 * N + 3 * M – 1. WK contains the following information on output: The second N locations contain the last step taken. The third N locations contain the last Gauss-Newton step. The fourth N locations contain an estimate of the gradient at the solution.

   IWK — Work vector of length 2 * N containing the permutations used in the QR factorization of the Jacobian at the solution.

2. Informational errors

Type	Code	Description
3	1	Both the actual and predicted relative reductions in the function are less than or equal to the relative function convergence tolerance.
3	2	The iterates appear to be converging to a noncritical point.
4	3	Maximum number of iterations exceeded.
4	4	Maximum number of function evaluations exceeded.
3	6	Five consecutive steps have been taken with the maximum step length.
2	7	Scaled step tolerance satisfied; the current point may be an approximate local solution, or the algorithm is making very slow progress and is not near a solution, or STEPTL is too big.

3. The first stopping criterion for BCLSF occurs when the norm of the function is less than the absolute function tolerance. The second stopping criterion occurs when the norm of the scaled gradient is less than the given gradient tolerance. The third stopping criterion for BCLSF occurs when the scaled distance between the last two steps is less than the step tolerance.

4. If the default parameters are desired for BCLSF, then set IPARAM(1) to zero and call the routine BCLSF. Otherwise, if any nondefault parameters are desired for IPARAM or RPARAM, then the following steps should be taken before calling BCLSF:

```
CALL U4LSF (IPARAM, RPARAM)
```

Set nondefault values for desired `IPARAM`, `RPARAM` elements.

Note that the call to `U4LSF` will set `IPARAM` and `RPARAM` to their default values so only nondefault values need to be set above.

The following is a list of the parameters and the default values:

IPARAM — Integer vector of length 6.

`IPARAM`(1) = Initialization flag.

`IPARAM`(2) = Number of good digits in the function.
Default: Machine dependent.

`IPARAM`(3) = Maximum number of iterations.
Default: 100.

`IPARAM`(4) = Maximum number of function evaluations.
Default: 400.

`IPARAM`(5) = Maximum number of Jacobian evaluations.
Default: 100.

`IPARAM`(6) = Internal variable scaling flag.
If `IPARAM`(6) = 1, then the values for `XSCALE` are set internally.
Default: 1.

RPARAM — Real vector of length 7.

`RPARAM`(1) = Scaled gradient tolerance.
The *i*-th component of the scaled gradient at x is calculated as

$$\frac{|g_i| * \max\left(|x_i|, 1/s_i\right)}{\|F(x)\|_2^2}$$

where

$$g_i = \left(J(x)^T F(x)\right)_i * \left(f_s\right)_i^2$$

$J(x)$ is the Jacobian, s = `XSCALE`, and f_s = `FSCALE`.
Default:

$$\sqrt{\varepsilon}, \sqrt[3]{\varepsilon}$$

in double where **ε** is the machine precision.

RPARAM(2) = Scaled step tolerance. (STEPTL)
The i-th component of the scaled step between two points *x* and *y* is computed as

$$\frac{|x_i - y_i|}{\max\left(|x_i|, 1/s_i\right)}$$

where *s* = XSCALE.
Default: $\varepsilon^{2/3}$ where ε is the machine precision.

RPARAM(3) = Relative function tolerance.
Default: $\max(10^{-10}, \varepsilon^{2/3})$, $\max(10^{-20}, \varepsilon^{2/3})$ in double where ε is the machine precision.

RPARAM(4) = Absolute function tolerance.
Default: $\max(10^{-20}\ \varepsilon^{2})$, $\max(10^{-40}, \varepsilon^{2})$ in double where ε is the machine precision.

RPARAM(5) = False convergence tolerance.
Default: 100 ε where ε is the machine precision.

RPARAM(6) = Maximum allowable step size.
Default: 1000 $\max(\varepsilon_1, \varepsilon_2)$ where

$$\varepsilon_1 = \sqrt{\sum_{i=1}^{n}\left(s_i t_i\right)^2}$$

$\varepsilon_2 = \|s\|_2$, *s* = XSCALE, and *t* = XGUESS.

RPARAM(7) = Size of initial trust region radius.
Default: based on the initial scaled Cauchy step.

If double precision is desired, then DU4LSF is called and RPARAM is declared double precision.

5. Users wishing to override the default print/stop attributes associated with error messages issued by this routine are referred to “Error Handling” in the Introduction.

Example

The nonlinear least squares problem

$$\min_{x\in\mathrm{R}^2} \frac{1}{2}\sum_{i=1}^{2} f_i(x)^2$$

$$\text{subject to } -2 \le x_1 \le 0.5$$

$$-1 \le x_2 \le 2$$

where

$$f_1(x) = 10\left(x_2 - x_1^2\right) \text{ and } f_2(x) = \left(1 - x_1\right)$$

is solved with an initial guess (−1.2, 1.0) and default values for parameters.

```
      USE BCLSF_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                 Declaration of variables
      INTEGER    M, N
      PARAMETER  (M=2, N=2)
!
      INTEGER    IPARAM(7), ITP, NOUT
      REAL       FSCALE(M), FVEC(M), X(N), XGUESS(N), XLB(N), XS(N), XUB(N)
      EXTERNAL   ROSBCK
!                                 Compute the least squares for the
!                                 Rosenbrock function.
      DATA XGUESS/-1.2E0, 1.0E0/
      DATA XLB/-2.0E0, -1.0E0/, XUB/0.5E0, 2.0E0/
!                                 All the bounds are provided
      ITP = 0
!                                 Default parameters are used
      IPARAM(1) = 0
!
      CALL BCLSF (ROSBCK, M, ITP, XLB, XUB, X, xguess=xguess, &
                 iparam=iparam, fvec=fvec)
!                                 Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) X, FVEC, IPARAM(3), IPARAM(4)
!
99999 FORMAT ('  The solution is ', 2F9.4, //, '  The function ', &
            'evaluated at the solution is ', /, 18X, 2F9.4, //, &
            '  The number of iterations is ', 10X, I3, /, '  The ', &
            'number of function evaluations is ', I3, /)
      END
!
      SUBROUTINE ROSBCK (M, N, X, F)
      INTEGER    M, N
      REAL       X(N), F(M)
!
      F(1) = 1.0E1*(X(2)-X(1)*X(1))
      F(2) = 1.0E0 - X(1)
      RETURN
      END
```

Output

```
The solution is     0.5000   0.2500

The function evaluated at the solution is
0.0000   0.5000

The number of iterations is            15
The number of function evaluations is  20
```

BCLSJ

more...

Solves a nonlinear least squares problem subject to bounds on the variables using a modified Levenberg-Marquardt algorithm and a user-supplied Jacobian.

Required Arguments

FCN — User-supplied subroutine to evaluate the function to be minimized. The usage is
`CALL FCN (M, N, X, F)`, where

`M` – Length of `F`. (Input)

`N` – Length of `X`. (Input)

`X` – The point at which the function is evaluated. (Input)
`X` should not be changed by `FCN`.

`F` – The computed function at the point `X`. (Output)

`FCN` must be declared `EXTERNAL` in the calling program.

JAC — User-supplied subroutine to evaluate the Jacobian at a point `X`. The usage is
`CALL JAC (M, N, X, FJAC, LDFJAC)`, where

`M` – Length of `F`. (Input)

`N` – Length of `X`. (Input)

`X` – The point at which the function is evaluated. (Input)
`X` should not be changed by `FCN`.

`FJAC` – The computed `M` by `N` Jacobian at the point `X`. (Output)

`LDFJAC` – Leading dimension of `FJAC`. (Input)

`JAC` must be declared `EXTERNAL` in the calling program.

M — Number of functions. (Input)

IBTYPE — Scalar indicating the types of bounds on variables. (Input)

IBTYPE	Action
0	User will supply all the bounds.
1	All variables are nonnegative.
2	All variables are nonpositive.
3	User supplies only the bounds on 1st variable, all other variables will have the same bounds.

XLB — Vector of length `N` containing the lower bounds on variables. (Input, if `IBTYPE` = 0; output, if `IBTYPE` = 1 or 2; input/output, if `IBTYPE` = 3)

XUB — Vector of length `N` containing the upper bounds on variables. (Input, if `IBTYPE` = 0; output, if `IBTYPE` = 1 or 2; input/output, if `IBTYPE` = 3)

X — Vector of length `N` containing the approximate solution. (Output)

Optional Arguments

N — Number of variables. (Input)
`N` must be less than or equal to `M`.
Default: `N` = `SIZE` (X,1).

XGUESS — Vector of length `N` containing the initial guess. (Input)
Default: `XGUESS` = 0.0.

XSCALE — Vector of length `N` containing the diagonal scaling matrix for the variables. (Input)
`XSCALE` is used mainly in scaling the gradient and the distance between two points. By default, the values for `XSCALE` are set internally. See `IPARAM`(6) in Comment 4.

FSCALE — Vector of length `M` containing the diagonal scaling matrix for the functions. (Input)
`FSCALE` is used mainly in scaling the gradient. In the absence of other information, set all entries to 1.0.
Default: `FSCALE` = 1.0.

IPARAM — Parameter vector of length 6. (Input/Output)
Set `IPARAM`(1) to zero for default values of `IPARAM` and `RPARAM`. See Comment 4.
Default: `IPARAM`= 0.

RPARAM — Parameter vector of length 7. (Input/Output)
See Comment 4.

FVEC — Vector of length `M` containing the residuals at the approximate solution. (Output)

FJAC — M by N matrix containing a finite difference approximate Jacobian at the approximate solution. (Output)

LDFJAC — Leading dimension of FJAC exactly as specified in the dimension statement of the calling program. (Input)
Default: LDFJAC = SIZE(FJAC,1).

FORTRAN 90 Interface

Generic: CALL BCLSJ (FCN, JAC, M, IBTYPE, XLB, XUB, X [, …])

Specific: The specific interface names are S_BCLSJ and D_BCLSJ.

FORTRAN 77 Interface

Single: CALL BCLSJ (FCN, JAC, M, N, XGUESS, IBTYPE, XLB, XUB, XSCALE, FSCALE, IPARAM, RPARAM, X, FVEC, FJAC, LDFJAC)

Double: The double precision name is DBCLSJ.

Description

The routine BCLSJ uses a modified Levenberg-Marquardt method and an active set strategy to solve nonlinear least squares problems subject to simple bounds on the variables. The problem is stated as follows:

$$\min_{x \in \mathbf{R}^n} \frac{1}{2} F(x)^T F(x) = \frac{1}{2} \sum_{i=1}^{m} f_i(x)^2$$

$$\text{subject to } l \le x \le u$$

where $m \ge n$, $F : \mathbf{R}^n \rightarrow \mathbf{R}^m$, and $f_i(x)$ is the i-th component function of $F(x)$. From a given starting point, an active set IA, which contains the indices of the variables at their bounds, is built. A variable is called a “free variable” if it is not in the active set. The routine then computes the search direction for the free variables according to the formula

$$d = -(J^T J + \mu I)^{-1} J^T F$$

where μ is the Levenberg-Marquardt parameter, $F = F(x)$, and J is the Jacobian with respect to the free variables. The search direction for the variables in IA is set to zero. The trust region approach discussed by Dennis and Schnabel (1983) is used to find the new point. Finally, the optimality conditions are checked. The conditions are

$$\|g(x_i)\| \le \varepsilon, \; l_i < x_i < u_i$$

$$g(x_i) < 0, \;\; x_i = u_i$$

$$g(x_i) > 0, x_i = l_i$$

where **ε** is a gradient tolerance. This process is repeated until the optimality criterion is achieved.

The active set is changed only when a free variable hits its bounds during an iteration or the optimality condition is met for the free variables but not for all variables in IA, the active set. In the latter case, a variable that violates the optimality condition will be dropped out of IA. For more detail on the Levenberg-Marquardt method, see Levenberg (1944) or Marquardt (1963). For more detailed information on active set strategy, see Gill and Murray (1976).

Comments

1. Workspace may be explicitly provided, if desired, by use of `B2LSJ/DB2LSJ`. The reference is:

```
CALL B2LSJ (FCN, JAC, M, N, XGUESS, IBTYPE, XLB, XUB,
   XSCALE, FSCALE, IPARAM, RPARAM, X, FVEC, FJAC, LDFJAC, WK,
   IWK)
```

   The additional arguments are as follows:

   WK — Work vector of length 11 * `N` + 3 * `M` − 1. `WK` contains the following information on output: The second `N` locations contain the last step taken. The third `N` locations contain the last Gauss-Newton step. The fourth `N` locations contain an estimate of the gradient at the solution.

   IWK — Work vector of length 2 * `N` containing the permutations used in the `QR` factorization of the Jacobian at the solution.

2. Informational errors

Type	**Code**	**Description**
3	1	Both the actual and predicted relative reductions in the function are less than or equal to the relative function convergence tolerance.
3	2	The iterates appear to be converging to a noncritical point.
4	3	Maximum number of iterations exceeded.
4	4	Maximum number of function evaluations exceeded.
3	6	Five consecutive steps have been taken with the maximum step length.
4	5	Maximum number of Jacobian evaluations exceeded.
2	7	Scaled step tolerance satisfied; the current point may be an approximate local solution, or the algorithm is making very slow progress and is not near a solution, or `STEPTL` is too big.

3. The first stopping criterion for `BCLSJ` occurs when the norm of the function is less than the absolute function tolerance. The second stopping criterion occurs when the norm of the scaled gradient is less than the given gradient tolerance. The third stopping criterion for `BCLSJ` occurs when the scaled distance between the last two steps is less than the step tolerance.

4. If the default parameters are desired for BCLSJ, then set IPARAM(1) to zero and call the routine BCLSJ. Otherwise, if any nondefault parameters are desired for IPARAM or RPARAM, then the following steps should be taken before calling BCLSJ:

   CALL U4LSF (IPARAM, RPARAM)

   Set nondefault values for desired IPARAM, RPARAM elements.

Note that the call to U4LSF will set IPARAM and RPARAM to their default values so only nondefault values need to be set above.

The following is a list of the parameters and the default values:

IPARAM — Integer vector of length 6.

IPARAM(1) = Initialization flag.

IPARAM(2) = Number of good digits in the function.
Default: Machine dependent.

IPARAM(3) = Maximum number of iterations.
Default: 100.

IPARAM(4) = Maximum number of function evaluations.
Default: 400.

IPARAM(5) = Maximum number of Jacobian evaluations.
Default: 100.

IPARAM(6) = Internal variable scaling flag.

If IPARAM(6) = 1, then the values for XSCALE are set internally.
Default: 1.

RPARAM — Real vector of length 7.

RPARAM(1) = Scaled gradient tolerance.
The *i*-th component of the scaled gradient at x is calculated as

$$\frac{|g_i| * \max\left(|x_i|, 1/s_i\right)}{\|F(x)\|_2^2}$$

where

$$g_i = \left(J(x)^T F(x)\right)_i * \left(f_s\right)_i^2$$

J(*x*) is the Jacobian, *s* = XSCALE, and f_s = FSCALE.
Default:

$$\sqrt{\varepsilon}, \sqrt[3]{\varepsilon}$$

in double where **ε** is the machine precision.

RPARAM(2) = Scaled step tolerance. (STEPTL)
The i-th component of the scaled step between two points x and y is computed as

$$\frac{|x_i - y_i|}{\max\left(|x_i|, 1/s_i\right)}$$

where s = XSCALE.
Default: $\varepsilon^{2/3}$ where ε is the machine precision.

RPARAM(3) = Relative function tolerance.
Default: $\max(10^{-10}, \varepsilon^{2/3})$, $\max(10^{-20}, \varepsilon^{2/3})$ in double where ε is the machine precision.

RPARAM(4) = Absolute function tolerance.
Default: $\max(10^{-20}, \varepsilon^2)$, $\max(10^{-40}, \varepsilon^2)$ in double where ε is the machine precision.

RPARAM(5) = False convergence tolerance.
Default: 100ε where ε is the machine precision.

RPARAM(6) = Maximum allowable step SIZE.
Default: $1000 \max(\varepsilon_1, \varepsilon_2)$ where

$$\varepsilon_1 = \sqrt{\sum_{i=1}^{n} \left(s_i t_i\right)^2}$$

$\varepsilon_2 = \|s\|_2$, s = XSCALE, and t = XGUESS.

RPARAM(7) = Size of initial trust region radius.
Default: based on the initial scaled Cauchy step.

If double precision is desired, then DU4LSF is called and RPARAM is declared double precision.

5. Users wishing to override the default print/stop attributes associated with error messages issued by this routine are referred to ERROR HANDLING in the Introduction.

Example

The nonlinear least squares problem

$$\min_{x \in R^2} \frac{1}{2} \sum_{i=1}^{2} f_i(x)^2$$

$$\text{subject to } -2 \le x_1 \le 0.5$$

$$-1 \le x_2 \le 2$$

where

$$f_1(x) = 10\left(x_2 - x_1^2\right) \text{ and } f_2(x) = \left(1 - x_1\right)$$

is solved with an initial guess (−1.2, 1.0) and default values for parameters.

```
      USE BCLSJ_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                 Declaration of variables
      INTEGER    LDFJAC, M, N
      PARAMETER  (LDFJAC=2, M=2, N=2)
!
      INTEGER    IPARAM(7), ITP, NOUT
      REAL       FVEC(M), RPARAM(7), X(N), XGUESS(N), XLB(N), XUB(N)
      EXTERNAL   ROSBCK, ROSJAC
!                                 Compute the least squares for the
!                                 Rosenbrock function.
      DATA XGUESS/-1.2E0, 1.0E0/
      DATA XLB/-2.0E0, -1.0E0/, XUB/0.5E0, 2.0E0/
!                                 All the bounds are provided
      ITP = 0
!                                 Default parameters are used
      IPARAM(1) = 0
!
      CALL BCLSJ (ROSBCK,ROSJAC,M,ITP,XLB,XUB,X,XGUESS=XGUESS, &
                 IPARAM=IPARAM, FVEC=FVEC)
!                                 Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) X, FVEC, IPARAM(3), IPARAM(4)
!
99999 FORMAT ('  The solution is ', 2F9.4, //, '  The function ', &
            'evaluated at the solution is ', /, 18X, 2F9.4, //, &
            '  The number of iterations is ', 10X, I3, /, '  The ', &
            'number of function evaluations is ', I3, /)
      END
!
      SUBROUTINE ROSBCK (M, N, X, F)
      INTEGER    M, N
      REAL       X(N), F(M)
!
      F(1) = 1.0E1*(X(2)-X(1)*X(1))
      F(2) = 1.0E0 - X(1)
      RETURN
      END
!
      SUBROUTINE ROSJAC (M, N, X, FJAC, LDFJAC)
      INTEGER    M, N, LDFJAC
      REAL       X(N), FJAC(LDFJAC,N)
!
      FJAC(1,1) = -20.0E0*X(1)
      FJAC(2,1) = -1.0E0
      FJAC(1,2) = 10.0E0
      FJAC(2,2) = 0.0E0
      RETURN
      END
```

Output

```
The solution is    0.5000   0.2500
```

```
The function evaluated at the solution is
0.0000   0.5000

The number of iterations is            13
The number of function evaluations is  21
```

BCNLS

more...

Solves a nonlinear least-squares problem subject to bounds on the variables and general linear constraints.

Required Arguments

FCN — User-supplied subroutine to evaluate the function to be minimized. The usage is `CALL FCN (M, N, X, F)`, where

`M` – Number of functions. (Input)

`N` – Number of variables. (Input)

`X` – Array of length `N` containing the point at which the function will be evaluated. (Input)

`F` – Array of length `M` containing the computed function at the point `X`. (Output)

The routine `FCN` must be declared `EXTERNAL` in the calling program.

M — Number of functions. (Input)

C — `MCON` × `N` matrix containing the coefficients of the `MCON` general linear constraints. (Input)

BL — Vector of length `MCON` containing the lower limit of the general constraints. (Input).

BU — Vector of length `MCON` containing the upper limit of the general constraints. (Input).

IRTYPE — Vector of length `MCON` indicating the types of general constraints in the matrix `C`. (Input)
Let `R(I)` = `C(I, 1)*X(1)` + … + `C(I, N)*X(N)`. Then the value of `IRTYPE(I)` signifies the following:

IRTYPE(I)	I-th CONSTRAINT
0	`BL(I).EQ.R(I).EQ.BU(I)`
1	`R(I).LE.BU(I)`
2	`R(I).GE.BL(I)`
3	`BL(I).LE.R(I).LE.BU(I)`

XLB — Vector of length N containing the lower bounds on variables; if there is no lower bound on a variable, then 1.0E30 should be set as the lower bound. (Input)

XUB — Vector of length N containing the upper bounds on variables; if there is no upper bound on a variable, then −1.0E30 should be set as the upper bound. (Input)

X — Vector of length N containing the approximate solution. (Output)

Optional Arguments

N — Number of variables. (Input)
Default: N = SIZE (C,2).

MCON — The number of general linear constraints for the system, not including simple bounds. (Input)
Default: MCON = SIZE (C,1).

LDC — Leading dimension of C exactly as specified in the dimension statement of the calling program. (Input)
LDC must be at least MCON.

Default: LDC = SIZE (C,1).

XGUESS — Vector of length N containing the initial guess. (Input)
Default: XGUESS = 0.0.

RNORM — The Euclidean length of components of the function $f(x)$ after the approximate solution has been found. (Output).

ISTAT — Scalar indicating further information about the approximate solution X. (Output)
See the Comments section for a description of the tolerances and the vectors IPARAM and RPARAM.

ISTAT	Meaning
1	The function $f(x)$ has a length less than TOLF = RPARAM(1). This is the expected value for ISTAT when an actual zero value of $f(x)$ is anticipated.
2	The function $f(x)$ has reached a local minimum. This is the expected value for ISTAT when a nonzero value of $f(x)$ is anticipated.
3	A small change (absolute) was noted for the vector x. A full model problem step was taken. The condition for ISTAT = 2 may also be satisfied, so that a minimum has been found. However, this test is made before the test for ISTAT = 2.

ISTAT	Meaning
4	A small change (relative) was noted for the vector *x*. A full model problem step was taken. The condition for ISTAT = 2 may also be satisfied, so that a minimum has been found. However, this test is made before the test for ISTAT = 2.
5	The number of terms in the quadratic model is being restricted by the amount of storage allowed for that purpose. It is suggested, but not required, that additional storage be given for the quadratic model parameters. This is accessed through the vector ***IPARAM***, documented below.
6	Return for evaluation of function and Jacobian if reverse communication is desired. See the Comments below.

FORTRAN 90 Interface

Generic: CALL BCNLS (FCN, M, C, BL, BU, IRTYPE, XLB, XUB, X [, …])

Specific: The specific interface names are S_BCNLS and D_BCNLS.

FORTRAN 77 Interface

Single: CALL BCNLS (FCN, M, N, MCON, C, LDC, BL, BU, IRTYPE, XLB, XUB, XGUESS, X, RNORM, ISTAT)

Double: The double precision name is DBCNLS.

Description

The routine BCNLS solves the nonlinear least squares problem

$$\min \sum_{i=1}^{m} f_i(x)^2$$

subject to

$$b_l \le Cx \le b_u$$
$$x_l \le x \le x_u$$

BCNLS is based on the routine DQED by R.J. Hanson and F.T. Krogh. The section of BCNLS that approximates, using finite differences, the Jacobian of *f(x)* is a modification of JACBF by D.E. Salane.

Comments

1. Workspace may be explicitly provided, if desired, by use of B2NLS/DB2NLS. The reference is:

```
CALL B2NLS (FCN, M, N, MCON, C, LDC, BL, BU, IRTYPE, XLB,
   XUB, XGUESS, X, RNORM,ISTAT, IPARAM, RPARAM, JAC, F, FJ,
   LDFJ, IWORK, LIWORK, WORK, LWORK)
```

The additional arguments are as follows:

IPARAM — Integer vector of length six used to change certain default attributes of BCNLS. (Input).
If the default parameters are desired for B2NLS, set IPARAM(1) to zero. Otherwise, if any nondefault parameters are desired for IPARAM or RPARAM, the following steps should be taken before calling B2NLS:

CALL B7NLS (IPARAM, RPARAM)

Set nondefault values for IPARAM and RPARAM.
If double precision is being used, DB7NLS should be called instead. Following is a list of parameters and the default values.

IPARAM(1) = Initialization flag.

IPARAM(2) = ITMAX, the maximum number of iterations allowed.
Default: 75

IPARAM(3) = a flag that suppresses the use of the quadratic model in the inner loop. If set to one, then the quadratic model is never used. Otherwise use the quadratic model where appropriate. This option decreases the amount of workspace as well as the computing overhead required. A user may wish to determine if the application really requires the use of the quadratic model.
Default: 0

IPARAM(4) = NTERMS, one more than the maximum number of terms used in the quadratic model.
Default: 5

IPARAM(5) = RCSTAT, a flag that determines whether forward or reverse communication is used. If set to zero, forward communication through functions FCN and JAC is used. If set to one, reverse communication is used, and the dummy routines B10LS/DB10LS and B11LS/DB11LS may be used in place of FCN and JAC, respectively. When BCNLS returns with ISTAT = 6, arrays F and FJ are filled with $f(x)$ and the Jacobian of $f(x)$, respectively. BCNLS is then called again.

Default: 0

IPARAM(6) = a flag that determines whether the analytic Jacobian, as supplied in JAC, is used, or if a finite difference approximation is computed. If set to zero, JAC is not accessed and finite differences are used. If set to one, JAC is used to compute the Jacobian.
Default: 0

RPARAM — Real vector of length 7 used to change certain default attributes of BCNLS. (Input)
For the description of RPARAM, we make the following definitions:

FCcurrent value of the length of $f(x)$
FBbest value of length of $f(x)$
FLvalue of length of $f(x)$ at the previous step
PVpredicted value of length of $f(x)$, after the step is taken, using the approximating model **ε** machine epsilon = amach(4).

The conditions |FB − PV| ≤ TOLSNR*FB and |FC − PV| ≤ TOLP*FB and |FC − FL| ≤ TOLSNR*FB together with taking a full model step, must be satisfied before the condition ISTAT = 2 is returned. (Decreasing any of the values for TOLF, TOLD, TOLX, TOLSNR, or TOLP will likely increase the number of iterations required for convergence.)

RPARAM(1) = TOLF, tolerance used for stopping when FC ≤ TOLF.

$$Default\ :\ \min\left(1.E-5, \sqrt{\varepsilon}\right)$$

RPARAM(2) = TOLX, tolerance for stopping when change to *x* values has length less than or equal to TOLX*length of *x* values.

$$Default\ :\ \min\left(1.E-5, \sqrt{\varepsilon}\right)$$

RPARAM(3) = TOLD, tolerance for stopping when change to *x* values has length less than or equal to TOLD.

$$Default\ :\ \min\left(1.E-5, \sqrt{\varepsilon}\right)$$

RPARAM(4) = TOLSNR, tolerance used in stopping condition ISTAT = 2.
Default: 1.E5

RPARAM(5) = TOLP, tolerance used in stopping condition ISTAT = 2.
Default: 1.E5

RPARAM(6) = TOLUSE, tolerance used to avoid values of *x* in the quadratic model's interpolation of previous points. Decreasing this value may result in more terms being included in the quadratic model.

$$Default{:}\sqrt{\varepsilon}$$

RPARAM(7) = COND, largest condition number to allow when solving for the quadratic model coefficients. Increasing this value may result in more terms being included in the quadratic model.
Default: 30

JAC — User-supplied subroutine to evaluate the Jacobian. The usage is
CALL JAC (M, N, X, FJAC, LDFJAC), where
M – Number of functions. (Input)
N – Number of variables. (Input)
X – Array of length N containing the point at which the Jacobian will be evaluated. (Input)
FJAC – The computed M × N Jacobian at the point X. (Output)
LDFJAC – Leading dimension of the array FJAC. (Input)
The routine JAC must be declared EXTERNAL in the calling program.

F — Real vector of length N used to pass *f*(*x*) if reverse communication (IPARAM(4)) is enabled. This array must be allocated regardless of the setting of (IPARAM(4)). (Input)

FJ — Real array of size M × N. It is used to store the Jacobian matrix of *f*(*x*) if reverse communication (IPARAM(4)) is enabled. This array must be allocated regardless of the setting of (IPARAM(4)). (Input)
Specifically,

$$FJ\left(i,j\right) = \frac{\partial f_i}{\partial x_j}$$

LDFJ — Leading dimension of FJ exactly as specified in the dimension statement of the calling program. (Input)

IWORK — Integer work vector of length LIWORK.

LIWORK — Length of work vector IWORK. LIWORK must be at least
5MCON + 12N + 47 + MAX(M, N)

WORK — Real work vector of length LWORK

LWORK — Length of work vector WORK. LWORK must be at least
41N + 6M + 11MCON + (M + MCON) (N + 1) + NA (NA + 7) + 8 MAX (M, N) + 99.
Where NA = MCON + 2N + 6.

2. Informational errors

Type	Code	Description
3	1	The function *f*(*x*) has reached a value that may be a local minimum. However, the bounds on the trust region defining the size of the step are being hit at each step. Thus, the situation is suspect. (Situations of this type can occur when the solution is at infinity at some of the components of the unknowns, *x*).
3	2	The model problem solver has noted a value for the linear or quadratic model problem residual vector length that is greater than or equal to the current value of the function, i.e. the Euclidean length of *f*(*x*). This situation probably means that the evaluation of *f (x)* has more uncertainty or noise than is possible to account for in the tolerances used to not a local minimum. The value of *x* is suspect, but a minimum has probably been found.
3	3	More than ITMAX iterations were taken to obtain the solution. The value obtained for *x* is suspect, although it is the best set of *x* values that occurred in the entire computation. The value of ITMAX can be increased though the IPARAM vector.

Examples

Example 1

This example finds the four variables x_1, x_2, x_3, x_4 that are in the model function

$$h(t) = x_1 e^{x_2 t} + x_3 e^{x_4 t}$$

There are values of *h(t)* at five values of *t*.

h(0.05) = 2.206

h(0.1) = 1.994

h(0.4) = 1.35

h(0.5) = 1.216

h(1.0) = 0.7358

There are also the constraints that x_2, $x_4 \le 0$, x_1, $x_3 \ge 0$, and x_2 and x_4 must be separated by at least 0.05. Nothing more about the values of the parameters is known so the initial guess is 0.

```
      USE BCNLS_INT
      USE UMACH_INT
      USE WRRRN_INT

      IMPLICIT   NONE
      INTEGER    MCON, N
      PARAMETER  (MCON=1, N=4)
!                                 SPECIFICATIONS FOR PARAMETERS
      INTEGER    LDC, M
      PARAMETER  (M=5, LDC=MCON)
!                                 SPECIFICATIONS FOR LOCAL VARIABLES
      INTEGER    IRTYPE(MCON), NOUT
      REAL       BL(MCON), C(MCON,N), RNORM, X(N), XLB(N), &
                XUB(N)
!                                 SPECIFICATIONS FOR SUBROUTINES
!                                 SPECIFICATIONS FOR FUNCTIONS
      EXTERNAL   FCN
!
      CALL UMACH (2, NOUT)
!                                 Define the separation between x(2)
!                                 and x(4)
      C(1,1) = 0.0
      C(1,2) = 1.0
      C(1,3) = 0.0
      C(1,4) = -1.0
      BL(1)  = 0.05
      IRTYPE(1) = 2
!                                 Set lower bounds on variables
      XLB(1) = 0.0
      XLB(2) = 1.0E30
      XLB(3) = 0.0
      XLB(4) = 1.0E30
!                                 Set upper bounds on variables
      XUB(1) = -1.0E30
      XUB(2) = 0.0
      XUB(3) = -1.0E30
      XUB(4) = 0.0
!
      CALL BCNLS (FCN, M, C, BL, BL, IRTYPE, XLB, XUB, X, RNORM=RNORM)
      CALL WRRRN ('X', X, 1, N, 1)
      WRITE (NOUT,99999) RNORM
99999 FORMAT (/, 'rnorm = ', E10.5)
      END
```

```
!
      SUBROUTINE FCN (M, N, X, F)
!                                  SPECIFICATIONS FOR ARGUMENTS
      INTEGER    M, N
      REAL       X(*), F(*)
!                                  SPECIFICATIONS FOR LOCAL VARIABLES
      INTEGER    I
!                                  SPECIFICATIONS FOR SAVE VARIABLES
      REAL       H(5), T(5)
      SAVE       H, T
!                                  SPECIFICATIONS FOR INTRINSICS
      INTRINSIC  EXP
      REAL       EXP
!
      DATA T/0.05, 0.1, 0.4, 0.5, 1.0/
      DATA H/2.206, 1.994, 1.35, 1.216, 0.7358/
!
      DO 10  I=1, M
         F(I) = X(1)*EXP(X(2)*T(I)) + X(3)*EXP(X(4)*T(I)) - H(I)
   10 CONTINUE
      RETURN
      END
```

Output

```
                    X
     1        2        3        4
   1.999   -1.000   0.500   -9.954
rnorm = .42425E-03
```

Example 2

This example solves the same problem as the last example, but reverse communication is used to evaluate *f*(*x*) and the Jacobian of *f*(*x*). The use of the quadratic model is turned off.

```
      USE B2NLS_INT
      USE UMACH_INT
      USE WRRRN_INT

      IMPLICIT   NONE
      INTEGER    LDC, LDFJ, M, MCON, N
      PARAMETER  (M=5, MCON=1, N=4, LDC=MCON, LDFJ=M)
!                                  Specifications for local variables
      INTEGER    I, IPARAM(6), IRTYPE(MCON), ISTAT, IWORK(1000), &
                LIWORK, LWORK, NOUT
      REAL      BL(MCON), C(MCON,N), F(M), FJ(M,N), RNORM, RPARAM(7), &
                WORK(1000), X(N), XGUESS(N), XLB(N), XUB(N)
      REAL       H(5), T(5)
      SAVE       H, T
      INTRINSIC  EXP
      REAL       EXP
!                                  Specifications for subroutines
      EXTERNAL   B7NLS
!                                  Specifications for functions
      EXTERNAL   B10LS, B11LS
!
      DATA T/0.05, 0.1, 0.4, 0.5, 1.0/
      DATA H/2.206, 1.994, 1.35, 1.216, 0.7358/
!
      CALL UMACH (2, NOUT)
!                                  Define the separation between x(2)
!                                  and x(4)
      C(1,1)    = 0.0
```

```
      C(1,2)    = 1.0
      C(1,3)    = 0.0
      C(1,4)    = -1.0
      BL(1)     = 0.05
      IRTYPE(1) = 2
!                                  Set lower bounds on variables
      XLB(1) = 0.0
      XLB(2) = 1.0E30
      XLB(3) = 0.0
      XLB(4) = 1.0E30
!                                  Set upper bounds on variables
      XUB(1) = -1.0E30
      XUB(2) = 0.0
      XUB(3) = -1.0E30
      XUB(4) = 0.0
!                                  Set initial guess to 0.0
      XGUESS = 0.0E0
!                                  Call B7NLS to set default parameters
      CALL B7NLS (IPARAM, RPARAM)
!                                  Suppress the use of the quadratic
!                                  model, evaluate functions and
!                                  Jacobian by reverse communication
      IPARAM(3) = 1
      IPARAM(5) = 1
      IPARAM(6) = 1
      LWORK     = 1000
      LIWORK    = 1000
!                                  Specify dummy routines for FCN
!                                  and JAC since we are using reverse
!                                  communication
   10 CONTINUE
      CALL B2NLS (B10LS, M, N, MCON, C, LDC, BL, BL, IRTYPE, XLB, &
                 XUB, XGUESS, X, RNORM, ISTAT, IPARAM, RPARAM, &
                 B11LS, F, FJ, LDFJ, IWORK, LIWORK, WORK, LWORK)
!
!                                  Evaluate functions if the routine
!                                  returns with ISTAT = 6
      IF (ISTAT .EQ. 6) THEN
         DO 20  I=1, M
            FJ(I,1) = EXP(X(2)*T(I))
            FJ(I,2) = T(I)*X(1)*FJ(I,1)
            FJ(I,3) = EXP(X(4)*T(I))
            FJ(I,4) = T(I)*X(3)*FJ(I,3)
            F(I) = X(1)*FJ(I,1) + X(3)*FJ(I,3) - H(I)
   20    CONTINUE
         GO TO 10
      END IF
!
      CALL WRRRN ('X', X, 1, N, 1)
      WRITE (NOUT,99999) RNORM
99999 FORMAT (/, 'rnorm = ', E10.5)
      END
```

Output

```
                    X
      1        2        3        4
   1.999   -1.000    0.500   -9.954
rnorm = .42413E-03
```

READ_MPS

This subroutine reads an MPS file containing a linear programming problem or a quadratic programming problem.

Required Arguments

FILENAME — Character string containing the name of the MPS file to be read. (Input)

MPS— A structure of IMSL defined derived type `s_MPS` containing the data read from the MPS file. (Output)

The IMSL defined derived type `s_MPS` consists of the following components:

Component	**Description**
character, allocatable :: `filename`	Name of the MPS file.
character (*len*=8) `name`	Name of the problem.
integer `nrows`	Number of rows in the constraint matrix.
integer `ncolumns`	Number of columns in the constraint matrix. This is also the number of variables.
integer `nonzeros`	Number of non-zeros in the constraint matrix.
integer `nhessian`	Number of non-zeros in the Hessian matrix. If zero, then there is no Hessian matrix.
integer `ninteger`	Number of variables required to be integer. This includes binary variables.
integer `nbinary`	Number of variables required to be binary (0 or 1).
real (kind(1e0)), allocatable :: `objective(:)`	A `real` array of length `ncolumns` containing the objective vector.
type (*s_SparseMatrixElement*), allocatable :: `constraint(:)`	A derived type array of length `nonzeros` and of type `s_SparseMatrixElement` containing the sparse matrix representation of the constraint matrix. See below for details.
type(*s_SparseMatrixElement*), allocatable :: `hessian(:)`	A derived type array of length `nhessian` and of type `s_SparseMatrixElement` containing the sparse matrix representation of the Hessian matrix. If `nhessian` is zero, then this field is not allocated.
real (kind(1e0)), allocatable ::`lower_range(:)`	A `real` array of length `nrows` containing the lower constraint bounds. If a constraint is unbounded below, the corresponding entry in `lower_range` is set to `negative_infinity`, defined below.

Component	Description	
real (kind(1e0)), allocatable ::`upper_range(:)`	A `real` array of length `nrows` containing the upper constraint bounds. If a constraint is unbounded above, the corresponding entry in `upper_range` is set to `positive_infinity`, defined below.	
real (kind(1e0)), allocatable :: `lower_bound(:)`	A `real` array of length `ncolumns` containing the lower variable bounds. If a variable is unbounded below, the corresponding entry in `lower_bound` is set to `negative_infinity`, defined below.	
real (kind(1e0)), allocatable :: `upper_bound(:)`	A `real` array of length `ncolumns` containing the upper variable bounds. If a variable is unbounded above, the corresponding entry in `upper_bound` is set to `positive_infinity`, defined below.	
integer, allocatable :: `variable_type(:)`	An `integer` array of length `ncolumns` containing the type of each variable. Variable types are:	
	0	Continuous
	1	Integer
	2	Binary (0 or 1)
	4	Semicontinuous
character (*len*=8) `name_objective`	Name of the set in ROWS used for the objective row.	
character (*len*=8) `name_rhs`	Name of the RHS set used.	
character (*len*=8) `name_ranges`	Name of the RANGES set used or the empty string if no RANGES section in the file.	
character (*len*=8) `name_bounds`	Name of the BOUNDS set used or the empty string if no BOUNDS section in the file.	
character (*len*=8), allocatable :: `name_row(:)`	Array of length `nrows` containing the row names. The name of the *i*-th constraint row is `name_row(i)`.	
character (*len*=8), allocatable :: `name_column(:)`	Array of length `ncolumns` containing the column names. The name of the *i*-th column and variable is `name_column(i)`.	
real (*kind* (*1e*0)) `positive_infinity`	Value used for a constraint or bound upper limit when the constraint or bound is unbounded above. This can be set using an optional argument. Default is 1.0e+30.	
real (*kind* (*1e*0)) `negative_infinity`	Value used for a constraint or bound lower limit when the constraint or bound is unbounded below. This can be set using an optional argument. Default is -1.0e+30.	

This derived type stores the constraint and Hessian matrices in a simple sparse matrix format of derived type `s_SparseMatrixElement` defined in the interface module `mp_types`. `s_SparseMatrixElement` consists of three components; a row index, a column index, and a value. For each non-zero element in the constraint and Hessian matrices an element of derived type `s_SparseMatrixElement` is stored. The following code fragment expands the sparse constraint matrix of the derived type `s_SparseMatrixElement` contained in `mps`, a derived type of type `s_MPS`, into a dense matrix:

```
!  allocate a matrix
integer nr = mps%nrows
integer nc = mps%ncolumns
real (kind(1e0)), allocatable :: matrix(:,:)
allocate(matrix(nr,nc))

matrix = 0.0e0
!  expand the sparse matrix
do k = 1, mps%nonzeros
      i = mps%constraint(k)%row
      j = mps%constraint(k)%column
      matrix(i,j) = mps%constraint(k)%value
end do
```

The IMSL derived type `d_MPS` is the double precision counterpart to `s_MPS`. The IMSL derived type `d_SparseMatrixElement` is the double precision counterpart to `s_SparseMatrixElement`.

To release the space allocated for this derived type use the following statement:

```
call mps_free(mps)
```

Optional Arguments

NUNIT— The unit number for reading an MPS file opened by the user. If `NUNIT` is not used, this subroutine opens the file indicated by `FILENAME` for reading and then closes it after reading. (Input)
By default, 7 is used.

OBJ — Character string of length 8 containing the name of the objective function set to be used. (Input)

An MPS file can contain multiple objective function sets.
By default, the first objective function set in the MPS file is used. This name is case sensitive.

RHS — Character string of length 8 containing the name of the `RHS` set to be used. (Input)
An MPS file can contain multiple RHS sets.
By default, the first `RHS` set in the MPS file is used. This name is case sensitive.

RANGES — Character string of length 8 containing the name of the `RANGES` set to be used. (Input)
An MPS file can contain multiple `RANGES` sets.
By default, the first `RANGES` set in the MPS file is used. This name is case sensitive.

BOUNDS — Character string of length 8 containing the name of the `BOUNDS` set to be used. (Input)
An MPS file can contain multiple `BOUNDS` sets.
By default, the first `BOUNDS` set in the MPS file is used. This name is case sensitive.

POS_INF — Value used for a constraint or bound upper limit when the constraint or bound is unbounded above. (Input)
Default: 1.0e+30.

NEG_INF — Value used for a constraint or bound lower limit when the constraint or bound is unbounded below. (Input)
Default: -1.0e+30.

FORTRAN 90 Interface

Generic: `CALL READ_MPS (FILENAME, MPS [, …])`

Specific: The specific interface names are `S_READ_MPS` and `D_READ_MPS`.

Description

An MPS file defines a linear or quadratic programming problem.

A linear programming problem is assumed to have the form:

$$\min_x c^T x$$

$$b_l \le Ax \le b_u$$

$$x_l \le x \le x_u$$

A quadratic programming problem is assumed to have the form:

$$\min_x \frac{1}{2} x^T Q x + c^T x$$

$$b_l \le Ax \le b_u$$

$$x_l \le x \le x_u$$

The following table maps this notation into the components in the derived type returned by `READ_MPS`:

C	`Objective`
A	`Constraint`
Q	`Hessian`
b_l	`lower_range`
b_u	`upper_range`

x_l	`lower_bound`
x_u	`upper_bound`

If the MPS file specifies an equality constraint or bound, the corresponding lower and upper values in the returned derived type will be exactly equal.

The problem formulation assumes that the constraints and bounds are two-sided. If a particular constraint or bound has no lower limit, then the corresponding component of the derived type is set to -1.0e+30. If the upper limit is missing, then the corresponding component of the derived type is set to +1.0e+30.

MPS File Format

There is some variability in the MPS format. This section describes the MPS format accepted by this reader.

An MPS file consists of a number of sections. Each section begins with a name in column 1. With the exception of the NAME section, the rest of this line is ignored. Lines with a '*' or '$' in column 1 are considered comment lines and are ignored.

The body of each section consists of lines divided into fields, as follows:

Field Number	**Columns**	**Contents**
1	2-3	Indicator
2	5-12	Name
3	15-22	Name
4	25-36	Value
5	40-47	Name
6	50-61	Value

The format limits MPS names to 8 characters and values to 12 characters. The names in fields 2, 3 and 5 are case sensitive. Leading and trailing blanks are ignored, but internal spaces are significant.

The sections in an MPS file are as follows.

- NAME
- ROWS
- COLUMNS
- RHS
- RANGES (optional)
- BOUNDS (optional)

- QUADRATIC (optional)
- ENDATA

Sections must occur in the above order.

MPS keywords, section names and indicator values, are case insensitive. Row, column and set names are case sensitive.

NAME Section

The NAME section contains a single line. A problem name can occur anywhere on the line after NAME and before column 62. The problem name is truncated to 8 characters.

ROWS Section

The ROWS section defines the name and type for each row. Field 1 contains the row type and field 2 contains the row name. Row type values are not case sensitive. Row names are case sensitive. The following row types are allowed:

Row Type	Meaning
E	Equality Constraint.
L	Less than or equal constraint
G	Greater than or equal constraint.
N	Objective or a free row.

COLUMNS Section

The COLUMNS section defines the nonzero entries in the objective and the constraint matrix. The row names here must have been defined in the ROWS section.

Field	Contents
2	Column name.
3	Row name.
4	Value for the entry whose row and column are given by fields 3 and 2.
5	Row name.
6	Value for the entry whose row and column are given by fields 5 and 2.

NOTE: Fields 5 and 6 are optional.

The COLUMNS section can also contain markers. These are indicated by the name 'MARKER' (with the quotes) in field 3 and the marker type in field 4 or 5.

Marker type 'INTORG' (with the quotes) begins an integer group. The marker type 'INTEND' (with the quotes) ends this group. The variables corresponding to the columns defined within this group are required to be integer.

RHS Section

The RHS section defines the right-hand side of the constraints. An MPS file can contain more than one RHS set, distinguished by the RHS set name. The row names here must be defined in the ROWS section.

Field	Contents
2	RHS set name.
3	Row name.
4	Value for the entry whose set and row are given by fields 2 and 3.
5	Row name.
6	Value for the entry whose set and row are given by fields 2 and 5.

NOTE: Fields 5 and 6 are optional.

RANGES Section

The optional RANGES section defines two-sided constraints. An MPS file can contain more than one range set, distinguished by the range set name. The row names here must have been defined in the ROWS section.

Field	Contents
2	Range set name.
3	Row name.
4	Value for the entry whose set and row are given by fields 2 and 3.
5	Row name.
6	Value for the entry whose set and row are given by fields 2 and 5.

NOTE: Fields 5 and 6 are optional.

Ranges change one-sided constraints, defined in the RHS section, into two-sided constraints. The two-sided constraint for row *i* depends on the range value, r_i, defined in this section. The right-hand side value, b_i, is defined in the RHS section. The two-sided constraints for row *i* are given in the following table:

Row Type	Lower Constraint	Upper Constraint
G	b_i	$b_i + \|r_i\|$
L	$b_i - \|r_i\|$	b_i
E	$b_i + \min(0, r_i)$	$b_i + \max(0, r_i)$

BOUNDS Section

The optional BOUNDS section defines bounds on the variables. By default, the bounds are $0 \le x_i \le \infty$. The bounds can also be used to indicate that a variable must be an integer.

More than one bound can be set for a single variable. For example, to set $2 \le x_i \le 6$, use a LO bound with value 2 to set $2 \le x_i$ and a UP bound with value 6 to add the condition $x_i \le 6$.

An MPS file can contain more than one bounds set, distinguished by the bound set name.

Field	Contents
1	Bounds type.
2	Bounds set name.
3	Column name
4	Value for the entry whose set and column are given by fields 2 and 3.
5	Column name.
6	Value for the entry whose set and column are given by fields 2 and 5.

NOTE: Fields 5 and 6 are optional.

The bound types are as follows. Here b_i are the bound values defined in this section, the x_i are the variables, and *I* is the set of integers.

Bounded Type	Definition	Formula
LO	Lower bound	$b_j \le x_i$
UP	Upper bound	$x_i \le b_i$

Bounded Type	Definition	Formula
FX	Fixed variable	$x_i = b_i$
FR	Free variable	$-\infty \le x_i \le \infty$
MI	Lower bound is minus infinity	$-\infty \le x_i$
PL	Upper bound is positive infinity	$x_i \le \infty$
BV	Binary variable (variable must be 0 or 1).	$x_i \in \{0,1\}$
UI	Upper bound and integer	$x_i \le b_i$ and $x_i \in I$
LI	Lower bound and integer	$b_i \le x_i$ and $x_i \in I$
SC	Semicontinuous	0 or $b_i \le x_i$

The bound type names are not case sensitive.

If the bound type is UP or UI and $b_j < 0$ then the lower bound is set to $-\infty$.

QUADRATIC Section

The optional QUADRATIC section defines the Hessian for quadratic programming problems. The names HESSIAN, QUADS, QUADOBJ, QSECTION, and QMATRIX are also recognized as beginning the QUADRATIC section.

Field	Contents
2	Column name.
3	Column name.
4	Value for the entry specified by fields 2 and 3.
5	Column name.
6	Value for the entry specified by fields 2 and 5.

NOTE: Fields 5 and 6 are optional.

ENDATA Section

The ENDATA section ends the MPS file.

Comments

Informational errors

Type	Code	
3	5	No objective coefficients found.
3	6	No RHS values found.
3	8	No range values found.
3	9	No bounds found.
4	3	Missing section title.
4	4	Error reading input file.
4	7	Invalid number.
4	11	Unexpected section header.
4	12	Unknown row type.
4	13	Out-of-order marker.
4	14	Unknown marker type.
4	15	Unknown column name.
4	16	Unknown bound type.
4	17	Unknown row name.
4	18	Unexpected section name.

Examples

Example 1

```
use read_mps_int
implicit none

TYPE(S_MPS) mps
CALL read_mps ('test.mps', mps)
End
```

Example 2

See Example 2 of DENSE_LP.

MPS_FREE

Deallocates the space allocated for the IMSL derived type `s_MPS`. This routine is usually used in conjunction with `READ_MPS`.

Required Arguments

`MPS` — A structure of IMSL defined derived type `s_MPS` containing the data read from the MPS file. (Input/Output)

The allocated components of `s_MPS` will be deallocated on output.

The IMSL defined derived type `s_MPS` consists of the following components:

Component	**Description**
character, allocatable :: `filename`	Name of the MPS file.
character (*len*=8) `name`	Name of the problem.
integer `nrows`	Number of rows in the constraint matrix.
integer `ncolumns`	Number of columns in the constraint matrix. This is also the number of variables.
integer `nonzeros`	Number of non-zeros in the constraint matrix.
integer `nhessian`	Number of non-zeros in the Hessian matrix. If zero, then there is no Hessian matrix.
integer `ninteger`	Number of variables required to be integer. This includes binary variables.
integer `nbinary`	Number of variables required to be binary (0 or 1).
real (kind(1e0)), allocatable :: `objective(:)`	A `real` array of length `ncolumns` containing the objective vector.
type (*s_SparseMatrixElement*), allocatable :: `constraint(:)`	A derived type array of length `nonzeros` and of type `s_SparseMatrixElement` containing the sparse matrix representation of the constraint matrix. See below for details.
type(*s_SparseMatrixElement*), allocatable :: `hessian(:)`	A derived type array of length `nhessian` and of type `s_SparseMatrixElement` containing the sparse matrix representation of the Hessian matrix. If `nhessian` is zero, then this field is not allocated.
real (kind(1e0)), allocatable ::`lower_range(:)`	A `real` array of length `nrows` containing the lower constraint bounds. If a constraint is unbounded below, the corresponding entry in `lower_range` is set to `negative_infinity`, defined below.

Component	Description	
real (kind(1e0)), allocatable ::`upper_range(:)`	A `real` array of length `nrows` containing the upper constraint bounds. If a constraint is unbounded above, the corresponding entry in `upper_range` is set to `positive_infinity`, defined below.	
real (kind(1e0)), allocatable :: `lower_bound(:)`	A `real` array of length `ncolumns` containing the lower variable bounds. If a variable is unbounded below, the corresponding entry in `lower_bound` is set to `negative_infinity`, defined below.	
real (kind(1e0)), allocatable :: `upper_bound(:)`	A `real` array of length `ncolumns` containing the upper variable bounds. If a variable is unbounded above, the corresponding entry in `upper_bound` is set to `positive_infinity`, defined below.	
integer, allocatable :: `variable_type(:)`	An `integer` array of length `ncolumns` containing the type of each variable. Variable types are:	
	0	Continous
	1	Integer
	2	Binary (0 or 1)
	3	Semicontinuous
character (*len*=8) `name_objective`	Name of the set in ROWS used for the objective row.	
character (*len*=8) `name_rhs`	Name of the RHS set used.	
character (*len*=8) `name_ranges`	Name of the RANGES set used or the empty string if no RANGES section in the file.	
character (*len*=8) `name_bounds`	Name of the BOUNDS set used or the empty string if no BOUNDS section in the file.	
character (*len*=8), allocatable :: `name_row(:)`	Array of length `nrows` containing the row names. The name of the *i*-th constraint row is `name_row(i)`.	
character (*len*=8), allocatable :: `name_column(:)`	Array of length `ncolumns` containing the column names. The name of the *i*-th column and variable is `name_column(i)`.	
real (*kind* (*1e*0)) `positive_infinity`	Value used for a constraint or bound upper limit when the constraint or bound is unbounded above. This can be set using an optional argument. Default is 1.0e+30.	
real (*kind* (*1e*0)) `negative_infinity`	Value used for a constraint or bound lower limit when the constraint or bound is unbounded below. This can be set using an optional argument. Default is -1.0e+30.	

This derived type stores the constraint and Hessian matrices in a simple sparse matrix format of derived type `s_SparseMatrixElement` defined in the interface module `mp_types`. `s_SparseMatrixElement` consists of three components; a row index, a column index, and a value. For each non-zero element in the constraint and Hessian matrices an element of derived type `s_SparseMatrixElement` is stored The following code fragment expands the sparse constraint matrix of the derived type `s_SparseMatrixElement` contained in `mps`, a derived type of type `s_MPS`, into a dense matrix:

```
!  allocate a matrix
integer nr = mps%nrows
integer nc = mps%ncolumns
real  (kind(1e0)), allocatable :: matrix(:,:)
allocate(matrix(nr,nc))

matrix = 0.0e0
!  expand the sparse matrix
do k = 1, mps%nonzeros
      i = mps%constraint(k)%row
      j = mps%constraint(k)%column
      matrix(i,j) = mps%constraint(k)%value
end do
```

The IMSL derived type `d_MPS` is the double precision counterpart to `s_MPS`. The IMSL derived type `d_SparseMatrixElement` is the double precision counterpart to `s_SparseMatrixElement`.

FORTRAN 90 Interface

Generic: CALL MPS_FREE (MPS)

Specific: The specific interface names are `S_MPS_FREE` and `D_MPS_FREE`.

Description

This subroutine simply issues deallocate statements for each of the arrays allocated in the IMSL derived type `s_MPS` defined above. It is supplied as a convenience utility to the user of `READ_MPS`.

Example

In the following example, the space that had been allocated to accommodate the IMSL derived type `S_MPS` is deallocated with a call to `MPS_FREE` after a call to `READ_MPS` was made.

```
use read_mps_int
use mps_free_int
implicit none

TYPE(S_MPS) mps
CALL read_mps ('test.mps', mps)
   .
   .
   .
call mps_free (mps)
end
```

DENSE_LP

Solves a linear programming problem using an active set strategy.

NOTE: DENSE_LP is available in double precision only.

Required Arguments

A — M by NVAR matrix containing the coefficients of the M constraints. (Input)

BL — Vector of length M containing the lower limit of the general constraints; if there is no lower limit on the I-th constraint, then BL(I) is not referenced. (Input)

BU — Vector of length M containing the upper limit of the general constraints; if there is no upper limit on the I-th constraint, then BU(I) is not referenced; if there are no range constraints, BL and BU can share the same storage locations. (Input)

C — Vector of length NVAR containing the coefficients of the objective function. (Input)

IRTYPE — Vector of length M indicating the types of general constraints in the matrix A. (Input)
Let R(I) = A(I, 1) * XSOL(1) + … + A(I, NVAR) * XSOL(NVAR). Then, the value of IRTYPE(I) signifies the following:

Irtype[I]	I-th Constraint
0	BL(I) = R(I) = BU(I)
1	R(I) ≤ BU(I)
2	R(I) ≥ BL(I)
3	BL(I) ≤ R(I) ≤ BU(I)
4	Ignore this constraint

OBJ — Value of the objective function. (Output)

XSOL — Vector of length NVAR containing the primal solution.(Output)

DSOL — Vector of length M containing the dual solution. (Output)

Optional Arguments

M — Number of constraints. (Input)
Default: M = SIZE (A,1).

NVAR — Number of variables. (Input)
Default: NVAR = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
LDA must be at least M.
Default: LDA = SIZE (A,1).

XLB — Vector of length NVAR containing the lower bound on the variables; if there is no lower bound on a variable, then 1.0D30 should be set as the lower bound. (Input)
Default: XLB = 0.0D0.

XUB — Vector of length NVAR containing the upper bound on the variables; if there is no upper bound on a variable, then −1.0D30 should be set as the upper bound. (Input)
Default: No upperbound enforced.

ITREF — The type if iterative refinement used. (Input)

ITREF	Refinement
0	No refinement
1	Iterative refinement
2	Use extended refinement. Iterate until no more progress.

Default: ITREF = 0.

ITERS — Number of iterations. (Output)

IERR — Status flag indicating which warning conditions were set upon completion. (Output)

IERR	Status
≥ 0	Solution found. **IERR** = 0 indicates there are no warning conditions. If the solution was found with warning conditions **IERR** is incremented by the number given below.
1	1 is added to the value returned if there are multiple solutions giving essentially the same minimum.

IERR	Status
2	2 is added to the value returned if there were some constraints discarded because they were too linearly dependent on other active constraints.
4	4 is added to the value returned if the constraints were not satisfied. L_1 minimization was applied to all (including bounds on simple variables) but the equalities, to approximate violated non-equalities as well as possible. If a feasible solution is possible then refinement may help
8	8 is added to the value returned if the algorithm appears to be cycling. Using refinement may help.

FORTRAN 90 Interface

Generic: CALL DENSE_LP (A, BL, BU, C, IRTYPE, OBJ, XSOL, DSOL [, …])

Specific: The specific interface name is D_DENSE_LP. This subroutine is available in double precision only.

Description

The routine DENSE_LP solves the linear programming problem

$$\min_{x \in R^n} c^T x$$

$$\text{subject to} \quad b_1 \le Ax \le b_u$$
$$x_l \le x \le x_u$$

where c is the objective coefficient vector, A is the coefficient matrix, and the vectors b_l, b_u, x_l and x_u are the lower and upper bounds on the constraints and the variables, respectively.

DENSE_LP uses an active set strategy.

Refer to the following paper for further information: Krogh, Fred, T. (2005), *An Algorithm for Linear Programming*, http://mathalacarte.com/fkrogh/pub/lp.pdf ,Tujunga, CA.

Comments

1. Informational errors

Type	Code	Description
1	1	Multiple solutions giving essentially the same solution exist.
3	1	Some constraints were discarded because they were too linearly dependent on other active constraints.
3	2	All constraints are not satisfied.
3	3	The algorithm appears to be cycling.
4	1	The problem appears vacuous.
4	2	The problem is unbounded.
4	3	An acceptable pivot could not be found.
4	4	The constraint bounds are inconsistent.
4	5	The variable bounds are inconsistent.

Examples

Example 1

The linear programming problem in the standard form

$$
\begin{array}{rl}
 & \min\ f(x) = -x_1 - 3x_2 \\
\text{subject to} & x_1 + x_2 + x_3 = 1.5 \\
 & x_1 + x_2 - x_4 = 0.5 \\
 & x_1 + x_5 = 1.0 \\
 & x_2 + x_6 = 1.0 \\
 & x_1 \geq 0,\ \text{for}\ i = 1,\ldots 6
\end{array}
$$

is solved.

```
      USE UMACH_INT
      USE WRRRN_INT
      USE DENSE_LP_INT
      IMPLICIT NONE
      INTEGER NOUT, M, NVAR
      PARAMETER (M=4, NVAR=6)
      DOUBLE PRECISION A(M, NVAR), B(M), C(NVAR), XSOL(NVAR), &
             DSOL(M), BL(M), BU(M), OBJ
      INTEGER IRTYPE(M)
      DATA A/1, 1, 1, 0, 1, 1, 0, 1, 1, 0, 0, 0, 0, -1, &
             0, 0, 0, 0, 1, 0, 0, 0, 0, 1/
      DATA B/1.5, 0.5, 1.0, 1.0/
      DATA C/-1.0, -3.0, 0.0, 0.0, 0.0, 0.0/
      DATA BL/1.5, 0.5, 1.0, 1.0/
      DATA BU/M*-1.D30/
      DATA IRTYPE/M*0/

      CALL UMACH(2, NOUT)
```

```
!                          Solve the LP problem
      CALL DENSE_LP (A, BL, BU, C, IRTYPE, OBJ, XSOL, DSOL)

      WRITE(NOUT, 99999) OBJ
      CALL WRRRN('Solution', XSOL, 1, NVAR, 1)
99999 FORMAT (' Objective', F9.4)
      END
```

Output

```
Objective  -3.5000

                    Solution
      1        2        3        4        5        6
  0.500    1.000    0.000    1.000    0.500    0.000
```

Example 2

This example demonstrates how `READ_MPS` can be used together with `DENSE_LP` to solve a linear programming problem defined in an MPS file. The MPS file used in this example is an *uncompressed* version of the file '`afiro`', available from `http://www.netlib.org/lp/data/`.

```
      USE UMACH_INT
      USE WRRRN_INT
      USE READ_MPS_INT
      USE DENSE_LP_INT
      IMPLICIT NONE
      REAL(KIND(1D0)) OBJ
      REAL(KIND(1D0)), ALLOCATABLE :: XSOL(:)
      REAL(KIND(1D0)), ALLOCATABLE :: DSOL(:)
      REAL(KIND(1D0)), ALLOCATABLE :: A(:,:)
      INTEGER, ALLOCATABLE :: IRTYPE(:)
      TYPE(D_MPS) PROBLEM
      CHARACTER NAME*256
      INTEGER I,J, K, NOUT

      CALL UMACH(2, NOUT)

!     READ LP PROBLEM FROM THE MPS FILE.
      NAME = 'afiro'
      CALL READ_MPS (NAME, PROBLEM)
      ALLOCATE (A(PROBLEM%NROWS, PROBLEM%NCOLUMNS))
      ALLOCATE (IRTYPE(PROBLEM%NROWS))
      ALLOCATE (XSOL(PROBLEM%NCOLUMNS))
      ALLOCATE (DSOL(PROBLEM%NROWS))
      A = 0
      IRTYPE = 3
!     FILL DENSE A
      DO K = 1, PROBLEM%NONZEROS
         I = PROBLEM%CONSTRAINT(K)%ROW
         J = PROBLEM%CONSTRAINT(K)%COLUMN
         A(I,J) = PROBLEM%CONSTRAINT(K)%VALUE
      ENDDO
!     CALL THE LP SOLVER
      CALL DENSE_LP (A, PROBLEM%LOWER_RANGE, PROBLEM%UPPER_RANGE, &
                    PROBLEM%OBJECTIVE, IRTYPE, OBJ, XSOL, DSOL, &
                    XLB=PROBLEM%LOWER_BOUND, XUB=PROBLEM%UPPER_BOUND)
      WRITE(NOUT, 99999) OBJ
      CALL WRRRN('Solution', XSOL, 1, PROBLEM%NROWS, 1)
```

```
      DEALLOCATE(A)
      DEALLOCATE(IRTYPE)
      DEALLOCATE(XSOL)
      DEALLOCATE(DSOL)
99999 FORMAT('Objective:  ', E16.7)
      END
```

Output

```
Objective:    -0.4647531E+03

                                 Solution
     1        2        3        4        5        6        7        8        9   10
  80.0     25.5     54.5     84.8     57.9      0.0      0.0      0.0      0.0  0.0

    11       12       13       14       15       16       17       18     19      20
   0.0      0.0     18.2     39.7     61.3    500.0    475.9     24.1    0.0   215.0

    21       22       23       24       25       26       27
 363.9      0.0      0.0      0.0      0.0      0.0      0.0
```

DLPRS

more...

Solves a linear programming problem via the revised simplex algorithm.

Required Arguments

A — M by NVAR matrix containing the coefficients of the M constraints. (Input)

BL — Vector of length M containing the lower limit of the general constraints; if there is no lower limit on the I-th constraint, then BL(I) is not referenced. (Input)

BU — Vector of length M containing the upper limit of the general constraints; if there is no upper limit on the I-th constraint, then BU(I) is not referenced; if there are no range constraints, BL and BU can share the same storage locations. (Input)

C — Vector of length NVAR containing the coefficients of the objective function. (Input)

IRTYPE — Vector of length M indicating the types of general constraints in the matrix A. (Input)
Let R(I) = A(I, 1) * XSOL(1) + … + A(I, NVAR) * XSOL(NVAR). Then, the value of IRTYPE(I) signifies the following:

IRTYPE(I)	I-th Constraint
0	BL(I).EQ.R(I).EQ.BU(I)
1	R(I).LE.BU(I)
2	R(I).GE.BL(I)
3	BL(I).LE.R(I).LE.BU(I)

OBJ — Value of the objective function. (Output)

XSOL — Vector of length NVAR containing the primal solution. (Output)

DSOL — Vector of length M containing the dual solution. (Output)

Optional Arguments

M — Number of constraints. (Input)
Default: M = SIZE (A,1).

NVAR — Number of variables. (Input)
Default: NVAR = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
LDA must be at least M.
Default: LDA = SIZE (A,1).

XLB — Vector of length NVAR containing the lower bound on the variables; if there is no lower bound on a variable, then 1.0E30 should be set as the lower bound. (Input)
Default: XLB = 0.0.

XUB — Vector of length NVAR containing the upper bound on the variables; if there is no upper bound on a variable, then −1.0E30 should be set as the upper bound. (Input)
Default: XUB = 3.4e38 for single precision and 1.79d + 308 for double precision.

FORTRAN 90 Interface

Generic:	CALL DLPRS (A, BL, BU, C, IRTYPE, OBJ, XSOL, DSOL [, …])
Specific:	The specific interface names are S_DLPRS and D_DLPRS.

FORTRAN 77 Interface

Single:	CALL DLPRS (M, NVAR, A, LDA, BL, BU, C, IRTYPE, XLB, XUB, OBJ, XSOL, DSOL)
Double:	The double precision name is DDLPRS.

Description

The routine DLPRS uses a revised simplex method to solve linear programming problems, i.e., problems of the form

$$\min_{x \in R^n} c^T x$$

$$\text{subject to} \quad b_1 \le A_x \le b_u$$
$$x_l \le x \le x_u$$

where *c* is the objective coefficient vector, *A* is the coefficient matrix, and the vectors b_l, b_u, x_l and x_u are the lower and upper bounds on the constraints and the variables, respectively.

For a complete description of the revised simplex method, see Murtagh (1981) or Murty (1983).

Comments

1. Workspace may be explicitly provided, if desired, by use of D2PRS/DD2PRS. The reference is:

```
CALL D2PRS (M, NVAR, A, LDA, BL, BU, C, IRTYPE, XLB, XUB, OBJ,
   XSOL, DSOL, AWK, LDAWK, WK, IWK)
```

   The additional arguments are as follows:

   AWK — Real work array of dimension 1 by 1. (AWK is not used in the new implementation of the revised simplex algorithm. It is retained merely for calling sequence consistency.)

   LDAWK — Leading dimension of AWK exactly as specified in the dimension statement of the calling program. LDAWK should be 1. (LDAWK is not used in the new implementation of the revised simplex algorithm. It is retained merely for calling sequence consistency.)

   WK — Real work vector of length M * (M + 28).

   IWK — Integer work vector of length 29 * M + 3 * NVAR.

2. Informational errors

Type	Code	Description
3	1	The problem is unbounded.
4	2	Maximum number of iterations exceeded.
3	3	The problem is infeasible.
4	4	Moved to a vertex that is poorly conditioned; using double precision may help.
4	5	The bounds are inconsistent.

Example

A linear programming problem is solved.

```
      USE DLPRS_INT
      USE UMACH_INT
      USE SSCAL_INT

      IMPLICIT   NONE
      INTEGER    LDA, M, NVAR
      PARAMETER  (M=2, NVAR=2, LDA=M)
!                                  M = number of constraints
!                                  NVAR = number of variables
!
      INTEGER    I, IRTYPE(M), NOUT
      REAL       A(LDA,NVAR), B(M), C(NVAR), DSOL(M), OBJ, XLB(NVAR), &
                XSOL(NVAR), XUB(NVAR)
!
!                                  Set values for the following problem
!
!                                  Max 1.0*XSOL(1) + 3.0*XSOL(2)
!
!                                  XSOL(1) + XSOL(2) .LE. 1.5
!                                  XSOL(1) + XSOL(2) .GE. 0.5
!
!                                  0 .LE. XSOL(1) .LE. 1
!                                  0 .LE. XSOL(2) .LE. 1
!
      DATA XLB/2*0.0/, XUB/2*1.0/
      DATA A/4*1.0/, B/1.5, .5/, C/1.0, 3.0/
      DATA IRTYPE/1, 2/
!                                  To maximize, C must be multiplied by
!                                  -1.
      CALL SSCAL (NVAR, -1.0E0, C, 1)
!                                  Solve the LP problem.  Since there is
!                                  no range constraint, only B is
!                                  needed.
      CALL DLPRS (A, B, B, C, IRTYPE, OBJ, XSOL, DSOL, &
                 XUB=XUB)
!                                  OBJ must be multiplied by -1 to get
!                                  the true maximum.
      OBJ = -OBJ
!                                  DSOL must be multiplied by -1 for
!                                  maximization.
      CALL SSCAL (M, -1.0E0, DSOL, 1)
!                                  Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) OBJ, (XSOL(I),I=1,NVAR), (DSOL(I),I=1,M)
!
99999 FORMAT (//, '   Objective       = ', F9.4, //, '   Primal ',&
             'Solution =', 2F9.4, //, '   Dual solution   =', 2F9.4)
!
      END
```

Output

```
 Objective       =    3.5000

 Primal Solution =   0.5000   1.0000

 Dual solution   =   1.0000   0.0000
```

SLPRS

Solves a sparse linear programming problem via the revised simplex algorithm.

Required Arguments

A — Vector of length NZ containing the coefficients of the M constraints. (Input)

IROW — Vector of length NZ containing the row numbers of the corresponding element in A. (Input)

JCOL — Vector of length NZ containing the column numbers of the corresponding elements in *A*. (Input)

BL — Vector of length M containing the lower limit of the general constraints; if there is no lower limit on the I-th constraint, then BL(I) is not referenced. (Input)

BU — Vector of length M containing the upper limit of the general constraints; if there is no upper limit on the I-th constraint, then BU(I) is not referenced. (Input)

C — Vector of length NVAR containing the coefficients of the objective function. (Input)

IRTYPE — Vector of length M indicating the types of general constraints in the matrix A. (Input)
Let R(I) = A(I, 1)*XSOL(1) + … + A(I, NVAR)*XSOL(NVAR)

IRTYPE(I)	I-th Constraint
0	BL(I) = R(I) = BU(I)
1	R(I) ≤ BU(I)
2	R(I) ≥ BL(I)
3	BL(I) ≤ R(I) ≤ BU(I)

OBJ — Value of the objective function. (Output)

XSOL — Vector of length NVAR containing the primal solution. (Output)

DSOL — Vector of length M containing the dual solution. (Output)

Optional Arguments

M — Number of constraints. (Input)
Default: M = SIZE (IRTYPE,1).

NVAR — Number of variables. (Input)
Default: `NVAR` = `SIZE` (`C`,1).

NZ — Number of nonzero coefficients in the matrix *A*. (Input)
Default: `NZ` = `SIZE` (`A`,1).

XLB — Vector of length `NVAR` containing the lower bound on the variables; if there is no lower bound on a variable, then 1.0E30 should be set as the lower bound. (Input)
Default: `XLB` = 0.0.

XUB — Vector of length `NVAR` containing the upper bound on the variables; if there is no upper bound on a variable, then −1.0E30 should be set as the upper bound. (Input)
Default: `XUB` = 3.4e38 for single precision and 1.79d + 308 for double precision.

FORTRAN 90 Interface

Generic: `CALL SLPRS` (`A`, `IROW`, `JCOL`, `BL`, `BU`, `C`, `IRTYPE`, `OBJ`, `XSOL`, `DSOL [, …]`)

Specific: The specific interface names are `S_SLPRS` and `D_SLPRS`.

FORTRAN 77 Interface

Single: `CALL SLPRS` (`M`, `NVAR`, `NZ`, `A`, `IROW`, `JCOL`, `BL`, `BU`, `C`, `IRTYPE`, `XLB`, `XUB`, `OBJ`, `XSOL`, `DSOL`)

Double: The double precision name is `DSLPRS`.

Description

This subroutine solves problems of the form

$$\min c^T x$$

subject to

$$b_l \le Ax \le b_u,$$
$$x_l \le x \le x_u$$

where c is the objective coefficient vector, A is the coefficient matrix, and the vectors b_l, b_u, x_l, and x_u are the lower and upper bounds on the constraints and the variables, respectively. `SLPRS` is designed to take advantage of sparsity in *A*. The routine is based on `DPLO` by Hanson and Hiebert.

Comments

Workspace may be explicitly provided, if desired, by use of S2PRS/DS2PRS. The reference is:

```
CALL S2PRS (M, NVAR, NZ, A, IROW, JCOL, BL, BU, C, IRTYPE,
   XLB, XUB, OBJ, XSOL, DSOL, IPARAM, RPARAM, COLSCL, ROWSCL,
   WORK, LW, IWORK, LIW)
```

The additional arguments are as follows:

IPARAM — Integer parameter vector of length 12. If the default parameters are desired for SLPRS, then set IPARAM(1) to zero and call the routine SLPRS. Otherwise, if any nondefault parameters are desired for IPARAM or RPARAM, then the following steps should be taken before calling SLPRS:

CALL S5PRS (IPARAM, RPARAM)

Set nondefault values for IPARAM and RPARAM.

Note that the call to S5PRS will set IPARAM and RPARAM to their default values so only nondefault values need to be set above.

IPARAM(1) = 0 indicates that a minimization problem is solved. If set to 1, a maximization problem is solved.
Default: 0

IPARAM(2) = switch indicating the maximum number of iterations to be taken before returning to the user. If set to zero, the maximum number of iterations taken is set to 3*(NVARS+M). If positive, that value is used as the iteration limit.
Default: IPARAM(2) = 0

IPARAM(3) = indicator for choosing how columns are selected to enter the basis. If set to zero, the routine uses the steepest edge pricing strategy which is the best local move. If set to one, the minimum reduced cost pricing strategy is used. The steepest edge pricing strategy generally uses fewer iterations than the minimum reduced cost pricing, but each iteration costs more in terms of the amount of calculation performed. However, this is very problem-dependent.
Default: IPARAM(3) = 0

IPARAM(4) = MXITBR, the number of iterations between recalculating the error in the primal solution is used to monitor the error in solving the linear system. This is an expensive calculation and every tenth iteration is generally enough.
Default: IPARAM(4) = 10

IPARAM(5) = NPP, the number of negative reduced costs (at most) to be found at each iteration of choosing a variable to enter the basis. If set to zero,
NPP = NVARS will be used, implying that all of the reduced costs are computed at each such step. This "Partial pricing" may increase the total number of iterations required. However, it decreases the number of calculation required at each iteration. The effect on overall efficiency is very problem-dependent. If set to some positive number, that value is used as NPP.
Default: IPARAM(5) = 0

IPARAM(6) = IREDFQ, the number of steps between basis matrix redecompositions. Redecompositions also occur whenever the linear systems for the primal and dual systems have lost half their working precision.
Default: IPARAM(6) = 50

IPARAM(7) = LAMAT, the length of the portion of WORK that is allocated to sparse matrix storage and decomposition. LAMAT must be greater than NZ + NVAR + 7.
Default: LAMAT = MAX (NZ + NVAR + 8, 4*NVAR + 7)

IPARAM(8) = LBM, the length of the portion of IWORK that is allocated to sparse matrix storage and decomposition. LBM must be positive.
Default: LBM = 14 * M

IPARAM(9) = switch indicating that partial results should be saved after the maximum number of iterations, IPARAM(2), or at the optimum. If IPARAM(9) is not zero, data essential to continuing the calculation is saved to a file, attached to unit number IPARAM(9). The data saved includes all the information about the sparse matrix A and information about the current basis. If IPARAM(9) is set to zero, partial results are not saved. It is the responsibility of the calling program to open the output file.

IPARAM(10) = switch indicating that partial results have been computed and stored on unit number IPARAM(10), if greater than zero. If IPARAM(10) is zero, a new problem is started.
Default: IPARAM(10) = 0

IPARAM(11) = switch indicating that the user supplies scale factors for the columns of the matrix *A*. If IPARAM(11) = 0, SLPRS computes the scale factors as the reciprocals of the max norm of each column. If IPARAM(11) is set to one, element I of the vector COLSCL is used as the scale factor for column I of the matrix *A*. The scaling is implicit, so no input data is actually changed.
Default: IPARAM(11) = 0

IPARAM(12) = switch indicating that the user supplied scale factors for the rows of the matrix *A*. If IPARAM(12) is set to zero, no row scaling is one. If IPARAM(12) is set to 1, element I of the vector ROWSCL is used as the scale factor for row I of the matrix *A*. The scaling is implicit, so no input data is actually changed.
Default: IPARAM(12) = 0

RPARAM — Real parameter vector of length 7.

RPARAM(1) = COSTSC, a scale factor for the vector of costs. Normally SLPRS computes this scale factor to be the reciprocal of the max norm if the vector costs after the column scaling has been applied. If RPARAM(1) is zero, SLPRS compute COSTSC.
Default: RPARAM(1) = 0.0

RPARAM(2) = ASMALL, the smallest magnitude of nonzero entries in the matrix *A*. If RPARAM(2) is nonzero, checking is done to ensure that all elements of *A* are at least as large as RPARAM(2). Otherwise, no checking is done.
Default: RPARAM(2) = 0.0

RPARAM(3) = ABIG, the largest magnitude of nonzero entries in the matrix *A*. If RPARAM(3) is nonzero, checking is done to ensure that all elements of *A* are no larger than RPARAM(3). Otherwise, no checking is done.
Default: RPARAM(3) = 0.0

RPARAM(4) = TOLLS, the relative tolerance used in checking if the residuals are feasible. RPARAM(4) is nonzero, that value is used as TOLLS, otherwise the default value is used.
Default: TOLLS = 1000.0*amach(4)

RPARAM(5) = PHI, the scaling factor used to scale the reduced cost error estimates. In some environments, it may be necessary to reset PHI to the range [0.01, 0.1], particularly on machines with short word length and working precision when solving a large problem. If RPARAM(5) is nonzero, that value is used as PHI, otherwise the default value is used.
Default: PHI = 1.0

RPARAM(6) = TOLABS, an absolute error test on feasibility. Normally a relative test is used with TOLLS (see RPARAM(4)). If this test fails, an absolute test will be applied using the value TOLABS.
Default: TOLABS = 0.0

RPARAM(7) = pivot tolerance of the underlying sparse factorization routine. If RPARAM(7) is set to zero, the default pivot tolerance is used, otherwise, the RPARAM(7) is used.
Default: RPARAM(7) = 0.1

COLSCL — Array of length NVARS containing column scale factors for the matrix *A*. (Input). COLSCL is not used if IPARAM(11) is set to zero.

ROWSCL — Array of length M containing row scale factors for the matrix *A*. (Input) ROWSCL is not used if IPARAM(12) is set to zero.

WORK — Work array of length LW.

LW — Length of real work array. LW must be at least 4*NVAR + 9*M + LAMAT + LBM + 4*(M+NVAR) + 2*NZ + NVAR + 1, where LAMAT = IPARAM(7) and LBM = IPARAM(8).

IWORK — Integer work array of length LIW.

LIW — Length of integer work array. LIW must be at least NVAR + 11*M + LAMAT + 2*LBM + 2*(M + NVAR), where LAMAT = IPARAM(7) and LBM = IPARAM(8).

Example

Solve a linear programming problem, with

$$A = \begin{bmatrix} 0 & 0.5 & & & \\ & 1 & 0.5 & & \\ & & 1 & \ddots & \\ & & & \ddots & 0.5 \\ & & & & 1 \end{bmatrix}$$

defined in sparse coordinate format.

```
      USE SLPRS_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    M, NVAR
      PARAMETER  (M=200, NVAR=200)
!                                 Specifications for local variables
      INTEGER    INDEX, IROW(3*M), J, JCOL(3*M), NOUT, NZ
      REAL       A(3*M), DSOL(M), OBJ, XSOL(NVAR)
      INTEGER    IRTYPE(M)
      REAL       B(M), C(NVAR), XL(NVAR), XU(NVAR)
!                                 Specifications for subroutines
      DATA B/199*1.7, 1.0/
      DATA C/-1.0, -2.0, -3.0, -4.0, -5.0, -6.0, -7.0, -8.0, -9.0, &
      -10.0, 190*-1.0/
      DATA XL/200*0.1/
      DATA XU/200*2.0/
      DATA IRTYPE/200*1/
!
      CALL UMACH (2, NOUT)
!                                 Define A
      INDEX = 1
      DO 10  J=2, M
!                                 Superdiagonal element
         IROW(INDEX) = J - 1
         JCOL(INDEX) = J
         A(INDEX)    = 0.5
!                                 Diagonal element
         IROW(INDEX+1) = J
         JCOL(INDEX+1) = J
         A(INDEX+1) = 1.0
         INDEX      = INDEX + 2
   10 CONTINUE
      NZ = INDEX - 1
!
!
      XL(4) = 0.2
      CALL SLPRS (A, IROW, JCOL, B, B, C, IRTYPE, OBJ, XSOL, DSOL, &
                  NZ=NZ, XLB=XL, XUB=XU)
!
      WRITE (NOUT,99999) OBJ
!
99999 FORMAT (/, 'The value of the objective function is ', E12.6)
!
      END
```

Output

```
The value of the objective function is -.280971E+03
```

TRAN

Solves a transportation problem.

Required Arguments

WCAP — Array of size `NW` containing the source (warehouse) capacities. (Input)

SREQ — Array of size `NS` containing the sink (store) requirements. (Input)

COST — Array of size `NW` by `NS` containing the cost matrix. (Input)
`COST(I, J)` is the per unit cost to ship from source `I` to sink `J`.

X — Array of size `NW` by `NS` containing the optimal routing. (Output)
`X(I, J)` units should be shipped from source `I` to sink `J`.

CMIN — Total cost of the optimal routing. (Output)

Optional Arguments

NW — Number of sources. (Input)
Default: `NW` = `SIZE(WCAP, 1)`.

NS — Number of sinks. (Input)
Default: `NS` = `SIZE(SREQ, 1)`.

MAXITN — Upper bound on the number of simplex steps. (Input)
Default: `MAXITN` = 0, means no limit.

DUAL — Array of size `NW` + `NS` containing the dual solution. (Output)

FORTRAN 90 Interface

Generic: `CALL TRAN (WCAP, SREQ, COST, X, CMIN [, …])`

Specific: The specific interface names are `S_TRAN` and `D_TRAN`.

Description

Routine `TRAN` solves the transportation problem.

Minimize

$$\sum_{i=1}^{NW} \sum_{j=1}^{NS} C_{ij} X_{ij}$$

subject to the constraints

$$\sum_{j=1}^{NS} X_{ij} \le W_i \quad \text{for} \quad i = 1, NW$$

and

$$\sum_{i=1}^{NW} X_{ij} = S_j \quad \text{for} \quad j = 1, NS$$

and

$$X_{ij} \ge 0$$

where C = COST, X = X, W = WCAP and S = SREQ.

The revised simplex method is used to solve a very sparse linear programming problem with NW + NS constraints and NW * NS variables. If NW = NS = k, the work per iteration is O(k^2), compared with O(k^3) when a dense simplex algorithm is used. For more details, see Sewell (2005).

DUAL(I) gives the decrease in total cost per unit increase in WCAP (I), for small increases, and −DUAL (NW+J) gives the increase in total cost per unit increase in SREQ (J).

Comments

Informational errors

Type	Code	Description
3	1	There is insufficient source capacity. The total source capacity is less than the total sink needs, so TRAN will return a solution which minimizes the cost to distribute everything in the sources, but does not fill all the sink needs.
4	2	The maximum number of iterations has been exceeded.

Example

In this example, there are two warehouses with capacities 40 and 20, and 3 stores, which need 25, 10 and 22 units, respectively.

```
      USE TRAN_INT
      IMPLICIT NONE
      INTEGER, PARAMETER :: NW=2, NS=3
      INTEGER            :: I, J, NOUT
      REAL               ::  X(NW,NS), COST(NW,NS), CMIN
!                                  WAREHOUSE CAPACITIES
      REAL               ::  WCAP(NW) =(/40, 20/)
!                                  STORE REQUIREMENTS
      REAL               :: SREQ(NS) =(/25, 10, 22/)
!                                  COSTS
      DATA COST/550,350,300,300,400,100/
!
      CALL UMACH(2, NOUT)
!                                  SOLVE TRANSPORTATION PROBLEM
!
      CALL TRAN(WCAP, SREQ, COST, X, CMIN)
!                                  PRINT RESULTS
      WRITE(NOUT, 99995)  CMIN
      DO I=1, NW
         DO J=1, NS
             WRITE (NOUT, 99996) X(I,J),I,J
         END DO
      END DO
 99995 FORMAT (' Minimum cost is ',F10.2)
 99996 FORMAT (' Ship ',F5.2,' units from warehouse ',I2, &
             ' to store ',I2)
      END
```

Output

```
Minimum cost is   19550.00
Ship 25.00 units from warehouse  1 to store  1
Ship 10.00 units from warehouse  1 to store  2
Ship  2.00 units from warehouse  1 to store  3
Ship  0.00 units from warehouse  2 to store  1
Ship  0.00 units from warehouse  2 to store  2
Ship 20.00 units from warehouse  2 to store  3
```

QPROG

Solves a quadratic programming problem subject to linear equality/inequality constraints.

Required Arguments

NEQ — The number of linear equality constraints. (Input)

A — `NCON` by `NVAR` matrix. (Input)
The matrix contains the equality contraints in the first `NEQ` rows followed by the inequality constraints.

B — Vector of length `NCON` containing right-hand sides of the linear constraints. (Input)

G — Vector of length `NVAR` containing the coefficients of the linear term of the objective function. (Input)

H — `NVAR` by `NVAR` matrix containing the Hessian matrix of the objective function. (Input)
`H` should be symmetric positive definite; if `H` is not positive definite, the algorithm attempts to solve the QP problem with `H` replaced by a `H` + `DIAGNL * I` such that
`H` + `DIAGNL * I` is positive definite. See Comment 3.

SOL — Vector of length `NVAR` containing solution. (Output)

Optional Arguments

NVAR — The number of variables. (Input)
Default: `NVAR` = `SIZE` (A,2).

NCON — The number of linear constraints. (Input)
Default: `NCON` = `SIZE` (A,1).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = `SIZE` (A,1).

LDH — Leading dimension of `H` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDH` = `SIZE` (H,1).

DIAGNL — Scalar equal to the multiple of the identity matrix added to `H` to give a positive definite matrix. (Output)

NACT — Final number of active constraints. (Output)

IACT — Vector of length NVAR containing the indices of the final active constraints in the first NACT positions. (Output)

ALAMDA — Vector of length NVAR containing the Lagrange multiplier estimates of the final active constraints in the first NACT positions. (Output)

MAXITN — This number is the maximum number of iterations allowed. (Input)
If MAXITN is set to 0 the iteration count is unbounded.
Default: MAXITN = 100000.

SMALL — This constant is used in the determination of the positive definiteness of the Hessian H. (Input)
SMALL is also used for the convergence criteria of a constraint violation.
Default: SMALL = 10.0 * machine precision for single precision and 1000.0*machine precision for double precision.

FORTRAN 90 Interface

Generic: CALL QPROG (NEQ, A, B, G, H, SOL [, …])

Specific: The specific interface names are S_QPROG and D_QPROG.

FORTRAN 77 Interface

Single: CALL QPROG (NVAR, NCON, NEQ, A, LDA, B, G, H, LDH, DIAGNL, SOL, NACT, IACT, ALAMDA)

Double: The double precision name is DQPROG.

Description

The routine QPROG is based on M.J.D. Powell's implementation of the Goldfarb and Idnani (1983) dual quadratic programming (QP) algorithm for convex QP problems subject to general linear equality/inequality constraints, i.e., problems of the form

$$\min_{x \in \mathrm{R}^n} g^T x + \frac{1}{2} x^T H x$$

$$\text{subject to } A_1 x = b_1$$

$$A_2 x \geq b_2$$

given the vectors b_1, b_2, and g and the matrices H, A_1, and A_2. H is required to be positive definite. In this case, a unique x solves the problem or the constraints are inconsistent. If H is not positive definite, a positive definite perturbation of H is used in place of H. For more details, see Powell (1983, 1985).

Comments

1. Workspace may be explicitly provided, if desired, by use of `Q2ROG/DQ2ROG`. The reference is:

   `CALL Q2ROG (NVAR, NCON, NEQ, A, LDA, B, G, H, LDH, DIAGNL, SOL, NACT, IACT, ALAMDA, WK)`

   The additional argument is:

   WK — Work vector of length (3 * `NVAR`**2 + 11 * `NVAR`)/2 + `NCON`.

2. Informational errors

Type	Code	Description
3	1	Due to the effect of computer rounding error, a change in the variables fail to improve the objective function value; usually the solution is close to optimum.
4	2	The system of equations is inconsistent. There is no solution.

3. If a perturbation of `H`, `H` + `DIAGNL` * `I`, was used in the `QP` problem, then `H` + `DIAGNL` * `I` should also be used in the definition of the Lagrange multipliers.

Example

The quadratic programming problem

$$\begin{aligned}
&\min f(x) = x_1^2 + x_2^2 + x_3^2 + x_4^2 + x_5^2 - 2x_2x_3 - 2x_4x_5 - 2x_1 \\
&\text{subject to} \quad x_1 + x_2 + x_3 + x_4 + x_5 = 5 \\
&\qquad\qquad\quad x_3 - 2x_4 - 2x_5 = -3
\end{aligned}$$

is solved.

```
      USE QPROG_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    LDA, LDH, NCON, NEQ, NVAR
      PARAMETER  (NCON=2, NEQ=2, NVAR=5, LDA=NCON, LDH=NVAR)
!
      INTEGER    K, NACT, NOUT
      REAL       A(LDA,NVAR), ALAMDA(NVAR), B(NCON), G(NVAR), &
```

```
                  H(LDH,LDH), SOL(NVAR)
!
!                                   Set values of A, B, G and H.
!                                   A = ( 1.0  1.0  1.0  1.0  1.0)
!                                       ( 0.0  0.0  1.0 -2.0 -2.0)
!
!                                   B = ( 5.0 -3.0)
!
!                                   G = (-2.0  0.0  0.0  0.0  0.0)
!
!                                   H = ( 2.0  0.0  0.0  0.0  0.0)
!                                       ( 0.0  2.0 -2.0  0.0  0.0)
!                                       ( 0.0 -2.0  2.0  0.0  0.0)
!                                       ( 0.0  0.0  0.0  2.0 -2.0)
!                                       ( 0.0  0.0  0.0 -2.0  2.0)
!
      DATA A/1.0, 0.0, 1.0, 0.0, 1.0, 1.0, 1.0, -2.0, 1.0, -2.0/
      DATA B/5.0, -3.0/
      DATA G/-2.0, 4*0.0/
      DATA H/2.0, 5*0.0, 2.0, -2.0, 3*0.0, -2.0, 2.0, 5*0.0, 2.0, &
          -2.0, 3*0.0, -2.0, 2.0/
!
      CALL QPROG (NEQ, A, B, G, H, SOL)
!
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) (SOL(K),K=1,NVAR)
99999 FORMAT ('  The solution vector is', /, '  SOL = (', 5F6.1, &
            '  )')
!
      END
```

Output

```
The solution vector is
SOL = (   1.0   1.0   1.0   1.0   1.0  )
```

LCONF

Minimizes a general objective function subject to linear equality/inequality constraints.

Required Arguments

FCN — User-supplied subroutine to evaluate the function to be minimized. The usage is
CALL FCN (N, X, F), where

N – Value of NVAR. (Input)

X – Vector of length N at which point the function is evaluated. (Input)
X should not be changed by FCN.

F – The computed function value at the point X. (Output)

FCN must be declared EXTERNAL in the calling program.

NEQ — The number of linear equality constraints. (Input)

A — NCON by NVAR matrix. (Input)
The matrix contains the equality constraint gradients in the first NEQ rows, followed by the inequality constraint gradients.

B — Vector of length NCON containing right-hand sides of the linear constraints. (Input)
Specifically, the constraints on the variables X(I), I = 1, …, NVAR are
A(K, 1) * X(1) + … + A(K, NVAR) * X(NVAR).EQ.B(K), K = 1, …, NEQ.A(K, 1) *
X(1) + … + A(K, NVAR) * X(NVAR).LE.B(K), K = NEQ + 1, …, NCON. Note that the data that define the equality constraints come before the data of the inequalities.

XLB — Vector of length NVAR containing the lower bounds on the variables; choose a very large negative value if a component should be unbounded below or set XLB(I) = XUB(I) to freeze the I-th variable. (Input)
Specifically, these simple bounds are XLB(I).LE.X(I), I = 1, …, NVAR.

XUB — Vector of length NVAR containing the upper bounds on the variables; choose a very large positive value if a component should be unbounded above. (Input)
Specifically, these simple bounds are X(I).LE.XUB(I), I = 1, …, NVAR.

SOL — Vector of length NVAR containing solution. (Output)

Optional Arguments

NVAR — The number of variables. (Input)
Default: NVAR = SIZE (A,2).

NCON — The number of linear constraints (excluding simple bounds). (Input)
Default: NCON = SIZE (A,1).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = SIZE (A,1).

XGUESS — Vector of length NVAR containing the initial guess of the minimum. (Input)
Default: XGUESS = 0.0.

ACC — The nonnegative tolerance on the first order conditions at the calculated solution. (Input)
Default: ACC = 1.e-4 for single precision and 1.d-8 for double precision.

MAXFCN — On input, maximum number of function evaluations allowed. (Input/ Output)
On output, actual number of function evaluations needed.
Default: MAXFCN = 400.

OBJ — Value of the objective function. (Output)

NACT — Final number of active constraints. (Output)

IACT — Vector containing the indices of the final active constraints in the first NACT positions. (Output)
Its length must be at least NCON + 2 * NVAR.

ALAMDA — Vector of length NVAR containing the Lagrange multiplier estimates of the final active constraints in the first NACT positions. (Output)

FORTRAN 90 Interface

Generic: CALL LCONF (FCN, NEQ, A, B, XLB, XUB, SOL [, …])

Specific: The specific interface names are S_LCONF and D_LCONF.

FORTRAN 77 Interface

Single: CALL LCONF (FCN, NVAR, NCON, NEQ, A, LDA, B, XLB, XUB, XGUESS, ACC, MAXFCN, SOL, OBJ, NACT, IACT, ALAMDA)

Double: The double precision name is DLCONF.

Description

The routine `LCONF` is based on M.J.D. Powell's `TOLMIN`, which solves linearly constrained optimization problems, i.e., problems of the form

$$\min_{x \in R^n} f(x)$$

$$\text{subject to} \quad A_1 x = b_1$$

$$A_2 x \le b_2$$

$$x_l \le x \le x_u$$

given the vectors b_1, b_2, x_l and x_u and the matrices A_1, and A_2.

The algorithm starts by checking the equality constraints for inconsistency and redundancy. If the equality constraints are consistent, the method will revise x^0, the initial guess provided by the user, to satisfy

$$A_1 x = b_1$$

Next, x^0 is adjusted to satisfy the simple bounds and inequality constraints. This is done by solving a sequence of quadratic programming subproblems to minimize the sum of the constraint or bound violations.

Now, for each iteration with a feasible x^k, let J_k be the set of indices of inequality constraints that have small residuals. Here, the simple bounds are treated as inequality constraints. Let I_k be the set of indices of active constraints. The following quadratic programming problem

$$\min f\left(x^k\right) + d^T \nabla f\left(x^k\right) + \frac{1}{2} d^T B^k d$$

$$\text{subject to} \quad a_j d = 0 \quad j \in I_k$$

$$a_j d \le 0 \quad j \in J_k$$

is solved to get (d^k, λ^k) where a_j is a row vector representing either a constraint in A_1 or A_2 or a bound constraint on x. In the latter case, the $a_j = e_i$ for the bound constraint $x_i \le (x_u)_i$ and $a_j = -e_i$ for the constraint $-x_i \le (-x_l)_i$. Here, e_i is a vector with a 1 as the i-th component, and zeroes elsewhere. λ^k are the Lagrange multipliers, and B^k is a positive definite approximation to the second derivative $\nabla^2 f(x^k)$.

After the search direction d^k is obtained, a line search is performed to locate a better point. The new point $x^{k+1} = x^k + \alpha^k d^k$ has to satisfy the conditions

$$f\left(x^k+\alpha^k d^k\right) \le f\left(x^k\right) + 0.1\alpha^k\left(d^k\right)^T \nabla f\left(x^k\right)$$

and

$$\left(d^k\right)^T \nabla f\left(x^k+\alpha^k d^k\right) \ge 0.7\left(d^k\right)^T \nabla f\left(x^k\right)$$

The main idea in forming the set J_k is that, if any of the inequality constraints restricts the step-length α^k, then its index is not in J_k. Therefore, small steps are likely to be avoided.

Finally, the second derivative approximation, B^k, is updated by the BFGS formula, if the condition

$$\left(d^k\right)^T \nabla f\left(x^k+\alpha^k d^k\right) - \nabla f\left(x^k\right) > 0$$

holds. Let $x^k \leftarrow x^{k+1}$, and start another iteration.

The iteration repeats until the stopping criterion

$$\|\nabla f\left(x^k\right) - A^k\lambda^k\|_2 \le \tau$$

is satisfied; here, τ is a user-supplied tolerance. For more details, see Powell (1988, 1989).

Since a finite-difference method is used to estimate the gradient for some single precision calculations, an inaccurate estimate of the gradient may cause the algorithm to terminate at a noncritical point. In such cases, high precision arithmetic is recommended. Also, whenever the exact gradient can be easily provided, routine LCONG should be used instead.

Comments

1. Workspace may be explicitly provided, if desired, by use of L2ONF/DL2ONF. The reference is:

```
CALL L2ONF (FCN, NVAR, NCON, NEQ, A, LDA, B, XLB, XUB,
   XGUESS, ACC, MAXFCN, SOL, OBJ, NACT, IACT, ALAMDA, IPRINT,
   INFO, WK)
```

   The additional arguments are as follows:

   IPRINT — Print option (see Comment 3). (Input)

   INFO — Informational flag (see Comment 3). (Output)

   WK — Real work vector of length `NVAR**2 + 11 * NVAR + NCON`.

2. Informational Errors

Type	Code	Description
4	4	The equality constraints are inconsistent.
4	5	The equality constraints and the bounds on the variables are found to be inconsistent.
4	6	No vector X satisfies all of the constraints. In particular, the current active constraints prevent any change in X that reduces the sum of constraint violations.
4	7	Maximum number of function evaluations exceeded.
4	9	The variables are determined by the equality constraints.

3. The following are descriptions of the arguments IPRINT and INFO:

   IPRINT — This argument must be set by the user to specify the frequency of printing during the execution of the routine LCONF. There is no printed output if IPRINT = 0. Otherwise, after ensuring feasibility, information is given every IABS(IPRINT) iterations and whenever a parameter called TOL is reduced. The printing provides the values of X(.), F(.) and G(.) = GRAD(F) if IPRINT is positive. If IPRINT is negative, this information is augmented by the current values of IACT(K) K = 1, …, NACT, PAR(K) K = 1, …, NACT and RESKT(I) I = 1, …, N. The reason for returning to the calling program is also displayed when IPRINT is nonzero.

   INFO — On exit from L2ONF, INFO will have one of the following integer values to indicate the reason for leaving the routine:

   INFO = 1 SOL is feasible, and the condition that depends on ACC is satisfied.

   INFO = 2 SOL is feasible, and rounding errors are preventing further progress.

   INFO = 3 SOL is feasible, but the objective function fails to decrease although a decrease is predicted by the current gradient vector.

   INFO = 4 In this case, the calculation cannot begin because LDA is less than NCON or because the lower bound on a variable is greater than the upper bound.

   INFO = 5 This value indicates that the equality constraints are inconsistent. These constraints include any components of X(.) that are frozen by setting XL(I) = XU(I).

   INFO = 6 In this case there is an error return because the equality constraints and the bounds on the variables are found to be inconsistent.

   INFO = 7 This value indicates that there is no vector of variables that satisfies all of the constraints. Specifically, when this return or an INFO = 6 return occurs, the current active constraints (whose indices are IACT(K), K = 1, …, NACT) prevent any change in X(.) that reduces the sum of constraint violations. Bounds are only included in this sum if INFO = 6.

   INFO = 8 Maximum number of function evaluations exceeded.

   INFO = 9 The variables are determined by the equality constraints.

Example

The problem from Schittkowski (1987)

$$\min f(x) = -x_1 x_2 x_3$$

$$\text{subject to} \qquad -x_1 - 2x_2 - 2x_3 \le 0$$

$$x_1 + 2\,x_2 + 2\,x_3 \le 72$$

$$0 \le x_1 \le 20$$

$$0 \le x_2 \le 11$$

$$0 \le x_3 \le 42$$

is solved with an initial guess $x_1 = 10$, $x_2 = 10$ and $x_3 = 10$.

```
      USE LCONF_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                 Declaration of variables
      INTEGER    NCON, NEQ, NVAR
      PARAMETER  (NCON=2, NEQ=0, NVAR=3)
!
      INTEGER    MAXFCN, NOUT
      REAL       A(NCON,NVAR), ACC, B(NCON), OBJ, &
                SOL(NVAR), XGUESS(NVAR), XLB(NVAR), XUB(NVAR)
      EXTERNAL   FCN
!
!                                 Set values for the following problem.
!
!                                 Min  -X(1)*X(2)*X(3)
!
!                                 -X(1) - 2*X(2) - 2*X(3)  .LE.   0
!                                  X(1) + 2*X(2) + 2*X(3)  .LE.  72
!
!                                 0  .LE.  X(1)  .LE.  20
!                                 0  .LE.  X(2)  .LE.  11
!                                 0  .LE.  X(3)  .LE.  42
!
      DATA A/-1.0, 1.0, -2.0, 2.0, -2.0, 2.0/, B/0.0, 72.0/
      DATA XLB/3*0.0/, XUB/20.0, 11.0, 42.0/, XGUESS/3*10.0/
      DATA ACC/0.0/, MAXFCN/400/
!
      CALL UMACH (2, NOUT)
!
      CALL LCONF (FCN, NEQ, A, B, XLB, XUB, SOL, XGUESS=XGUESS,  &
                 MAXFCN=MAXFCN, ACC=ACC, OBJ=OBJ)
!
      WRITE (NOUT,99998) 'Solution:'
      WRITE (NOUT,99999) SOL
      WRITE (NOUT,99998) 'Function value at solution:'
      WRITE (NOUT,99999) OBJ
      WRITE (NOUT,99998) 'Number of function evaluations:', MAXFCN
      STOP
99998 FORMAT (//, ' ', A, I4)
99999 FORMAT (1X, 5F16.6)
      END
!
```

```
      SUBROUTINE FCN (N, X, F)
      INTEGER    N
      REAL       X(*), F
!
      F = -X(1)*X(2)*X(3)
      RETURN
      END
```

Output

```
Solution:
 20.000000       11.000000       15.000000

Function value at solution:
-3300.000000

Number of function evaluations:   5
```

LCONG

Minimizes a general objective function subject to linear equality/inequality constraints.

Required Arguments

FCN — User-supplied subroutine to evaluate the function to be minimized. The usage is
CALL FCN (N, X, F), where

N – Value of NVAR. (Input)

X – Vector of length N at which point the function is evaluated. (Input)
X should not be changed by FCN.

F – The computed function value at the point X. (Output)

FCN must be declared EXTERNAL in the calling program.

GRAD — User-supplied subroutine to compute the gradient at the point X. The usage is
CALL GRAD (N, X, G), where

N – Value of NVAR. (Input)

X – Vector of length N at which point the function is evaluated. (Input)
X should not be changed by GRAD.

G – Vector of length N containing the values of the gradient of the objective function evaluated at the point X. (Output)

GRAD must be declared EXTERNAL in the calling program.

NEQ — The number of linear equality constraints. (Input)

A — NCON by NVAR matrix. (Input)
The matrix contains the equality constraint gradients in the first NEQ rows, followed by the inequality constraint gradients.

B — Vector of length NCON containing right-hand sides of the linear constraints. (Input)
Specifically, the constraints on the variables X(I), I = 1, …, NVAR are A(K, 1) * X(1) + … + A(K, NVAR) * X(NVAR).EQ.B(K), K = 1, …,
NEQ.A(K, 1) * X(1) + … + A(K, NVAR) * X(NVAR).LE.B(K), K = NEQ + 1, …, NCON. Note that the data that define the equality constraints come before the data of the inequalities.

XLB — Vector of length NVAR containing the lower bounds on the variables; choose a very large negative value if a component should be unbounded below or set
XLB(I) = XUB(I) to freeze the I-th variable. (Input)
Specifically, these simple bounds are XLB(I).LE.X(I), I = 1, …, NVAR.

XUB — Vector of length NVAR containing the upper bounds on the variables; choose a very large positive value if a component should be unbounded above. (Input)
Specifically, these simple bounds are X(I).LE. XUB(I), I = 1, …, NVAR.

SOL — Vector of length NVAR containing solution. (Output)

Optional Arguments

NVAR — The number of variables. (Input)
Default: NVAR = SIZE (A,2).

NCON — The number of linear constraints (excluding simple bounds). (Input)
Default: NCON = SIZE (A,1).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = SIZE (A,1).

XGUESS — Vector of length NVAR containing the initial guess of the minimum. (Input)
Default: XGUESS = 0.0.

ACC — The nonnegative tolerance on the first order conditions at the calculated solution. (Input)
Default: ACC = 1.e-4 for single precision and 1.d-8 for double precision.

MAXFCN — On input, maximum number of function evaluations allowed.(Input/ Output)
On output, actual number of function evaluations needed.
Default: MAXFCN = 400.

OBJ — Value of the objective function. (Output)

NACT — Final number of active constraints. (Output)

IACT — Vector containing the indices of the final active constraints in the first NACT positions. (Output)
Its length must be at least NCON + 2 * NVAR.

ALAMDA — Vector of length NVAR containing the Lagrange multiplier estimates of the final active constraints in the first NACT positions. (Output)

FORTRAN 90 Interface

Generic: CALL LCONG (FCN, GRAD, NEQ, A, B, XLB, XUB, SOL [, …])

Specific: The specific interface names are S_LCONG and D_LCONG.

FORTRAN 77 Interface

Single: CALL LCONG (FCN, GRAD, NVAR, NCON, NEQ, A, LDA, B, XLB, XUB, XGUESS, ACC, MAXFCN, SOL, OBJ, NACT, IACT, ALAMDA)

Double: The double precision name is DLCONG.

Description

The routine LCONG is based on M.J.D. Powell's TOLMIN, which solves linearly constrained optimization problems, i.e., problems of the form

$$\min_{x \in R^n} f(x)$$

$$\text{subject to } A_1 x = b_1$$

$$A_2 x \le b_2$$

$$x_l \le x \le x_u$$

given the vectors b_1, b_2, x_l and x_u and the matrices A_1, and A_2.

The algorithm starts by checking the equality constraints for inconsistency and redundancy. If the equality constraints are consistent, the method will revise x^0, the initial guess provided by the user, to satisfy

$$A_1 x = b_1$$

Next, x^0 is adjusted to satisfy the simple bounds and inequality constraints. This is done by solving a sequence of quadratic programming subproblems to minimize the sum of the constraint or bound violations.

Now, for each iteration with a feasible x^k, let J_k be the set of indices of inequality constraints that have small residuals. Here, the simple bounds are treated as inequality constraints. Let I_k be the set of indices of active constraints. The following quadratic programming problem

$$\min f\left(x^k\right) + d^T \nabla f\left(x^k\right) + \frac{1}{2} d^T B^k d$$

$$\text{subject to } a_j d = 0 \quad j \in I_k$$

$$a_j d \le 0 \quad j \in J_k$$

is solved to get (d^k, λ^k) where a_j is a row vector representing either a constraint in A_1 or A_2 or a bound constraint on x. In the latter case, the $a_j = e_i$ for the bound constraint $x_i \le (x_u)_i$ and $a_j = -e_i$ for the constraint $-x_i \le (-x_l)_i$. Here, e_i is a vector with a 1 as the i-th component, and zeroes elsewhere. λ^k are the Lagrange multipliers, and B^k is a positive definite approximation to the second derivative $\nabla^2 f(x^k)$.

After the search direction d^k is obtained, a line search is performed to locate a better point. The new point $x^{k+1} = x^k + \alpha^k d^k$ has to satisfy the conditions

$$f\left(x^k + \alpha^k d^k\right) \le f\left(x^k\right) + 0.1\alpha^k\left(d^k\right)^T \nabla f\left(x^k\right)$$

and

$$\left(d^k\right)^T \nabla f\left(x^k + \alpha^k d^k\right) \ge 0.7\left(d^k\right)^T \nabla f\left(x^k\right)$$

The main idea in forming the set J_k is that, if any of the inequality constraints restricts the step-length α^k, then its index is not in J_k. Therefore, small steps are likely to be avoided.

Finally, the second derivative approximation, B^k, is updated by the BFGS formula, if the condition

$$\left(d^k\right)^T \nabla f\left(x^k + \alpha^k d^k\right) - \nabla f\left(x^k\right) > 0$$

holds. Let $x^k \leftarrow x^{k+1}$, and start another iteration.

The iteration repeats until the stopping criterion

$$\|\nabla f\left(x^k\right) - A^k \lambda^k\|_2 \le \tau$$

is satisfied; here, τ is a user-supplied tolerance. For more details, see Powell (1988, 1989).

Comments

1. Workspace may be explicitly provided, if desired, by use of L2ONG/DL2ONG. The reference is:

```
CALL L2ONG (FCN, GRAD, NVAR, NCON, NEQ, A, LDA, B, XLB, XUB,
   XGUESS, ACC, MAXFCN, SOL, OBJ, NACT, IACT, ALAMDA, IPRINT,
   INFO, WK)
```

   The additional arguments are as follows:

   IPRINT — Print option (see Comment 3). (Input)

   INFO — Informational flag (see Comment 3). (Output)

   WK — Real work vector of length NVAR**2 + 11 * NVAR + NCON.

2. Informational errors

Type	Code	Description
4	4	The equality constraints are inconsistent.
4	5	The equality constraints and the bounds on the variables are found to be inconsistent.
4	6	No vector X satisfies all of the constraints. In particular, the current active constraints prevent any change in X that reduces the sum of constraint violations.
4	7	Maximum number of function evaluations exceeded.
4	9	The variables are determined by the equality constraints.

3. The following are descriptions of the arguments IPRINT and INFO:

IPRINT — This argument must be set by the user to specify the frequency of printing during the execution of the routine LCONG. There is no printed output if IPRINT = 0. Otherwise, after ensuring feasibility, information is given every IABS(IPRINT) iterations and whenever a parameter called TOL is reduced. The printing provides the values of X(.), F(.) and G(.) = GRAD(F) if IPRINT is positive. If IPRINT is negative, this information is augmented by the current values of IACT(K) K = 1, ..., NACT, PAR(K) K = 1, ..., NACT and RESKT(I) I = 1, ..., N. The reason for returning to the calling program is also displayed when IPRINT is nonzero.

INFO — On exit from L2ONG, INFO will have one of the following integer values to indicate the reason for leaving the routine:

INFO = 1 SOL is feasible and the condition that depends on ACC is satisfied.

INFO = 2 SOL is feasible and rounding errors are preventing further progress.

INFO = 3 SOL is feasible but the objective function fails to decrease although a decrease is predicted by the current gradient vector.

INFO = 4 In this case, the calculation cannot begin because LDA is less than NCON or because the lower bound on a variable is greater than the upper bound.

INFO = 5 This value indicates that the equality constraints are inconsistent. These constraints include any components of X(.) that are frozen by setting XL(I) = XU(I).

INFO = 6 In this case, there is an error return because the equality constraints and the bounds on the variables are found to be inconsistent.

INFO = 7 This value indicates that there is no vector of variables that satisfies all of the constraints. Specifically, when this return or an INFO = 6 return occurs, the current active constraints (whose indices are IACT(K), K = 1, ..., NACT) prevent any change in X(.) that reduces the sum of constraint violations, where only bounds are included in this sum if INFO = 6.

INFO = 8 Maximum number of function evaluations exceeded.

INFO = 9 The variables are determined by the equality constraints.

Example

The problem from Schittkowski (1987)

$$\min f(x) = -x_1 \; x_2 \; x_3$$

$$\text{subject to} \quad -x_1 - 2x_2 - 2x_3 \le 0$$

$$x_1 + 2\,x_2 + 2\,x_3 \le 72$$

$$0 \le x_1 \le 20$$

$$0 \le x_2 \le 11$$

$$0 \le x_3 \le 42$$

is solved with an initial guess x_1 = 10, x_2= 10 and x_3 = 10.

```
      USE LCONG_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                  Declaration of variables
      INTEGER    NCON, NEQ, NVAR
      PARAMETER  (NCON=2, NEQ=0, NVAR=3)
!
      INTEGER    MAXFCN, NOUT
      REAL       A(NCON,NVAR), ACC, B(NCON), OBJ, &
                 SOL(NVAR), XGUESS(NVAR), XLB(NVAR), XUB(NVAR)
      EXTERNAL   FCN, GRAD
!
!                                  Set values for the following problem.
!
!                                  Min  -X(1)*X(2)*X(3)
!
!                                  -X(1) - 2*X(2) - 2*X(3)  .LE.   0
!                                   X(1) + 2*X(2) + 2*X(3)  .LE.  72
!
!                                  0  .LE.  X(1)  .LE.  20
!                                  0  .LE.  X(2)  .LE.  11
!                                  0  .LE.  X(3)  .LE.  42
!
      DATA A/-1.0, 1.0, -2.0, 2.0, -2.0, 2.0/, B/0.0, 72.0/
      DATA XLB/3*0.0/, XUB/20.0, 11.0, 42.0/, XGUESS/3*10.0/
      DATA ACC/0.0/, MAXFCN/400/
!
      CALL UMACH (2, NOUT)
!
      CALL LCONG (FCN, GRAD, NEQ, A, B, XLB, XUB, SOL, XGUESS=XGUESS, &
                  ACC=ACC, MAXFCN=MAXFCN, OBJ=OBJ)
!
      WRITE (NOUT,99998) 'Solution:'
      WRITE (NOUT,99999) SOL
      WRITE (NOUT,99998) 'Function value at solution:'
      WRITE (NOUT,99999) OBJ
      WRITE (NOUT,99998) 'Number of function evaluations:', MAXFCN
      STOP
99998 FORMAT (//, ' ', A, I4)
99999 FORMAT (1X, 5F16.6)
      END
```

```
!
      SUBROUTINE FCN (N, X, F)
      INTEGER    N
      REAL       X(*), F
!
      F = -X(1)*X(2)*X(3)
      RETURN
      END
!
      SUBROUTINE GRAD (N, X, G)
      INTEGER    N
      REAL       X(*), G(*)
!
      G(1) = -X(2)*X(3)
      G(2) = -X(1)*X(3)
      G(3) = -X(1)*X(2)
      RETURN
      END
```

Output

```
Solution:
20.000000       11.000000       15.000000

Function value at solution:
-3300.000000

Number of function evaluations:   5
```

LIN_CON_TRUST_REGION

more...

Minimizes a function of N variables subject to linear constraints using a derivative-free, interpolation-based trust-region method.

NOTE: Routine LIN_CON_TRUST_REGION is available in double precision only.

Required Arguments

FCN — User-supplied subroutine to evaluate the function to be minimized. The usage is CALL FCN (N, X, F), where

N – Length of X. (Input)

X – Array of length N, the point at which the function is evaluated. (Input) X should not be changed by FCN.

F – The computed function value at the point X. (Output)

FCN must be declared EXTERNAL in the calling program.

NPT – The number of interpolation conditions, which is required to be in the interval [N+2,(N+1)*(N+2)/2]. Typical choices are NPT=N+6 and NPT=2*N+1. Larger values tend to be highly inefficient when the number of variables is substantial, due to the amount of work and extra difficulty of adjusting more points. (Input)

A – Array of size M by N containing the constraints. The constraints are of the form

$$a_i^T x \le b_i \;,\; i = 1, \ldots, m$$

where $a_i = \left(a_{i1}, \ldots, a_{in}\right)^T$ denotes the *i*-th constraint. (Input)

B – Array of size M containing the right-hand sides of the constraints. (Input)

RHOBEG – The initial value of a trust region radius, 0 < RHOEND <= RHOBEG. Typically, RHOBEG should be about 1/10 of the greatest expected change to a variable. (Input)

RHOEND – The final value of a trust region radius, 0 < RHOEND <= RHOBEG. Variable RHOEND should indicate the accuracy that is required in the final values of the variables. (Input)

X – Array of size N containing the computed solution. (Output)

Optional Arguments

M – Number of constraints. (Input)
Default: `M = SIZE (A,1)`.

N – Number of variables. (Input)
Default: `N = SIZE (X,1)`.

IPRINT – Parameter indicating the desired output level. (Input)

IPRINT	Action
0	No output printed
1	Output printed only upon return from `LIN_CON_TRUST_REGION`.
2	The best feasible vector of variables so far and the corresponding value of the objective function are printed whenever `RHO` is reduced, where `RHO` is the current lower bound on the trust region radius.
3	Output each new value of `FVALUE` with its variables.

Default: `IPRINT` = 0.

XGUESS – Array of size `N` that contains an initial guess to the minimum. If the initial guess is not feasible, then it is replaced by a feasible starting point determined as the solution of a constrained linear least-squares problem. (Input)
Default: `XGUESS` = 0.0.

MAXFCN – On input, maximum allowed number of function evaluations. (Input/Output)
On output, actual number of function evaluations needed.
Default: `MAXFCN` = 200.

FVALUE – Function value at the computed solution. (Output)

FORTRAN 90 Interface

Generic: `CALL LIN_CON_TRUST_REGION` (`FCN`, `NPT`, `A`, `B`, `RHOBEG`, `RHOEND`, `X` [, …])

Specific: The specific interface name is `D_LIN_CON_TRUST_REGION`. This subroutine is available in double precision only.

Description

The routine LIN_CON_TRUST_REGION implements a trust-region method that forms quadratic models by interpolation to solve linearly constrained optimization problems of the form

$$\begin{array}{rl} \min & f(x) \\ \text{subject to} & Ax \le b \end{array}$$

where $f(x)$ is a function of *n* variables, $A \in R^{m \times n}$ is the constraint matrix, $x \in R^n$ and $b \in R^m$.

Usually, many degrees of freedom remain in each new model after satisfying the interpolation conditions. These remaining degrees of freedom are taken up by minimizing the Frobenius norm of the change to the second derivative matrix of the model, see *Powell (2004)*.

One new function value is calculated at each iteration, usually at a point where the current model predicts a reduction in the least value so far reached by the objective function subject to the linear constraints. Alternatively, the algorithm may choose a new vector of variables to replace an interpolation point that is too far away for reliability, in which case this new point need not satisfy the linear constraints.

Routine LIN_CON_TRUST_REGION is based on the LINCOA algorithm by *Michael J.D. Powell (2014)*.

Comments

1. Informational errors

Type	**Code**	**Description**
4	1	A row of input matrix A is equal to zero.
4	2	The problem is infeasible.
4	3	The maximum number of function evaluations is exceeded.
4	4	Computer rounding errors prevent further refinement of X.
4	5	Algorithm has stopped because the denominator of the updating formula is zero.

2. Since LIN_CON_TRUST_REGION uses only function-value information at each step to determine a new approximate minimum, it could be quite inefficient on smooth problems compared to other methods, such as those implemented in routine LCONF, which takes into account derivative information at each iteration. Hence, routine LIN_CON_TRUST_REGION should be used only as a last resort if derivatives are available.

Example

In this example, Rosenbrock's post office problem,

$$\min f(x) = -x_1 x_2 x_3$$

subject to

$$x_1 + 2x_2 + 2x_3 - 72 \le 0$$
$$x_1 + 2x_2 + 2x_3 \ge 0$$
$$0 \le x_i \le 42, \quad i = 1, 2, 3$$

is solved with an initial feasible guess (`10.0, 10.0, 10.0`), and the solution is printed.

```
      USE LIN_CON_TRUST_REGION_INT
      USE UMACH_INT

      IMPLICIT NONE
!               Variable declarations
      INTEGER, PARAMETER :: M = 8, N = 3, NPT = 7
!
      INTEGER :: K, NOUT
      DOUBLE PRECISION :: RHOBEG, RHOEND, FVALUE
      DOUBLE PRECISION :: A(M,N), B(M), X(N)
!
!               Initialization (feasible starting point)
!               XGUESS = (10.0, 10.0, 10.0)
!
      DOUBLE PRECISION :: XGUESS(N) = (/ 10.0, 10.0, 10.0 /)
      EXTERNAL FCN
!
      RHOBEG = 1.0D0
      RHOEND = 1.0D-9
!
      A(:,1) = (/ 1.0, -1.0, 1.0, -1.0, 0.0, 0.0, 0.0, 0.0 /)
      A(:,2) = (/ 2.0, -2.0, 0.0, 0.0, 1.0, -1.0, 0.0, 0.0 /)
      A(:,3) = (/ 2.0, -2.0, 0.0, 0.0, 0.0, 0.0, 1.0, -1.0 /)
      B(:) = (/ 72.0, 0.0, 42.0, 0.0, 42.0, 0.0, 42.0, 0.0 /)
!
      CALL LIN_CON_TRUST_REGION (FCN, NPT, A, B, RHOBEG, RHOEND, X, &
                   XGUESS=XGUESS, FVALUE=FVALUE)
!
      CALL UMACH (2, NOUT)
      WRITE (NOUT, 99999) (X(K),K=1,N), FVALUE
99999 FORMAT ('  The best estimate for the minimum value of the', /, &
             '  function is X = (', 3(2X,F5.2), ')', /, '  with ', &
             'function value FVALUE = ', E13.6)
!
      END
!               External function to be minimized
      SUBROUTINE FCN (N, X, F)
      INTEGER :: N
      DOUBLE PRECISION :: X(N), F
!
      F = -X(1) * X(2) * X(3)
      RETURN
      END
```

Output

```
The best estimate for the minimum value of the
function is X = (  24.00  12.00  12.00)
with function value FVALUE = -0.345600E+04
```

NNLPF

Solves a general nonlinear programming problem using a sequential equality constrained quadratic programming method.

Required Arguments

FCN — User-supplied subroutine to evaluate the objective function and constraints at a given point. The internal usage is CALL FCN (X, IACT, RESULT, IERR), where

X – The point at which the objective function or constraint is evaluated. (Input)

IACT – Integer indicating whether evaluation of the objective function is requested or evaluation of a constraint is requested. If IACT is zero, then an objective function evaluation is requested. If IACT is nonzero then the value if IACT indicates the index of the constraint to evaluate. IACT = 1 to ME for equality constraints and IACT = ME +1 to M for inequality constraints. (Input)

RESULT – If IACT is zero, then RESULT is the computed function value at the point X. If IACT is nonzero, then RESULT is the computed constraint value at the point X. (Output)

IERR – Logical variable. On input IERR is set to .FALSE. If an error or other undesirable condition occurs during evaluation, then IERR should be set to .TRUE. Setting IERR to .TRUE. will result in the step size being reduced and the step being tried again. (If IERR is set to .TRUE. for XGUESS, then an error is issued.)

The routine FCN must be use-associated in a user module that uses NNLPF_INT, or else declared EXTERNAL in the calling program. If FCN is a separately compiled routine, not in a module, then it must be declared EXTERNAL.

M — Total number of constraints. (Input)

ME — Number of equality constraints. (Input)

IBTYPE — Scalar indicating the types of bounds on variables. (Input)

IBTYPE	Action
0	User will supply all the bounds.
1	All variables are nonnegative.
2	All variables are nonpositive.
3	User supplies only the bounds on 1st variable, all other variables will have the same bounds.

XLB — Vector of length N containing the lower bounds on variables. (Input, if IBTYPE = 0; output, if IBTYPE = 1 or 2; input/output, if IBTYPE = 3)
If there is no lower bound for a variable, then the corresponding XLB value should be set to -Huge(X(1)).

XUB — Vector of length N containing the upper bounds on variables. (Input, if IBTYPE = 0; output, if IBTYPE = 1 or 2; input/output, if IBTYPE = 3).
If there is no upper bound for a variable, then the corresponding XUB value should be set to Huge(X(1)).

X — Vector of length N containing the computed solution. (Output)

Optional Arguments

N — Number of variables. (Input)
Default: N = SIZE(X).

XGUESS — Vector of length N containing an initial guess of the solution. If XGUESS is located outside or in the boundary region of the bound constraints set, then the algorithm first projects XGUESS into the interior of the bound constraints set before starting the main computations. (Input)
Default: XGUESS = x, where x is the vector with the smallest l_2 – norm that satisfies the bounds.

XSCALE — Vector of length N setting the internal scaling of the variables. The initial value given and the objective function and gradient evaluations however are always in the original unscaled variables. The first internal variable is obtained by dividing values X(I) by XSCALE(I). (Input)
In the absence of other information, set all entries to 1.0.
Default: XSCALE(:) = 1.0.

IPRINT — Parameter indicating the desired output level. (Input)

IPRINT	Action
0	No output printed.
1	One line of intermediate results is printed in each iteration.
2	Lines of intermediate results summarizing the most important data for each step are printed.

IPRINT	Action
3	Lines of detailed intermediate results showing all primal and dual variables, the relevant values from the working set, progress in the backtracking and etc are printed
4	Lines of detailed intermediate results showing all primal and dual variables, the relevant values from the working set, progress in the backtracking, the gradients in the working set, the quasi-Newton updated and etc are printed.

Default: IPRINT = 0.

MAXITN — Maximum number of iterations allowed. (Input)
Default: MAXITN = 200.

EPSDIF — Relative precision in gradients. (Input)
Default: EPSDIF = epsilon(1)

TAU0 — A universal bound describing how much the unscaled penalty-term may deviate from zero. (Input)
NNLPF assumes that within the region described by

$$\sum_{i=1}^{M_e} |g_i(x)| - \sum_{i=M_e+1}^{M} \min\left(0, g_i(x)\right) \le \mathrm{TAU0}$$

all functions may be evaluated safely. The initial guess, however, may violate these requirements. In that case an initial feasibility improvement phase is run by NNLPF until such a point is found. A small TAU0 diminishes the efficiency of NNLPF, because the iterates then will follow the boundary of the feasible set closely. Conversely, a large TAU0 may degrade the reliability of the code.
Default TAU0 = 1.E0

DEL0 — In the initial phase of minimization a constraint is considered binding if

$$\frac{g_i(x)}{\max\left(1, \|\nabla g_i(x)\|\right)} \le \mathrm{DEL0} \qquad i = M_e + 1, \dots, M$$

Good values are between .01 and 1.0. If DEL0 is chosen too small then identification of the correct set of binding constraints may be delayed. Contrary, if DEL0 is too large, then the method will often escape to the full regularized SQP method, using individual slack variables for any active constraint, which is quite costly. For well-scaled problems DEL0=1.0 is reasonable. (Input)
Default: DEL0 = .5*TAU0

EPSFCN – Relative precision of the function evaluation routine. (Input)
Default: EPSFCN = epsilon(1)

DTYPE – Type of numerical differentiation to be used. (Input)
Default: IDTYPE = 1

IDTYPE	Action
1	Use a forward difference quotient with discretization stepsize 0.1 ($\text{EPSFCN}^{1/2}$) componentwise relative.
2	Use the symmetric difference quotient with discretization stepsize 0.1 ($\text{EPSFCN}^{1/3}$) componentwise relative
3	Use the sixth order approximation computing a Richardson extrapolation of three symmetric difference quotient values. This uses a discretization stepsize 0.01($\text{EPSFCN}^{1/7}$)

TAUBND – Amount by which bounds may be violated during numerical differentiation. Bounds are violated by TAUBND (at most) only if a variable is on a bound and finite differences are taken for gradient evaluations. (Input)
Default: TAUBND = 1.E0

SMALLW — Scalar containing the error allowed in the multipliers. For example, a negative multiplier of an inequality constraint is accepted (as zero) if its absolute value is less than SMALLW. (Input)
Default: SMALLW = exp(2*log(epsilon(x(1)))/3) (= epsilon(x(1))$^{2/3}$)

DELMIN — Scalar which defines allowable constraint violations of the final accepted result. Constraints are satisfied if $|g_i(x)| \le$ DELMIN , and $g_j(x) >$ (−DELMIN) respectively. (Input)
Default: DELMIN = min(DEL0/10, max(EPSDIF, min(DEL0/10, max(1.E-6*DEL0, SMALLW))))

SCFMAX — Scalar containing the bound for the internal automatic scaling of the objective function. (Input)
Default: SCFMAX = 1.0E4

FVALUE — Scalar containing the value of the objective function at the computed solution. (Output)

LGMULT— Vector of length M containing the Lagrange multiplier estimates of the constraints. (Output)

CONSTRES — Vector of length M containing the constraint residuals. (Output)

FORTRAN 90 Interface

Generic: CALL NNLPF (FCN, M, ME, IBTYPE, XLB, XUB, X [, …])

Specific: The specific interface names are S_NNLPF and D_NNLPF .

Description

The routine `NNLPF` provides an interface to a licensed version of subroutine `DONLP2`, a FORTRAN code developed by Peter Spellucci (1998). It uses a sequential equality constrained quadratic programming method with an active set technique, and an alternative usage of a fully regularized mixed constrained subproblem in case of nonregular constraints (i.e. linear dependent gradients in the "working sets"). It uses a slightly modified version of the Pantoja-Mayne update for the Hessian of the Lagrangian, variable dual scaling and an improved Armjijo-type stepsize algorithm. Bounds on the variables are treated in a gradient-projection like fashion. Details may be found in the following two papers:

P. Spellucci: *An SQP method for general nonlinear programs using only equality constrained subproblems*. Math. Prog. 82, (1998), 413-448.

P. Spellucci: *A new technique for inconsistent problems in the SQP method*. Math. Meth. of Oper. Res. 47, (1998), 355-500. (published by Physica Verlag, Heidelberg, Germany).

The problem is stated as follows:

$$\min_{x \in R^n} f(x)$$

$$\begin{aligned} \text{subject to} \quad & g_j(x) = 0, \quad \text{for} \quad j = 1, \ldots, m_e \\ & g_j(x) \geq 0, \quad \text{for} \quad j = m_e + 1, \ldots, m \\ & x_l \leq x \leq x_u \end{aligned}$$

Although default values are provided for optional input arguments, it may be necessary to adjust these values for some problems. Through the use of optional arguments, `NNLPF` allows for several parameters of the algorithm to be adjusted to account for specific characteristics of problems. The DONLP2 Users Guide provides detailed descriptions of these parameters as well as strategies for maximizing the perfomance of the algorithm. The DONLP2 Users Guide is available in the "*help*" subdirectory of the main IMSL product installation directory. In addition, the following are a number of guidelines to consider when using `NNLPF`.

- A good initial starting point is very problem specific and should be provided by the calling program whenever possible. See optional argument `XGUESS`.
- Gradient approximation methods can have an effect on the success of `NNLPF`. Selecting a higher order approximation method may be necessary for some problems. See optional argument `IDTYPE`.
- If a two sided constraint $l_i \leq g_i(x) \leq u_i$ is transformed into two constraints $g_{2i}(x) \geq 0$ and $g_{2i+1}(x) \geq 0$, then choose $\text{DEL0} < \frac{1}{2}(u_i - l_i)/\max\{1, \|\nabla g_i(x)\|\}$, or at least try to provide an estimate for that value. This will increase the efficiency of the algorithm. See optional argument `DEL0`.

- The parameter IERR provided in the interface to the user supplied function FCN can be very useful in cases when evaluation is requested at a point that is not possible or reasonable. For example, if evaluation at the requested point would result in a floating point exception, then setting IERR to .TRUE. and returning without performing the evaluation will avoid the exception. NNLPF will then reduce the stepsize and try the step again. Note, if IERR is set to .TRUE. for the initial guess, then an error is issued.

Comments

1. Informational errors

Type	Code	Description
4	1	Constraint evaluation returns an error with current point.
4	2	Objective evaluation returns an error with current point.
4	3	Working set is singular in dual extended QP.
4	4	QP problem is seemingly infeasible.
4	5	A stationary point located or termination criteria too strong.
4	8	Maximum number of iterations exceeded.
4	9	Stationary point not feasible.
4	10	Very slow primal progress.
4	11	The problem is singular.
4	12	Matrix of gradients of binding constraints is singular or very ill-conditioned.
4	13	Small changes in the penalty function.

Example

The problem

$$\begin{aligned} \min \ F(x) &= (x_1 - 2)^2 + (x_2 - 1)^2 \\ \text{subject to} \quad g_1(x) &= x_1 - 2x_2 + 1 = 0 \\ g_2(x) &= -x_1^2/4 - x_2^2 + 1 \geq 0 \end{aligned}$$

is solved.

```
      USE NNLPF_INT
      USE WRRRN_INT

      IMPLICIT    NONE
      INTEGER     IBTYPE, M, ME
```

```
      PARAMETER  (IBTYPE=0, M=2, ME=1)
!
      REAL(KIND(1E0)) FVALUE, X(2), XGUESS(2), XLB(2), XUB(2)
      EXTERNAL FCN
!
      XLB = -HUGE(X(1))
      XUB = HUGE(X(1))
!
      CALL NNLPF (FCN, M, ME, IBTYPE, XLB, XUB, X)
!
      CALL WRRRN ('The solution is', X)
      END

      SUBROUTINE FCN (X, IACT, RESULT, IERR)
      INTEGER    IACT
      REAL(KIND(1E0)) X(*), RESULT
      LOGICAL IERR
!
      SELECT CASE (IACT)
      CASE(0)
         RESULT = (X(1)-2.0E0)**2 + (X(2)-1.0E0)**2
      CASE(1)
         RESULT = X(1) - 2.0E0*X(2) + 1.0E0
      CASE(2)
         RESULT = -(X(1)**2)/4.0E0 - X(2)**2 + 1.0E0
      END SELECT
      RETURN
      END
```

Output

```
The solution is
 1   0.8229
 2   0.9114
```

NNLPG

Solves a general nonlinear programming problem using a sequential equality constrained quadratic programming method with user supplied gradients.

Required Arguments

FCN — User-supplied subroutine to evaluate the objective function and constraints at a given point. The internal usage is CALL FCN (X, IACT, RESULT, IERR), where

X – The point at which the objective function or constraint is evaluated. (Input)

IACT – Integer indicating whether evaluation of the objective function is requested or evaluation of a constraint is requested. If IACT is zero, then an objective function evaluation is requested. If IACT is nonzero then the value if IACT indicates the index of the constraint to evaluate. IACT = 1 to ME for equality constraints and IACT = ME +1 to M for inequality constraints. (Input)

RESULT – If IACT is zero, then RESULT is the computed objective function value at the point X. If IACT is nonzero, then RESULT is the computed constraint value at the point X. (Output)

IERR – Logical variable. On input IERR is set to .FALSE. If an error or other undesirable condition occurs during evaluation, then IERR should be set to .TRUE. Setting IERR to .TRUE. will result in the step size being reduced and the step being tried again. (If IERR is set to .TRUE. for XGUESS, then an error is issued.)

The routine FCN must be use-associated in a user module that uses NNLPG_INT, or else declared EXTERNAL in the calling program. If FCN is a separately compiled routine, not in a module, then it must be declared EXTERNAL.

GRAD — User-supplied subroutine to evaluate the gradients at a given point. The usage is CALL GRAD (X, IACT, RESULT), where

X – The point at which the gradient of the objective function or gradient of a constraint is evaluated. (Input)

IACT – Integer indicating whether evaluation of the function gradient is requested or evaluation of a constraint gradient is requested. If IACT is zero, then an objective function gradient evaluation is requested. If IACT is nonzero then the value if IACT indicates the index of the constraint gradient to evaluate. (Input)
IACT = 1 to ME for equality constraints and IACT = ME +1 to M for inequality constraints.

RESULT – If IACT is zero, then RESULT is the computed gradient of the objective function at the point X. If IACT is nonzero, then RESULT is the computed gradient of the requested constraint value at the point X. (Output)

The routine GRAD must be use-associated in a user module that uses NNLPG_INT, or else declared EXTERNAL in the calling program. If GRAD is a separately compiled routine, not in a module, then is must be declared EXTERNAL

M — Total number of constraints. (Input)

ME — Number of equality constraints. (Input)

IBTYPE — Scalar indicating the types of bounds on variables. (Input)

IBTYPE	Action
0	User will supply all the bounds.
1	All variables are nonnegative.
2	All variables are nonpositive.
3	User supplies only the bounds on 1st variable, all other variables will have the same bounds.

XLB — Vector of length N containing the lower bounds on the variables. (Input, if IBTYPE = 0; output, if IBTYPE = 1 or 2; input/output, if IBTYPE = 3) If there is no lower bound on a variable, then the corresponding XLB value should be set to −huge(x(1)).

XUB — Vector of length N containing the upper bounds on the variables. (Input, if IBTYPE = 0; output, if IBTYPE = 1 or 2; input/output, if IBTYPE = 3) If there is no upper bound on a variable, then the corresponding XUB value should be set to huge(x(1)).

X — Vector of length N containing the computed solution. (Output)

Optional Arguments

N — Number of variables. (Input)
Default: N = SIZE(X).

XGUESS — Vector of length N containing an initial guess of the solution. If XGUESS is located outside or in the boundary region of the bound constraints set, then the algorithm first projects XGUESS into the interior of the bound constraints set before starting the main computations. (Input)
Default: XGUESS = x, where x is the vector with the smallest l_2 – norm that satisfies the bounds.

IPRINT — Parameter indicating the desired output level. (Input)

IPRINT	Action
0	No output printed.
1	One line of intermediate results is printed in each iteration.
2	Lines of intermediate results summarizing the most important data for each step are printed.
3	Lines of detailed intermediate results showing all primal and dual variables, the relevant values from the working set, progress in the backtracking and etc are printed
4	Lines of detailed intermediate results showing all primal and dual variables, the relevant values from the working set, progress in the backtracking, the gradients in the working set, the quasi-Newton updated and etc are printed.

Default: IPRINT = 0.

MAXITN — Maximum number of iterations allowed. (Input)
Default: MAXITN = 200.

DEL0 — In the initial phase of minimization a constraint is considered binding if

$$\frac{g_i(x)}{\max\left(1,\|\nabla g_i(x)\|\right)} \le \mathrm{DEL0} \qquad i = M_e + 1, \ldots, M$$

Good values are between .01 and 1.0. If DEL0 is chosen too small then identification of the correct set of binding constraints may be delayed. Contrary, if DEL0 is too large, then the method will often escape to the full regularized SQP method, using individual slack variables for any active constraint, which is quite costly. For well-scaled problems DEL0=1.0 is reasonable. (Input)
Default: DEL0 = .5*TAU0

TAU0 — A universal bound describing how much the unscaled penalty-term may deviate from zero. (Input)
NNLPG assumes that within the region described by

$$\sum_{i=1}^{M_e} |g_i(x)| - \sum_{i=M_e+1}^{M} \min\left(0, g_i(x)\right) \le \texttt{TAU0}$$

all functions may be evaluated safely. The initial guess however, may violate these requirements. In that case an initial feasibility improvement phase is run by NNLPG until such a point is found. A small TAU0 diminishes the efficiency of NNLPG, because the iterates then will follow the boundary of the feasible set closely. Conversely, a large TAU0 may degrade the reliability of the code.
Default: TAU0 = 1.E0

SMALLW — Scalar containing the error allowed in the multipliers. For example, a negative multiplier of an inequality constraint is accepted (as zero) if its absolute value is less than SMALLW. (Input)
Default: SMALLW = exp(2*log(epsilon(x(1)))/3) (= epsilon(x(1))$^{2/3}$)

DELMIN — Scalar which defines allowable constraint violations of the final accepted result. Constraints are satisfied if $|g_i(x)| \le$ DELMIN, and $g_j(x) \ge$ (−DELMIN) respectively. (Input)
Default: DELMIN **=** min(DEL0/10, max(1.E-6*DEL0, SMALLW))

SCFMAX — Scalar containing the bound for the internal automatic scaling of the objective function. (Input)
Default: SCFMAX = 1.0E4

FVALUE — Scalar containing the value of the objective function at the computed solution. (Output)

LGMULT — Vector of length M containing the Lagrange multiplier estimates of the constraints. (Output)

CONSTRES — Vector of length M containing the constraint residuals. (Output)

FORTRAN 90 Interface

Generic: CALL NNLPG (FCN, GRAD, M, ME, IBTYPE, XLB, XUB, X [, …])

Specific: The specific interface names are S_NNLPG and D_NNLPG.

Description

The routine NNLPG provides an interface to a licensed version of subroutine DONLP2, a FORTRAN code developed by Peter Spellucci (1998). It uses a sequential equality constrained quadratic programming method with an active set technique, and an alternative usage of a fully regularized mixed constrained subproblem in case of nonregular constraints (i.e. linear dependent gradients in the “working sets”). It uses a slightly modified version of the Pantoja-Mayne update for the Hessian of the Lagrangian, variable dual scaling and an improved Armjijo-type stepsize algorithm. Bounds on the variables are treated in a gradient-projection like fashion. Details may be found in the following two papers:

P. Spellucci: *An SQP method for general nonlinear programs using only equality constrained subproblems*. Math. Prog. 82, (1998), 413-448.

P. Spellucci: *A new technique for inconsistent problems in the SQP method*. Math. Meth. of Oper. Res. 47, (1998), 355-500. (published by Physica Verlag, Heidelberg, Germany).

The problem is stated as follows:

$$\min_{x \in R^n} f(x)$$

$$\begin{aligned} \text{subject to} \quad & g_j(x) = 0, \quad \text{for} \quad j = 1, \dots, m_e \\ & g_j(x) \geq 0, \quad \text{for} \quad j = m_e + 1, \dots, m \\ & x_l \leq x \leq x_u \end{aligned}$$

Although default values are provided for optional input arguments, it may be necessary to adjust these values for some problems. Through the use of optional arguments, NNLPG allows for several parameters of the algorithm to be adjusted to account for specific characteristics of problems. The DONLP2 Users Guide provides detailed descriptions of these parameters as well as strategies for maximizing the perfomance of the algorithm. The DONLP2 Users Guide is available in the "*help*" subdirectory of the main IMSL product installation directory. In addition, the following are a number of guidelines to consider when using NNLPG.

- A good initial starting point is very problem specific and should be provided by the calling program whenever possible. See optional argument XGUESS.
- If a two sided constraint $l_i \leq g_i(x) \leq u_i$ is transformed into two constraints $g_{2i}(x) \geq 0$ and $g_{2i+1}(x) \geq 0$, then choose $\text{DEL0} < \frac{1}{2}(u_i - l_i)/max\{1, \|\nabla g_i(x)\|\}$, or at least try to provide an estimate for that value. This will increase the efficiency of the algorithm. See optional argument DEL0.
- The parameter IERR provided in the interface to the user supplied function FCN can be very useful in cases when evaluation is requested at a point that is not possible or reasonable. For example, if evaluation at the requested point would result in a floating point exception, then setting IERR to .TRUE. and returning without performing the evaluation will avoid the exception. NNLPG will then reduce the stepsize and try the step again. Note, if IERR is set to .TRUE. for the initial guess, then an error is issued.

Comments

1. Informational errors

Type	Code	Description
4	1	Constraint evaluation returns an error with current point.
4	2	Objective evaluation returns an error with current point.
4	3	Working set is singular in dual extended QP.
4	4	QP problem is seemingly infeasible.
4	5	A stationary point located or termination criteria too strong.
4	8	Maximum number of iterations exceeded.
4	9	Stationary point not feasible.
4	10	Very slow primal progress.
4	11	The problem is singular.
4	12	Matrix of gradients of binding constraints is singular or very ill-conditioned.
4	13	Small changes in the penalty function.

Examples

Example 1

The problem

$$\min\ F(x) = (x_1 - 2)^2 + (x_2 - 1)^2$$
$$\text{subject to}\quad g_1(x) = x_1 - 2x_2 + 1 = 0$$
$$g_2(x) = -x_1^2/4 - x_2^2 + 1 \geq 0$$

is solved.

```
      USE NNLPG_INT
      USE WRRRN_INT

      IMPLICIT   NONE
      INTEGER    IBTYPE, M, ME
      PARAMETER  (IBTYPE=0, M=2, ME=1)
!
      REAL(KIND(1E0)) FVALUE, X(2), XGUESS(2), XLB(2), XUB(2)
      EXTERNAL FCN, GRAD
!
      XLB = -HUGE(X(1))
      XUB = HUGE(X(1))
!
      CALL NNLPG (FCN, GRAD, M, ME, IBTYPE, XLB, XUB, X)
!
```

```
      CALL WRRRN ('The solution is', X)
      END

      SUBROUTINE FCN (X, IACT, RESULT, IERR)
      INTEGER    IACT
      REAL(KIND(1E0)) X(*), RESULT
      LOGICAL IERR
!
      SELECT CASE (IACT)
      CASE(0)
         RESULT = (X(1)-2.0E0)**2 + (X(2)-1.0E0)**2
      CASE(1)
         RESULT = X(1) - 2.0E0*X(2) + 1.0E0
      CASE(2)
         RESULT = -(X(1)**2)/4.0E0 - X(2)**2 + 1.0E0
      END SELECT
      RETURN
      END

      SUBROUTINE GRAD (X, IACT, RESULT)
      INTEGER    IACT
      REAL(KIND(1E0)) X(*),RESULT(*)
!
      SELECT CASE (IACT)
      CASE(0)
         RESULT (1) = 2.0E0*(X(1)-2.0E0)
         RESULT (2) = 2.0E0*(X(2)-1.0E0)
      CASE(1)
         RESULT (1) = 1.0E0
         RESULT (2) = -2.0E0
      CASE(2)
         RESULT (1) = -0.5E0*X(1)
         RESULT (2) = -2.0E0*X(2)
      END SELECT
      RETURN
      END
```

Output

```
The solution is
1   0.8229
2   0.9114
```

Example 2

The same problem from Example 1 is solved, but here we use central differences to compute the gradient of the first constraint. This example demonstrates how `NNLPG` can be used in cases when analytic gradients are known for only a portion of the constraints and/or objective function. The subroutine `CDGRD` is used to compute an approximation to the gradient of the first constraint.

```
      USE NNLPG_INT
      USE CDGRD_INT
      USE WRRRN_INT

      IMPLICIT   NONE
      INTEGER    IBTYPE, M, ME
      PARAMETER  (IBTYPE=0, M=2, ME=1)
!
      REAL(KIND(1E0)) FVALUE, X(2), XGUESS(2), XLB(2), XUB(2)
      EXTERNAL FCN, GRAD
!
```

```
       XLB = -HUGE(X(1))
       XUB = HUGE(X(1))
!
       CALL NNLPG (FCN, GRAD, M, ME, IBTYPE, XLB, XUB, X)
!
       CALL WRRRN ('The solution is', X)
       END

       SUBROUTINE FCN (X, IACT, RESULT, IERR)
       INTEGER    IACT
       REAL(KIND(1E0)) X(2), RESULT
       LOGICAL IERR
       EXTERNAL CONSTR1
!
       SELECT CASE (IACT)
       CASE(0)
          RESULT = (X(1)-2.0E0)**2 + (X(2)-1.0E0)**2
       CASE(1)
          CALL CONSTR1(2, X, RESULT)
       CASE(2)
          RESULT = -(X(1)**2)/4.0E0 - X(2)**2 + 1.0E0
       END SELECT
       RETURN
       END

       SUBROUTINE GRAD (X, IACT, RESULT)
       USE CDGRD_INT
       INTEGER    IACT
       REAL(KIND(1E0)) X(2),RESULT(2)
       EXTERNAL CONSTR1
!
       SELECT CASE (IACT)
       CASE(0)
          RESULT (1) = 2.0E0*(X(1)-2.0E0)
          RESULT (2) = 2.0E0*(X(2)-1.0E0)
       CASE(1)
          CALL CDGRD(CONSTR1, X, RESULT)
       CASE(2)
          RESULT (1) = -0.5E0*X(1)
          RESULT (2) = -2.0E0*X(2)
       END SELECT
       RETURN
       END

       SUBROUTINE CONSTR1 (N, X, RESULT)
       INTEGER N
       REAL(KIND(1E0)) X(*), RESULT
       RESULT = X(1) - 2.0E0*X(2) + 1.0E0
       RETURN
       END
```

Output

```
 The solution is
 1   0.8229
 2   0.9114
```

CDGRD

Approximates the gradient using central differences.

Required Arguments

FCN — User-supplied subroutine to evaluate the function to be minimized. The usage is
CALL FCN (N, X, F), where

N – Length of X. (Input)

X – The point at which the function is evaluated. (Input)
X should not be changed by FCN.

F – The computed function value at the point X. (Output)

FCN must be declared EXTERNAL in the calling program.

XC — Vector of length N containing the point at which the gradient is to be estimated. (Input)

GC — Vector of length N containing the estimated gradient at XC. (Output)

Optional Arguments

N — Dimension of the problem. (Input)
Default: N = SIZE (XC,1).

XSCALE — Vector of length N containing the diagonal scaling matrix for the variables. (Input)
In the absence of other information, set all entries to 1.0.
Default: XSCALE = 1.0.

EPSFCN — Estimate for the relative noise in the function. (Input)
EPSFCN must be less than or equal to 0.1. In the absence of other information, set EPSFCN to 0.0.
Default: EPSFCN = 0.0.

FORTRAN 90 Interface

Generic: CALL CDGRD (FCN, XC, GC [, …])

Specific: The specific interface names are S_CDGRD and D_CDGRD.

FORTRAN 77 Interface

Single: CALL CDGRD (FCN, N, XC, XSCALE, EPSFCN, GC)

Double: The double precision name is DCDGRD.

Description

The routine CDGRD uses the following finite-difference formula to estimate the gradient of a function of n variables at x:

$$\frac{f\left(x+h_i e_i\right)-f\left(x-h_i e_i\right)}{2h_i} \quad \text{for } i=1,\ \ldots,\ n$$

where

$$h_i=\varepsilon^{1/3}\max\left\{|x_i|,1/s_j\right\}sign\left(x_i\right),$$

ε is the machine epsilon, s_i is the scaling factor of the i-th variable, and e_i is the i-th unit vector. For more details, see Dennis and Schnabel (1983).

Since the finite-difference method has truncation error, cancellation error, and rounding error, users should be aware of possible poor performance. When possible, high precision arithmetic is recommended.

Comments

This is Description A5.6.4, Dennis and Schnabel, 1983, page 323.

Example

In this example, the gradient of $f(x) = x_1 - x_1x_2 - 2$ is estimated by the finite-difference method at the point (1.0, 1.0).

```
      USE CDGRD_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    I, N, NOUT
      PARAMETER  (N=2)
      REAL       EPSFCN, GC(N), XC(N)
      EXTERNAL   FCN
!                                 Initialization.
      DATA XC/2*1.0E0/
!                                 Set function noise.
      EPSFCN = 0.01
!
      CALL CDGRD (FCN, XC, GC, EPSFCN=EPSFCN)
!
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) (GC(I),I=1,N)
99999 FORMAT ('  The gradient is', 2F8.2, /)
```

```
!
      END
!
      SUBROUTINE FCN (N, X, F)
      INTEGER    N
      REAL       X(N), F
!
      F = X(1) - X(1)*X(2) - 2.0E0
!
      RETURN
      END
```

Output

```
The gradient is    0.00   -1.00
```

FDGRD

Approximates the gradient using forward differences.

Required Arguments

FCN — User-supplied subroutine to evaluate the function to be minimized. The usage is
`CALL FCN (N, X, F)`, where

`N` – Length of X. (Input)

`X` – The point at which the function is evaluated. (Input)
X should not be changed by `FCN`.

`F` – The computed function value at the point X. (Output)

`FCN` must be declared `EXTERNAL` in the calling program.

XC — Vector of length `N` containing the point at which the gradient is to be estimated. (Input)

FC — Scalar containing the value of the function at `XC`. (Input)

GC — Vector of length `N` containing the estimated gradient at `XC`. (Output)

Optional Arguments

N — Dimension of the problem. (Input)
Default: `N` = `SIZE` (XC,1).

XSCALE — Vector of length `N` containing the diagonal scaling matrix for the variables. (Input)
In the absence of other information, set all entries to 1.0.
Default: `XSCALE` = 1.0.

EPSFCN — Estimate of the relative noise in the function. (Input)
`EPSFCN` must be less than or equal to 0.1. In the absence of other information, set `EPSFCN` to 0.0.
Default: `EPSFCN` = 0.0.

FORTRAN 90 Interface

Generic: `CALL FDGRD (FCN, XC, FC, GC [, …])`

Specific: The specific interface names are `S_FDGRD` and `D_FDGRD`.

FORTRAN 77 Interface

Single: CALL FDGRD (FCN, N, XC, XSCALE, FC, EPSFCN GC)

Double: The double precision name is DFDGRD.

Description

The routine FDGRD uses the following finite-difference formula to estimate the gradient of a function of *n* variables at *x*:

$$\frac{f\left(x+h_i e_i\right)-f\left(x\right)}{h_i} \quad \text{for } i=1,\ \ldots,n$$

where $h_i = \varepsilon^{1/2} \max\{|x_i|, 1/s_i\} \operatorname{sign}(x_i)$, ε is the machine epsilon, e_i is the *i*-th unit vector, and s_i is the scaling factor of the *i*-th variable. For more details, see Dennis and Schnabel (1983).

Since the finite-difference method has truncation error, cancellation error, and rounding error, users should be aware of possible poor performance. When possible, high precision arithmetic is recommended. When accuracy of the gradient is important, IMSL routine CDGRD should be used.

Comments

This is Description A5.6.3, Dennis and Schnabel, 1983, page 322.

Example

In this example, the gradient of $f(x) = x_1 - x_1 x_2 - 2$ is estimated by the finite-difference method at the point (1.0, 1.0).

```
      USE FDGRD_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    I, N, NOUT
      PARAMETER  (N=2)
      REAL       EPSFCN, FC, GC(N), XC(N)
      EXTERNAL   FCN
!                                  Initialization.
      DATA XC/2*1.0E0/
!                                  Set function noise.
      EPSFCN = 0.01
!                                  Get function value at current
!                                  point.
      CALL FCN (N, XC, FC)
!
      CALL FDGRD (FCN, XC, FC, GC, EPSFCN=EPSFCN)
!
```

```
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) (GC(I),I=1,N)
99999 FORMAT ('  The gradient is', 2F8.2, /)
!
      END
!
      SUBROUTINE FCN (N, X, F)
      INTEGER    N
      REAL       X(N), F
!
      F = X(1) - X(1)*X(2) - 2.0E0
!
      RETURN
      END
```

Output

```
The gradient is    0.00   -1.00
```

FDHES

Approximates the Hessian using forward differences and function values.

Required Arguments

FCN — User-supplied subroutine to evaluate the function to be minimized. The usage is `CALL FCN (N, X, F)`, where

`N` – Length of `X`. (Input)

`X` – The point at which the function is evaluated. (Input)
`X` should not be changed by `FCN`.

`F` – The computed function value at the point `X`. (Output)

`FCN` must be declared `EXTERNAL` in the calling program.

XC — Vector of length `N` containing the point at which the Hessian is to be approximated. (Input)

FC — Function value at `XC`. (Input)

H — `N` by `N` matrix containing the finite difference approximation to the Hessian in the lower triangle. (Output)

Optional Arguments

N — Dimension of the problem. (Input)
Default: `N` = `SIZE` (`XC`,1).

XSCALE — Vector of length `N` containing the diagonal scaling matrix for the variables. (Input)
In the absence of other information, set all entries to 1.0.
Default: `XSCALE` = 1.0.

EPSFCN — Estimate of the relative noise in the function. (Input)
`EPSFCN` must be less than or equal to 0.1. In the absence of other information, set `EPSFCN` to 0.0.
Default: `EPSFCN` = 0.0.

LDH — Row dimension of `H` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDH` = `SIZE` (`H`,1).

FORTRAN 90 Interface

Generic: CALL FDHES (FCN, XC, FC, H [, …])

Specific: The specific interface names are S_FDHES and D_FDHES.

FORTRAN 77 Interface

Single: CALL FDHES (FCN, N, XC, XSCALE, FC, EPSFCN, H, LDH)

Double: The double precision name is DFDHES.

Description

The routine FDHES uses the following finite-difference formula to estimate the Hessian matrix of function *f* at *x*:

$$\frac{f\left(x+h_ie_i+h_je_j\right)-f\left(x+h_ie_i\right)-f\left(x+h_je_j\right)+f\left(x\right)}{h_ih_j}$$

Where

$$h_i=\varepsilon^{1/3}\max\left\{|x_i|,1/s_i\right\}sign\left(x_i\right),\ h_j=\varepsilon^{1/3}\max\left\{|x_j|,1/s_j\right\}sign\left(x_j\right),$$

ε is the machine epsilon or user-supplied estimate of the relative noise, s_i and s_j are the scaling factors of the *i*-th and *j*-th variables, and e_i and e_j are the *i*-th and *j*-th unit vectors, respectively. For more details, see Dennis and Schnabel (1983).

Since the finite-difference method has truncation error, cancellation error, and rounding error, users should be aware of possible poor performance. When possible, high precision arithmetic is recommended.

Comments

1. Workspace may be explicitly provided, if desired, by use of F2HES/DF2HES. The reference is:

   ```
   CALL F2HES (FCN, N, XC, XSCALE, FC, EPSFCN, H, LDH, WK1, WK2)
   ```

   The additional arguments are as follows:

   WK1 — Real work vector of length N.

   WK2 — Real work vector of length N.

2. This is Description A5.6.2 from Dennis and Schnabel, 1983; page 321.

Example

The Hessian is estimated for the following function at (1,−1)

$$f(x) = x_1^2 - x_1 x_2 - 2$$

```
      USE FDHES_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                  Declaration of variables
      INTEGER    N, LDHES, NOUT
      PARAMETER  (N=2, LDHES=2)
      REAL       XC(N), FVALUE, HES(LDHES,N), EPSFCN
      EXTERNAL   FCN
!                                    Initialization
      DATA XC/1.0E0,-1.0E0/
!                                    Set function noise
      EPSFCN = 0.001
!                                    Evaluate the function at
!                                    current point
      CALL FCN (N, XC, FVALUE)
!                                  Get Hessian forward difference
!                                  approximation
      CALL FDHES (FCN, XC, FVALUE, HES, EPSFCN=EPSFCN)
!
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) ((HES(I,J),J=1,I),I=1,N)
99999 FORMAT ('  The lower triangle of the Hessian is', /,&
               5X,F10.2,/,5X,2F10.2,/)
!
      END
!
      SUBROUTINE FCN (N, X, F)
!                                   SPECIFICATIONS FOR ARGUMENTS
      INTEGER N
      REAL    X(N), F
!
      F = X(1)*(X(1) - X(2)) - 2.0E0
!
      RETURN
      END
```

Output

```
 The lower triangle of the Hessian is
  2.00
 -1.00       0.00
```

GDHES

Approximates the Hessian using forward differences and a user-supplied gradient.

Required Arguments

GRAD — User-supplied subroutine to compute the gradient at the point `X`. The usage is `CALL GRAD (N, X, G)`, where

`N` – Length of `X` and `G`. (Input)

`X` – The point at which the gradient is evaluated. (Input)
`X` should not be changed by `GRAD`.

`G` – The gradient evaluated at the point `X`. (Output)

`GRAD` must be declared `EXTERNAL` in the calling program.

XC — Vector of length `N` containing the point at which the Hessian is to be estimated. (Input)

GC — Vector of length `N` containing the gradient of the function at `XC`. (Input)

H — `N` by `N` matrix containing the finite-difference approximation to the Hessian in the lower triangular part and diagonal. (Output)

Optional Arguments

N — Dimension of the problem. (Input)
Default: `N` = `SIZE` (`XC`,1).

XSCALE — Vector of length `N` containing the diagonal scaling matrix for the variables. (Input)
In the absence of other information, set all entries to 1.0.
Default: `XSCALE` = 1.0.

EPSFCN — Estimate of the relative noise in the function. (Input)
`EPSFCN` must be less than or equal to 0.1. In the absence of other information, set `EPSFCN` to 0.0.
Default: `EPSFCN` = 0.0.

LDH — Leading dimension of `H` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDH` = `SIZE` (`H`,1).

FORTRAN 90 Interface

Generic: `CALL GDHES (GRAD, XC, GC, H [, …])`

Specific: The specific interface names are `S_GDHES` and `D_GDHES`.

FORTRAN 77 Interface

Single: `CALL GDHES (GRAD, N, XC, XSCALE, GC, EPSFCN, H, LDH)`

Double: The double precision name is `DGDHES`.

Description

The routine `GDHES` uses the following finite-difference formula to estimate the Hessian matrix of function *F* at *x*:

$$\frac{g\left(x+h_j e_j\right)-g\left(x\right)}{h_j}$$

where

$$h_j=\varepsilon^{1/3}\max\left\{|x_j|,1/s_j\right\}sign\left(x_j\right),$$

ε is the machine epsilon, s_j is the scaling factor of the *j*-th variable, *g* is the analytic gradient of *F* at *x*, and e_j is the *j*-th unit vector. For more details, see Dennis and Schnabel (1983).

Since the finite-difference method has truncation error, cancellation error, and rounding error, users should be aware of possible poor performance. When possible, high precision arithmetic is recommended.

Comments

1. Workspace may be explicitly provided, if desired, by use of `G2HES`/`DG2HES`. The reference is:

   ```
   CALL G2HES (GRAD, N, XC, XSCALE, GC, EPSFCN, H, LDH, WK)
   ```

   The additional argument is

   WK — Work vector of length `N`.

2. This is Description A5.6.1, Dennis and Schnabel, 1983; page 320.

Example

The Hessian is estimated by the finite-difference method at point (1.0, 1.0) from the following gradient functions:

$$g_1 = 2x_1x_2 - 2$$
$$g_2 = x_1x_1 + 1$$

```
      USE GDHES_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                 Declaration of variables
      INTEGER    N, LDHES, NOUT
      PARAMETER  (N=2, LDHES=2)
      REAL       XC(N), GC(N), HES(LDHES,N)
      EXTERNAL   GRAD
!
      DATA XC/2*1.0E0/
!                                 Set function noise
!                                 Evaluate the gradient at the
!                                 current point
      CALL GRAD (N, XC, GC)
!                                 Get Hessian forward-difference
!                                 approximation
      CALL GDHES (GRAD, XC, GC, HES)
!
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) ((HES(I,J),J=1,N),I=1,N)
99999 FORMAT ('  THE HESSIAN IS', /, 2(5X,2F10.2,/),/)
!
      END
!
      SUBROUTINE GRAD (N, X, G)
!                                  SPECIFICATIONS FOR ARGUMENTS
      INTEGER N
      REAL    X(N), G(N)
!
      G(1) = 2.0E0*X(1)*X(2) - 2.0E0
      G(2) = X(1)*X(1) + 1.0E0
!
      RETURN
      END
```

Output

```
THE HESSIAN IS
2.00      2.00
2.00      0.00
```

DDJAC

Approximates the Jacobian of *m* functions in *n* unknowns using divided differences.

Required Arguments

FCN — User-supplied `subroutine` to evaluate functions. The usage is
`CALL FCN (INDX, Y, F [,…])` where

Required Arguments

`INDX` — Index of the variable whose derivative is to be computed. (Input)
`DDJAC` will set this argument to the index of the variable whose derivative is being computed. In those cases where there is a mix of finite differencing taking place along with additional analytic terms being computed, (see `METHOD = 2`), `DDJAC` will make two calls to `FCN` each time a new function evaluation is needed, once with `INDX` positive and a second time with `INDX` negative.

`Y` — Array containing the point at which the function is to be computed. (Input)

`F` — Array of length `M`, where `M` is the number of functions to be evaluated at point `Y`, containing the function values of the equations at point `Y`. (Output)

Normally, the user will return the values of the functions evaluated at point `Y` in `F`. However, when the function can be broken into two parts, a part which is known analytically and a part to be differenced, `FCN` will be called by `DDJAC` once with `INDX` positive for the portion to be differenced and again with `INDX` negative for the portion which is known analytically. In the case where `METHOD=2` has been chosen, `FCN` must be writtten to handle the known analytic portion separate from the part to be differenced. (See *Example 4* for an example where `METHOD=2` is used.)

Optional Arguments

`FCN_DATA` — A derived type, `s_fcn_data`, which may be used to pass additional integer or floating point information to or from the user-supplied subroutine. For a detailed description of this argument see `FCN_DATA` below. (Input/Output)

`FCN` must be declared `EXTERNAL` in the calling program.

Y — Array of length `N` containing the point at which the Jacobian is to be evaluated. (Input)

F — Array of length `M` containing the function values of the equations at point `Y`. (Output)

FJAC — Two dimensional array of which the first `M` by `N` subarray contains the estimated Jacobian. (Input/Output)
On input the user may set entries of columns that are to be accumulated to initial values (See the optional argument `METHOD`). On final output, `FJAC` will contain the estimated Jacobian.

Optional Arguments

M — The number of equations. (Input)
Default: `M = SIZE (F)`.

N — The number of variables. (Input)
Default: `N = SIZE (Y)`.

YSCALE — Array of length `N` containing the diagonal scaling matrix for the variables. (Input)
`YSCALE` can also be used to provide appropriate signs for the increments.
Default: `YSCALE` = 1.0.

METHOD — Array of length `N` containing the methods used to compute the derivatives. (Input)
`METHOD`(*i*) is the method to be used for the *i*-th variable. `METHOD`(*i*) can be one of the values in the following table:

Value	Description
0	Indicates one-sided differences.
1	Indicates central differences.
2	Indicates the accumulation of the result from whatever type of differences have been specified previously into initial values of the Jacobian
3	Indicates a variable is to be skipped

Default: One-sided differences are used for all variables.

FACTOR — Array of length `N` containing the percentage factor for differencing. (Input)
For each divided difference for variable *j* the increment used is *del*. The value of *del* is computed as follows: First define $\sigma = sign(\mathtt{YSCALE}(j))$. If the user has set the elements of array `YSCALE` to non-default values, then define $y_a = |\mathtt{YSCALE}(j)|$. Otherwise, $y_a = |Y(j)|$ and $\sigma = 1$. Finally, compute $del = \sigma y_a\ \mathtt{FACTOR}(j)$. By changing the sign of `YSCALE`(*j*), the difference *del* can have any desired orientation, such as staying within bounds on variable *j*. For central differences, a reduced factor is used for *del* that normally results in relative errors as small as machine precision to the 2/3 power. The elements of `FACTOR` must be such that machine precision to the 3/4 power <= `FACTOR`(*j*) <= 0.1
Default: All elements of `FACTOR` are set to `sqrt (machine precision)`.

ISTATUS — Array of length 10 which contains status information that might prove useful to the user wanting to gain better control over the differencing parameters. (Output)
This information can often be ignored. The following table describes the diagnostic information which is returned in each of the entries of `ISTATUS`:

index	Description
1	The number of times a function evaluation was computed.
2	The number of columns in which three attempts were made to increase a percentage factor for differencing (i.e. a component in the FACTOR array) but the computed *del* remained unacceptably small relative to Y[*j*] or YSCALE[*j*]. In such cases the percentage factor is set to the square root of machine precision.
3	The number of columns in which the computed *del* was zero to machine precision because Y[*j*] or YSCALE[*j*] was zero. In such cases *del* is set to the square root of machine precision.
4	The number of Jacobian columns which had to be recomputed because the largest difference formed in the column was close to zero relative to scale, where $$scale = \max(\lvert f_i(y)\rvert, \lvert f_i(y + del \times e_j)\rvert)$$ and *i* denotes the row index of the largest difference in the column currently being processed. *index* = 10 gives the last column where this occurred.
5	The number of columns whose largest difference is close to zero relative to scale after the column has been recomputed.
6	The number of times scale information was not available for use in the roundoff and truncation error tests. This occurs when $$\min(\lvert f_i(y)\rvert, \lvert f_i(y + del \times e_j)\rvert) = 0$$ Where *i* is the index of the largest difference for the column currently being processed.
7	The number of times the increment for differencing (*del*) was computed and had to be increased because (YSCALE[*j*] + *del*) − YSCALE[*j*]) was too small relative to Y[*j*] or YSCALE[*j*].
8	The number of times a component of the FACTOR array was reduced because changes in function values were large and excess truncation error was suspected. *index* = 9 gives the last column in which this occurred.
9	The index of the last column where the corresponding component of the FACTOR array had to be reduced because excessive truncation error was suspected.
10	The index of the last column where the difference was small and the column had to be recomputed with an adjusted increment (see *index* = 4). The largest derivative in this column may be inaccurate due to excessive roundoff error.

FCN_DATA — A derived type, `s_fcn_data`, which may be used to pass additional information to/from the user-supplied subroutine. (Input/Output)

The derived type, `s_fcn_data`, is defined as:

```
type s_fcn_data
    real(kind(1e0)), pointer, dimension(:) :: rdata
    integer, pointer, dimension(:) :: idata
 end type
```

in module `mp_types`. The double precision counterpart to `s_fcn_data` is named `d_fcn_data`. The user must include a `use mp_types` statement in the calling program to define this derived type.

FORTRAN 90 Interface

Generic: `CALL DDJAC (FCN,Y, F, FJAC [, …])`

Specific: The specific interface names are `S_DDJAC` and `D_DDJAC`.

Description

Computes the Jacobian matrix for a function $f(y)$ with m components in n independent variables. `DDJAC` uses divided finite differences to compute the Jacobian. This subroutine is designed for use in numerical methods for solving nonlinear problems where a Jacobian is evaluated repeatedly at neighboring arguments. For example this occurs in a Gauss-Newton method for solving non-linear least squares problems or a non-linear optimization method.

`DDJAC` is suited for applications where the Jacobian is a dense matrix. All cases $m < n$, $m = n$, or $m > n$ are allowed. Both one-sided and central divided differences can be used.

The design allows for computation of derivatives in a variety of contexts. Note that a gradient should be considered as the special case with $m = 1$, $n \geq 1$. A derivative of a single function of one variable is the case $m = 1$, $n = 1$. Any non-linear solving routine that optionally requests a Jacobian or gradient can use `DDJAC`. This should be considered if there are special properties or scaling issues associated with $f(y)$. Use the argument `METHOD` to specify different differencing options for numerical differentiation. These can be combined with some analytic subexpressions or other known relationships.

The divided differences are computed using values of the independent variables at the initial point $y_j = y$, and differenced points $y_e = y + del \times e_j$. Here the e_j, $j = 1,…,n$, are the unit coordinate vectors.

The value for each difference *del* depends on the variable *j*, the differencing method, and the scaling for that variable. This difference is computed internally. See FACTOR for computational details. The evaluation of $f(y_e)$ is normally done by the user-provided argument FCN, using the values y_e. The index *j*, values y_e, and output F are arguments to FCN.

The computational kernel of DDJAC performs the following steps:

1. Evaluates the equations at the point Y using FCN.
2. Computes the Jacobian.
3. Computes the difference at y_e.

There are four examples provided which illustrate various ways to use DDJAC. A discussion of the expected errors for the difference methods is found in *A First Course in Numerical Analysis*, Anthony Ralston, McGraw-Hill, NY, (1965).

Examples

Example 1

In this example, the Jacobian matrix of

$$f_1(x) = x_1x_2 - 2$$
$$f_2(x) = x_1 - x_1x_2 + 1$$

is estimated by the finite-difference method at the point (1.0, 1.0).

```
      USE DDJAC_INT
      USE WRRRN_INT
      IMPLICIT  NONE

      INTEGER, PARAMETER :: N=2, M=2
      REAL      FJAC(M,N), Y(N), F(M)
      EXTERNAL  FCN

      DATA Y/2*1.0/
!                                  Get Jacobian one-sided difference
!                                  approximation
      CALL DDJAC (FCN, Y, F, FJAC)
      CALL WRRRN ("The Jacobian is:", FJAC)
      END


      SUBROUTINE FCN (INDX, Y, F)
      INTEGER INDX
      REAL    Y(*), F(*)

      F(1) = Y(1)*Y(2) - 2.0
      F(2) = Y(1) - Y(1)*Y(2) + 1.0

      RETURN
```

```
      END
```

Output

```
The Jacobian is:
          1        2
 1    1.000    1.000
 2    0.000   -1.000
```

Example 2

A simple use of DDJAC is shown. The gradient of the function $f\left(y_1, y_2\right) = a\exp\left(by_1\right) + cy_1y_2^2$.

is required for values $a = 2.5e6, b = 3.4, c = 4.5, y_1 = 2.1, y_2 = 3.2$.

The analytic gradient of this function is:

$$grad\left(f\right) = [a\exp\left(by_1\right) + cy_2^2, 2cy_1cy_2]$$

```
      USE DDJAC_INT
      USE UMACH_INT
      IMPLICIT  NONE

      INTEGER, PARAMETER :: N=2, M=1
      INTEGER    J, NOUT
      REAL       FJAC(M,N), Y(N), F(M), SCALE(N)
      EXTERNAL   FCN

      DATA Y/2.1, 3.2/ SCALE/1.0, 8000.0/
!                                 Get Gradient one-sided difference
!                                 approximation
      CALL DDJAC (FCN, Y, F, FJAC, YSCALE=SCALE)
!                                 Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) (FJAC(1,J),J=1,N)
99999 FORMAT ('  The Numerical Gradient is (', 2e15.4,' )')
      END


      SUBROUTINE FCN (INDX, Y, F)
      INTEGER INDX
      REAL    A, B, C, Y(*), F(*)

      A = 2500000.
      B = 3.4
      C = 4.5

      F(1) =  A * EXP (B * Y(1)) + C * Y(1) * Y(2) * Y(2)

      RETURN
      END
```

Output

```
  The Numerical Gradient is (     0.1073E+11     0.9268E+02 )
```

Example 3

This example uses the same data as in *Example 2*. Here we assume that the second component of the gradient is analytically known. Therefore only the first gradient component needs numerical approximation. The input values of array METHOD specify that numerical differentiation with respect to y_2 is skipped.

```
      USE DDJAC_INT
      USE UMACH_INT
      IMPLICIT  NONE

      INTEGER, PARAMETER :: N=2, M=1
      INTEGER    J, NOUT, METHOD(2)
      REAL       FJAC(M,N), Y(N), F(M), SCALE(N)
      EXTERNAL   FCN

      DATA Y/2.1, 3.2/ SCALE/1.0, 8000.0/
!                                   Initialize second component
!                                   of Jacobian since it is
!                                   known analytically and can be
!                                   skipped
      FJAC(1,2) = 2.0 * 4.5 * Y(1) * Y(2)
!                                  Set METHOD to skip the second
!                                  component
      METHOD(1) = 0
      METHOD(2) = 3
!                                  Get Gradient approximation

      CALL DDJAC (FCN, Y, F, FJAC, YSCALE=SCALE, METHOD=METHOD)
!                                  Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) (FJAC(1,J),J=1,N)
99999 FORMAT ('  The Numerical Gradient is (', 2e15.4,' )')
      END


      SUBROUTINE FCN (INDX, Y, F)
      INTEGER INDX
      REAL    A, B, C, Y(*), F(*)

      A = 2500000.
      B = 3.4
      C = 4.5

      F(1) =  A * EXP (B * Y(1)) + C * Y(1) * Y(2) * Y(2)

      RETURN
      END
```

Output

```
  The Numerical Gradient is (     0.1073E+11     0.6048E+02 )
```

Example 4

This example uses the same data as in *Example 2*. An alternate examination of the function

$$f\left(y_1, y_2\right) = a\exp\left(by_1\right) + cy_1y_2^2$$

shows that the first term on the right-hand side need be evaluated just when computing the first partial. The additive term cy_2^2 occurs when computing the partial with respect to y_1. Also the first term does not depend on the second variable. Thus the first term can be left out of the function evaluation when computing the partial with respect to y_2, potentially avoiding cancellation errors. The input values of array `METHOD` allow `DDJAC` to use these facts and obtain greater accuracy using a minimum number of computations of the exponential function

```
      USE DDJAC_INT
      USE UMACH_INT
      USE MP_TYPES
      IMPLICIT  NONE

      INTEGER, PARAMETER :: N=2, M=1
      INTEGER   J, NOUT, METHOD(2)
      REAL      FJAC(M,N), Y(N), F(M), SCALE(N)
      REAL, TARGET :: RDATA(3)
      TYPE(S_FCN_DATA) USER_DATA
      EXTERNAL  FCN

      DATA Y/2.1, 3.2/ SCALE/1.0, 8000.0/

!                                   Set up to pass some extra
!                                   information to the function
      RDATA(1) = 2500000.0
      RDATA(2) = 3.4
      RDATA(3) = 4.5
      USER_DATA%RDATA => RDATA
!                                   Initialize first component
!                                   of function since it is
!                                   known
      FJAC(1,1) = 4.5 * Y(2) * Y(2)
!                                  Set METHOD to accumulate for
!                                  part of the first partial,
!                                  one-sided differences for
!                                  the second
      METHOD(1) = 2
      METHOD(2) = 0
!                                  Get Gradient approximation

      CALL DDJAC (FCN, Y, F, FJAC, YSCALE=SCALE, METHOD=METHOD, &
                  FCN_DATA=USER_DATA)
!                                  Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) (FJAC(1,J),J=1,N)
99999 FORMAT ('  The Numerical Gradient is (', 2e15.4,' )')
      END


      SUBROUTINE FCN (INDX, Y, F, FCN_DATA)
      USE MP_TYPES
      IMPLICIT  NONE

      INTEGER INDX
      REAL    A, B, C, Y(*), F(*)
      TYPE(S_FCN_DATA) FCN_DATA

      A = FCN_DATA%RDATA(1)
      B = FCN_DATA%RDATA(2)
      C = FCN_DATA%RDATA(3)
```

```
!                                  Handle both the differenced
!                                  part and the part that is
!                                  known analytically for each
!                                  dependent variable
      SELECT CASE(INDX)
         CASE (1)
            F(1)=A*EXP(B*Y(1))

         CASE(-1)
            F(1)= C*Y(2)**2

         CASE(2)
            F(1)   = C*Y(1)*Y(2)**2

         CASE(-2)
            F(1)=0
       END SELECT

      RETURN
      END
```

Output

```
  The Numerical Gradient is (      0.1073E+11      0.6046E+02 )
```

FDJAC

Approximates the Jacobian of M functions in N unknowns using forward differences.

Required Arguments

FCN — User-supplied subroutine to evaluate the function to be minimized. The usage is CALL FCN (M, N, X, F), where

M – Length of F. (Input)

N – Length of X. (Input)

X – The point at which the function is evaluated. (Input)
X should not be changed by FCN.

F – The computed function at the point X. (Output)

FCN must be declared EXTERNAL in the calling program.

XC — Vector of length N containing the point at which the gradient is to be estimated. (Input)

FC — Vector of length M containing the function values at XC. (Input)

FJAC — M by N matrix containing the estimated Jacobian at XC. (Output)

Optional Arguments

M — The number of functions. (Input)
Default: M = SIZE (FC,1).

N — The number of variables. (Input)
Default: N = SIZE (XC,1).

XSCALE — Vector of length N containing the diagonal scaling matrix for the variables. (Input)
In the absence of other information, set all entries to 1.0.
Default: XSCALE = 1.0.

EPSFCN — Estimate for the relative noise in the function. (Input)
EPSFCN must be less than or equal to 0.1. In the absence of other information, set EPSFCN to 0.0.
Default: EPSFCN = 0.0.

LDFJAC — Leading dimension of FJAC exactly as specified in the dimension statement of the calling program. (Input)
Default: LDFJAC = SIZE (FJAC,1).

FORTRAN 90 Interface

Generic: `CALL FDJAC (FCN, XC, FC, FJAC [, …])`

Specific: The specific interface names are `S_FDJAC` and `D_FDJAC`.

FORTRAN 77 Interface

Single: `CALL FDJAC (FCN, M, N, XC, XSCALE, FC, EPSFCN, FJAC, LDFJAC)`

Double: The double precision name is `DFDJAC`.

Description

The routine `FDJAC` uses the following finite-difference formula to estimate the Jacobian matrix of function f at x:

$$\frac{f\left(x+h_j e_j\right)-f(x)}{h_j}$$

where e_j is the j-th unit vector, $h_j = \varepsilon^{1/2} \max\{|x_j|, 1/s_j\} \operatorname{sign}(x_j)$, ε is the machine epsilon, and s_j is the scaling factor of the j-th variable. For more details, see Dennis and Schnabel (1983).

Since the finite-difference method has truncation error, cancellation error, and rounding error, users should be aware of possible poor performance. When possible, high precision arithmetic is recommended.

Comments

1. Workspace may be explicitly provided, if desired, by use of `F2JAC/DF2JAC`. The reference is:

   ```
   CALL F2JAC (FCN, M, N, XC, XSCALE, FC, EPSFCN, FJAC, LDFJAC,
   WK)
   ```

   The additional argument is:

   WK — Work vector of length M.

2. This is Description A5.4.1, Dennis and Schnabel, 1983, page 314.

Example

In this example, the Jacobian matrix of

$$f_1(x) = x_1 x_2 - 2$$
$$f_2(x) = x_1 - x_1 x_2 + 1$$

is estimated by the finite-difference method at the point (1.0, 1.0).

```
      USE FDJAC_INT
      USE UMACH_INT

      IMPLICIT  NONE
!                                  Declaration of variables
      INTEGER   N, M, LDFJAC, NOUT
      PARAMETER (N=2, M=2, LDFJAC=2)
      REAL      FJAC(LDFJAC,N), XC(N), FC(M), EPSFCN
      EXTERNAL  FCN!
      DATA XC/2*1.0E0/
!                                  Set function noise
      EPSFCN = 0.01
!                                  Evaluate the function at the
!                                  current point
      CALL FCN (M, N, XC, FC)
!                                  Get Jacobian forward-difference
!                                  approximation
      CALL FDJAC (FCN, XC, FC, FJAC, EPSFCN=EPFSCN)
!                                  Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) ((FJAC(I,J),J=1,N),I=1,M)
99999 FORMAT ('  The Jacobian is', /, 2(5X,2F10.2,/),/)
!
      END
!
      SUBROUTINE FCN (M, N, X, F)
!                                   SPECIFICATIONS FOR ARGUMENTS
      INTEGER M, N
      REAL    X(N), F(M)
!
      F(1) = X(1)*X(2) - 2.0E0
      F(2) = X(1) - X(1)*X(2) + 1.0E0
!
      RETURN
      END
```

Output

```
The Jacobian is
1.00       1.00
0.00      -1.00
```

CHGRD

Checks a user-supplied gradient of a function.

Required Arguments

FCN — User-supplied subroutine to evaluate the function of which the gradient will be checked. The usage is

CALL FCN (N, X, F), where

N – Length of X. (Input)

X – The point at which the function is evaluated. (Input)
X should not be changed by FCN.

F – The computed function value at the point X. (Output)

FCN must be declared EXTERNAL in the calling program.

GRAD — Vector of length N containing the estimated gradient at X. (Input)

X — Vector of length N containing the point at which the gradient is to be checked. (Input)

INFO — Integer vector of length N. (Output)

INFO(I) = 0 means the user-supplied gradient is a poor estimate of the numerical gradient at the point X(I).

INFO(I) = 1 means the user-supplied gradient is a good estimate of the numerical gradient at the point X(I).

INFO(I) = 2 means the user-supplied gradient disagrees with the numerical gradient at the point X(I), but it might be impossible to calculate the numerical gradient.

INFO(I) = 3 means the user-supplied gradient and the numerical gradient are both zero at X(I), and, therefore, the gradient should be rechecked at a different point.

Optional Arguments

N — Dimension of the problem. (Input)
Default: N = SIZE (X,1).

FORTRAN 90 Interface

Generic: CALL CHGRD (FCN, GRAD, X, INFO [, …])

Specific: The specific interface names are S_CHGRD and D_CHGRD.

FORTRAN 77 Interface

Single: `CALL CHGRD (FCN, GRAD, N, X, INFO)`

Double: The double precision name is `DCHGRD`.

Description

The routine `CHGRD` uses the following finite-difference formula to estimate the gradient of a function of *n* variables at *x*:

$$g_i(x) = \frac{f(x + h_i e_i) - f(x)}{h_i} \quad \text{for } i = 1, \ \ldots, n$$

where $h_i = \varepsilon^{1/2} \max\{|x_i|, 1/s_i\} \operatorname{sign}(x_i)$, ε is the machine epsilon, e_i is the *i*-th unit vector, and s_i is the scaling factor of the *i*-th variable.

The routine `CHGRD` checks the user-supplied gradient $\nabla f(x)$ by comparing it with the finite-difference gradient $g(x)$. If

$$\left| g_i(x) - (\nabla f(x))_i \right| < \tau \left| (\nabla f(x))_i \right|$$

where $\tau = \varepsilon^{1/4}$, then $(\nabla f(x))_i$, which is the *i*-th element of $\nabla f(x)$, is declared correct; otherwise, `CHGRD` computes the bounds of calculation error and approximation error. When both bounds are too small to account for the difference, $(\nabla f(x))_i$ is reported as incorrect. In the case of a large error bound, `CHGRD` uses a nearly optimal stepsize to recompute $g_i(x)$ and reports that $(\nabla f(x))_i$ is correct if

$$\left| g_i(x) - (\nabla f(x))_i \right| < 2\tau \left| (\nabla f(x))_i \right|$$

Otherwise, $(\nabla f(x))_i$ is considered incorrect unless the error bound for the optimal step is greater than $\tau \, |(\nabla f(x))_i|$. In this case, the numeric gradient may be impossible to compute correctly. For more details, see Schnabel (1985).

Comments

1. Workspace may be explicitly provided, if desired, by use of `C2GRD/DC2GRD`. The reference is:

   `CALL C2GRD (FCN, GRAD, N, X, INFO, FX, XSCALE, EPSFCN, XNEW)`

   The additional arguments are as follows:

   FX — The functional value at `X`.

   XSCALE — Real vector of length `N` containing the diagonal scaling matrix.

   EPSFCN — The relative "noise" of the function `FCN`.

XNEW — Real work vector of length `N`.

2. Informational errors

Type	Code	Description
4	1	The user-supplied gradient is a poor estimate of the numerical gradient.

Example

The user-supplied gradient of

$$f(x) = x_1 + x_2 e^{-(t - x_3)^2 / x_4}$$

at (625, 1, 3.125, 0.25) is checked where t = 2.125.

```
      USE CHGRD_INT
      USE WRIRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    N
      PARAMETER  (N=4)
!
      INTEGER    INFO(N)
      REAL       GRAD(N), X(N)
      EXTERNAL   DRIV, FCN
!
!                                 Input values for point X
!                                 X = (625.0, 1.0, 3.125, .25)
!
      DATA X/625.0E0, 1.0E0, 3.125E0, 0.25E0/
!
      CALL DRIV (N, X, GRAD)
!
      CALL CHGRD (FCN, GRAD, X, INFO)
      CALL WRIRN ('The information vector', INFO, 1, N, 1)
!
      END
!
      SUBROUTINE FCN (N, X, FX)
      INTEGER    N
      REAL       X(N), FX
!
      REAL       EXP
      INTRINSIC  EXP
!
      FX = X(1) + X(2)*EXP(-1.0E0*(2.125E0-X(3))**2/X(4))
      RETURN
      END
!
      SUBROUTINE DRIV (N, X, GRAD)
      INTEGER    N
      REAL       X(N), GRAD(N)
!
      REAL       EXP
      INTRINSIC  EXP
!
```

```
      GRAD(1) = 1.0E0
      GRAD(2) = EXP(-1.0E0*(2.125E0-X(3))**2/X(4))
      GRAD(3) = X(2)*EXP(-1.0E0*(2.125E0-X(3))**2/X(4))*2.0E0/X(4)* &
                (2.125-X(3))
      GRAD(4) = X(2)*EXP(-1.0E0*(2.125E0-X(3))**2/X(4))* &
                (2.125E0-X(3))**2/(X(4)*X(4))
      RETURN
      END
```

Output

```
The information vector
1   2   3   4
1   1   1   1
```

CHHES

Checks a user-supplied Hessian of an analytic function.

Required Arguments

GRAD — User-supplied subroutine to compute the gradient at the point X. The usage is
CALL GRAD (N, X, G), where

N – Length of X and G. (Input)

X – The point at which the gradient is evaluated. X should not be changed by GRAD. (Input)

G – The gradient evaluated at the point X. (Output)

GRAD must be declared EXTERNAL in the calling program.

HESS — User-supplied subroutine to compute the Hessian at the point X. The usage is
CALL HESS (N, X, H, LDH), where

N – Length of X. (Input)

X – The point at which the Hessian is evaluated. (Input)
X should not be changed by HESS.

H – The Hessian evaluated at the point X. (Output)

LDH – Leading dimension of H exactly as specified in in the dimension statement of the calling program. (Input)

HESS must be declared EXTERNAL in the calling program.

X — Vector of length N containing the point at which the Hessian is to be checked. (Input)

INFO — Integer matrix of dimension N by N. (Output)

INFO(I, J) = 0 means the Hessian is a poor estimate for function I at the point X(J).

INFO(I, J) = 1 means the Hessian is a good estimate for function I at the point X(J).

INFO(I, J) = 2 means the Hessian disagrees with the numerical Hessian for function I at the point X(J), but it might be impossible to calculate the numerical Hessian.

INFO(I, J) = 3 means the Hessian for function I at the point X(J) and the numerical Hessian are both zero, and, therefore, the gradient should be rechecked at a different point.

Optional Arguments

N — Dimension of the problem. (Input)
Default: N = SIZE (X,1).

LDINFO — Leading dimension of `INFO` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDINFO` = `SIZE` (`INFO`,1).

FORTRAN 90 Interface

Generic: `CALL CHHES` (`GRAD`, `HESS`, `X`, `INFO` [, …])

Specific: The specific interface names are `S_CHHES` and `D_CHHES`.

FORTRAN 77 Interface

Single: `CALL CHHES` (`GRAD`, `HESS`, `N`, `X`, `INFO`, `LDINFO`)

Double: The double precision name is `DCHHES`.

Description

The routine `CHHES` uses the following finite-difference formula to estimate the Hessian of a function of *n* variables at *x*:

$$B_{ij}(x) = \left(g_i\left(x + h_j e_j\right) - g_i(x)\right)/h_j \quad \text{for } j = 1, \ \dots, n$$

where

$$h_j = \varepsilon^{1/2} \quad \max\{|x_j|, \ 1/s_j\} \ \text{sign}(x_j),$$

ε is the machine epsilon,

$$e_j$$

is the *j*-th unit vector,

$$s_j$$

is the scaling factor of the *j*-th variable, and

$$g_i(x)$$

is the gradient of the function with respect to the *i*-th variable.

Next, `CHHES` checks the user-supplied Hessian *H*(*x*) by comparing it with the finite difference approximation *B*(*x*). If

$$|B_{ij}(x) - H_{ij}(x)| < \tau \quad |H_{ij}(x)|$$

where

$$\tau = \varepsilon^{1/4},$$

then

$$H_{ij}(x)$$

is declared correct; otherwise, `CHHES` computes the bounds of calculation error and approximation error. When both bounds are too small to account for the difference,

$$H_{ij}(x)$$

is reported as incorrect. In the case of a large error bound, `CHHES` uses a nearly optimal stepsize to recompute

$$B_{ij}(x)$$

and reports that

$$B_{ij}(x)$$

is correct if

$$|B_{ij}(x) - H_{ij}(x)| < 2\,\tau\;|H_{ij}(x)|$$

Otherwise, $H_{ij}(x)$ is considered incorrect unless the error bound for the optimal step is greater than $\tau\;|H_{ij}(x)|$. In this case, the numeric approximation may be impossible to compute correctly. For more details, see Schnabel (1985).

Comments

Workspace may be explicitly provided, if desired, by use of `C2HES/DC2HES`. The reference is

```
CALL C2HES (GRAD, HESS, N, X, INFO, LDINFO, G, HX, HS,
   XSCALE, EPSFCN, INFT, NEWX)
```

The additional arguments are as follows:

G — Vector of length `N` containing the value of the gradient `GRD` at `X`.

HX — Real matrix of dimension `N` by `N` containing the Hessian evaluated at `X`.

HS — Real work vector of length `N`.

XSCALE — Vector of length `N` used to store the diagonal scaling matrix for the variables.

EPSFCN — Estimate of the relative noise in the function.

INFT — Vector of length `N`. For `I` = 1 through `N`, `INFT` contains information about the Jacobian.

NEWX — Real work array of length `N`.

Example

The user-supplied Hessian of

$$f(x) = 100\left(x_2 - x_1^2\right)^2 + \left(1 - x_1\right)^2$$

at (−1.2, 1.0) is checked, and the error is found.

```
      USE CHHES_INT

      IMPLICIT   NONE
      INTEGER    LDINFO, N
      PARAMETER  (N=2, LDINFO=N)
!
      INTEGER    INFO(LDINFO,N)
      REAL       X(N)
      EXTERNAL   GRD, HES
!
!                                Input values for X
!                                  X = (-1.2, 1.0)
!
      DATA X/-1.2, 1.0/
!
      CALL CHHES (GRD, HES, X, INFO)
!
      END
!
      SUBROUTINE GRD (N, X, UG)
      INTEGER    N
      REAL       X(N), UG(N)
!
      UG(1) = -400.0*X(1)*(X(2)-X(1)*X(1)) + 2.0*X(1) - 2.0
      UG(2) = 200.0*X(2) - 200.0*X(1)*X(1)
      RETURN
      END
!
      SUBROUTINE HES (N, X, HX, LDHS)
      INTEGER    N, LDHS
      REAL       X(N), HX(LDHS,N)
!
      HX(1,1) = -400.0*X(2) + 1200.0*X(1)*X(1) + 2.0
      HX(1,2) = -400.0*X(1)
      HX(2,1) = -400.0*X(1)
!                                 A sign change is made to HX(2,2)
!
      HX(2,2) = -200.0
      RETURN
      END
```

Output

```
*** FATAL    ERROR 1 from CHHES.  The Hessian evaluation with respect to
***          X(2) and X(2) is a poor estimate.
```

CHJAC

Checks a user-supplied Jacobian of a system of equations with M functions in N unknowns.

Required Arguments

FCN — User-supplied subroutine to evaluate the function to be minimized. The usage is
CALL FCN (M, N, X, F), where

M – Length of F. (Input)

N – Length of X. (Input)

X – The point at which the function is evaluated. (Input)
X should not be changed by FCN.

F – The computed function value at the point X. (Output)

FCN must be declared EXTERNAL in the calling program.

JAC — User-supplied subroutine to evaluate the Jacobian at a point X. The usage is
CALL JAC (M, N, X, FJAC, LDFJAC), where

M – Length of F. (Input)

N – Length of X. (Input)

X – The point at which the function is evaluated. (Input)
X should not be changed by FCN.

FJAC – The computed M by N Jacobian at the point X. (Output)

LDFJAC – Leading dimension of FJAC. (Input)

JAC must be declared EXTERNAL in the calling program.

X — Vector of length N containing the point at which the Jacobian is to be checked. (Input)

INFO — Integer matrix of dimension M by N. (Output)

INFO(I, J) = 0 means the user-supplied Jacobian is a poor estimate for function I at the point X(J).

INFO(I, J) = 1 means the user-supplied Jacobian is a good estimate for function I at the point X(J).

INFO(I, J) = 2 means the user-supplied Jacobian disagrees with the numerical Jacobian for function I at the point X(J), but it might be impossible to calculate the numerical Jacobian.

INFO(I, J) = 3 means the user-supplied Jacobian for function I at the point X(J) and the numerical Jacobian are both zero. Therefore, the gradient should be rechecked at a different point.

Optional Arguments

M — The number of functions in the system of equations. (Input)
Default: M = SIZE (INFO,1).

N — The number of unknowns in the system of equations. (Input)
Default: N = SIZE (X,1).

LDINFO — Leading dimension of INFO exactly as specified in the dimension statement of the calling program. (Input)
Default: LDINFO = SIZE (INFO,1).

FORTRAN 90 Interface

Generic: CALL CHJAC (FCN, JAC, X, INFO [, …])

Specific: The specific interface names are S_CHJAC and D_CHJAC.

FORTRAN 77 Interface

Single: CALL CHJAC (FCN, JAC, M, N, X, INFO, LDINFO)

Double: The double precision name is DCHJAC.

Description

The routine CHJAC uses the following finite-difference formula to estimate the gradient of the i-th function of n variables at x:

$$g_{ij}(x) = (f_i(x + h_j e_j) - f_i(x))/h_j \text{ for } j = 1, \ldots, n$$

where $h_j = \varepsilon^{1/2} \max\{|x_j|, 1/s_j\} \operatorname{sign}(x_j)$, ε is the machine epsilon, e_j is the j-th unit vector, and s_j is the scaling factor of the j-th variable.

Next, CHJAC checks the user-supplied Jacobian $J(x)$ by comparing it with the finite difference gradient $g_i(x)$. If

$$|g_{ij}(x) - J_{ij}(x)| < \tau \; |J_{ij}(x)|$$

where $\tau = \varepsilon^{1/4}$, then $J_{ij}(x)$ is declared correct; otherwise, CHJAC computes the bounds of calculation error and approximation error. When both bounds are too small to account for the difference, $J_{ij}(x)$ is reported as incorrect. In the case of a large error bound, CHJAC uses a nearly optimal stepsize to recompute $g_{ij}(x)$ and reports that $J_{ij}(x)$ is correct if

$$|g_{ij}(x) - J_{ij}(x)| < 2\,\tau\,|J_{ij}(x)|$$

Otherwise, $J_{ij}(x)$ is considered incorrect unless the error bound for the optimal step is greater than $\tau\,|J_{ij}(x)|$. In this case, the numeric gradient may be impossible to compute correctly. For more details, see Schnabel (1985).

Comments

1. Workspace may be explicitly provided, if desired, by use of C2JAC/DC2JAC. The reference is:

```
CALL C2JAC (FCN, JAC, N, X, INFO, LDINFO, FX, FJAC, GRAD,
   XSCALE, EPSFCN, INFT, NEWX)
```

   The additional arguments are as follows:

   FX — Vector of length M containing the value of each function in FCN at X.

   FJAC — Real matrix of dimension M by N containing the Jacobian of FCN evaluated at X.

   GRAD — Real work vector of length N used to store the gradient of each function in FCN.

   XSCALE — Vector of length N used to store the diagonal scaling matrix for the variables.

   EPSFCN — Estimate of the relative noise in the function.

   INFT — Vector of length N. For I = 1 through N, INFT contains information about the Jacobian.

   NEWX — Real work array of length N.

2. Informational errors

Type	Code	Description
4	1	The user-supplied Jacobian is a poor estimate of the numerical Jacobian.

Example

The user-supplied Jacobian of

$$f_1 = 1 - x_1$$
$$f_2 = 10\left(x_2 - x_1^2\right)$$

at (−1.2, 1.0) is checked.

```
      USE CHJAC_INT
      USE WRIRN_INT

      IMPLICIT   NONE
      INTEGER    LDINFO, N
      PARAMETER  (M=2,N=2,LDINFO=M)
!
      INTEGER    INFO(LDINFO,N)
```

```
      REAL       X(N)
      EXTERNAL   FCN, JAC
!
!                                  Input value for X
!                                     X = (-1.2, 1.0)
!
      DATA X/-1.2, 1.0/
!
      CALL CHJAC (FCN, JAC, X, INFO)
      CALL WRIRN ('The information matrix', INFO)
!
      END
!
      SUBROUTINE FCN (M, N, X, F)
      INTEGER    M, N
      REAL       X(N), F(M)
!
      F(1) = 1.0 - X(1)
      F(2) = 10.0*(X(2)-X(1)*X(1))
      RETURN
      END
!
      SUBROUTINE JAC (M, N, X, FJAC, LDFJAC)
      INTEGER    M, N, LDFJAC
      REAL       X(N), FJAC(LDFJAC,N)
!
      FJAC(1,1) = -1.0
      FJAC(1,2) = 0.0
      FJAC(2,1) = -20.0*X(1)
      FJAC(2,2) = 10.0
      RETURN
      END
```

Output

```
*** WARNING  ERROR 2 from C2JAC.  The numerical value of the Jacobian
***          evaluation for function 1 at the point X(2) = 1.000000E+00 and
***          the user-supplied value are both zero.  The Jacobian for this
***          function should probably be re-checked at another value for
***          this point.

The information matrix
    1   2
1   1   3
2   1   1
```

GGUES

Generates points in an N-dimensional space.

Required Arguments

A — Vector of length N. (Input)
See B.

B — Real vector of length N. (Input)
A and B define the rectangular region in which the points will be generated, i.e., A(I) < S(I) < B(I) for I = 1, 2, …, N. Note that if B(I) < A(I), then B(I) < S(I) < A(I).

K — The number of points to be generated. (Input)

IDO — Initialization parameter. (Input/Output)
IDO must be set to zero for the first call. GGUES resets IDO to 1 and returns the first generated point in S. Subsequent calls should be made with IDO = 1.

S — Vector of length N containing the generated point. (Output)
Each call results in the next generated point being stored in S.

Optional Arguments

N — Dimension of the space. (Input)
Default: N = SIZE (B,1).

FORTRAN 90 Interface

Generic: CALL GGUES (A, B, K, IDO, S [, …])

Specific: The specific interface names are S_GGUES and D_GGUES.

FORTRAN 77 Interface

Single: CALL GGUES (N, A, B, K, IDO, S)

Double: The double precision name is DGGUES.

Description

The routine GGUES generates starting points for algorithms that optimize functions of several variables or, almost equivalently, algorithms that solve simultaneous nonlinear equations.

The routine GGUES is based on systematic placement of points to optimize the dispersion of the set. For more details, see Aird and Rice (1977).

Comments

1. Workspace may be explicitly provided, if desired, by use of G2UES/DG2UES. The reference is:

   CALL G2UES (N, A, B, K, IDO, S, WK, IWK)

   The additional arguments are:

   WK — Work vector of length N. WK must be preserved between calls to G2UES.

   IWK — Work vector of length 10. IWK must be preserved between calls to G2UES.

2. Informational error

Type	Code	Description
4	1	Attempt to generate more than K points.

3. The routine GGUES may be used with any nonlinear optimization routine that requires starting points. The rectangle to be searched (defined by A, B, and N) must be determined; and the number of starting points, K, must be chosen. One possible use for GGUES would be to call GGUES to generate a point in the chosen rectangle. Then, call the nonlinear optimization routine using this point as an initial guess for the solution. Repeat this process K times. The number of iterations that the optimization routine is allowed to perform should be quite small (5 to 10) during this search process. The best (or best several) point(s) found during the search may be used as an initial guess to allow the optimization routine to determine the optimum more accurately. In this manner, an N dimensional rectangle may be effectively searched for a global optimum of a nonlinear function. The choice of K depends upon the nonlinearity of the function being optimized. A function with many local optima requires a larger value than a function with only a few local optima.

Example

We want to search the rectangle with vertices at coordinates (1, 1), (3, 1), (3, 2), and (1, 2) ten times for a global optimum of a nonlinear function. To do this, we need to generate starting points. The following example illustrates the use of GGUES in this process:

```
      USE GGUES_INT
      USE UMACH_INT
```

```
      IMPLICIT   NONE
!                              Variable Declarations
      INTEGER    N
      PARAMETER  (N=2)
!
      INTEGER    IDO, J, K, NOUT
      REAL       A(N), B(N), S(N)
!                              Initializations
!
!                              A    = ( 1.0, 1.0)
!                              B    = ( 3.0, 2.0)
!
      DATA A/1.0, 1.0/
      DATA B/3.0, 2.0/
!
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99998)
99998 FORMAT ('  Point Number', 7X, 'Generated Point')
!
      K = 10
      IDO = 0
      DO 10  J=1, K
         CALL GGUES (A, B, K, IDO, S)
!
         WRITE (NOUT,99999) J, S(1), S(2)
99999    FORMAT (1X, I7, 14X, '(', F4.1, ',', F6.3, ')')
!
   10 CONTINUE
!
      END
```

Output

```
Point Number       Generated Point
 1                ( 1.5, 1.125)
 2                ( 2.0, 1.500)
 3                ( 2.5, 1.750)
 4                ( 1.5, 1.375)
 5                ( 2.0, 1.750)
 6                ( 1.5, 1.625)
 7                ( 2.5, 1.250)
 8                ( 1.5, 1.875)
 9                ( 2.0, 1.250)
10                ( 2.5, 1.500)
```

Basic Matrix/Vector Operations

Routines

Basic Linear Algebra Subprograms

The basic linear algebra subprograms, normally referred to as the BLAS, are routines for low-level operations such as dot products, matrix times vector, and matrix times matrix. Lawson et al. (1979) published the original set of 38 BLAS. The IMSL BLAS collection includes these 38 subprograms plus additional ones that extend their functionality. Since Dongarra et al. (1988 and 1990) published extensions to this set, it is customary to refer to the original 38 as Level 1 BLAS. The Level 1 operations are performed on one or two vectors of data. An extended set of subprograms perform operations involving a matrix and one or two vectors. These are called the Level 2 BLAS (see *Specification of the Level 2 BLAS*). An additional extended set of operations on matrices is called the Level 3 BLAS (see *Specification of the Level 3 BLAS*).

Users of the BLAS will often benefit from using versions of the BLAS supplied by hardware vendors, if available. This can provide for more efficient execution of many application programs. The BLAS provided by IMSL are written in FORTRAN. Those supplied by vendors may be written in other languages, such as assembler. The documentation given below for the BLAS is compatible with a vendor's version of the BLAS that conforms to the published specifications.

Programming Notes for Level 1 BLAS

The Level 1 BLAS do not follow the usual IMSL naming conventions. Instead, the names consist of a prefix of one or more of the letters "`I`", "`S`", "`D`", "`C`", and "`Z`"; a root name; and sometimes a suffix. For subprograms involving a mixture of data types, the output type is indicated by the first prefix letter. The suffix denotes a variant algorithm. The prefix denotes the type of the operation according to the following table:

`I`	Integer		
`S`	Real	`C`	Complex
`D`	Double	`Z`	Double Complex
`SD`	Single and Double	`CZ`	Single and Double Complex
`DQ`	Double and Quadruple	`ZQ`	Double and Quadruple Complex

Vector arguments have an increment parameter that specifies the storage space or stride between elements. The correspondence between the vectors *x* and *y* and the arguments `SX` and `SY`, and `INCX` and `INCY` is

$$x_i = \begin{cases} \mathrm{SX}\left(\left(\mathrm{I}-1\right) * \mathrm{INCX}+1\right) & \text{if INCX} \geq 0 \\ \mathrm{SX}\left(\left(\mathrm{I}-\mathrm{N}\right) * \mathrm{INCX}+1\right) & \text{if INCX} < 0 \end{cases}$$

$$y_i = \begin{cases} \mathrm{SY}\left(\left(\mathrm{I}-1\right) * \mathrm{INCY}+1\right) & \text{if INCY} \geq 0 \\ \mathrm{SY}\left(\left(\mathrm{I}-\mathrm{N}\right) * \mathrm{INCY}+1\right) & \text{if INCY} < 0 \end{cases}$$

Function subprograms `SXYZ` and `DXYZ` refer to a third vector argument *z*. The storage increment `INCZ` for *z* is defined like `INCX` and `INCY`. In the Level 1 BLAS, only positive values of `INCX` are allowed for operations that have a single vector argument. The loops in all of the Level 1 BLAS process the vector arguments in order of increasing *i*. For `INCX`, `INCY`, `INCZ` < 0, this implies processing in reverse storage order.

The function subprograms in the Level 1 BLAS are all illustrated by means of an assignment statement. For example, see `SDOT`. Any value of a function subprogram can be used in an expression or as a parameter passed to a subprogram as long as the data types agree.

Descriptions of the Level 1 BLAS Subprograms

The set of Level 1 BLAS are summarized in *Table 6*. This table also lists the page numbers where the subprograms are described in more detail.

Specification of the Level 1 BLAS

With the definitions,

$$\mathrm{MX} = \max \{1, 1 + (N - 1)|\mathrm{INCX}|\}$$

$$\mathrm{MY} = \max \{1, 1 + (N - 1)|\mathrm{INCY}|\}$$

$$\mathrm{MZ} = \max \{1, 1 + (N - 1)|\mathrm{INCZ}|\}$$

the subprogram descriptions assume the following FORTRAN declarations:

```
IMPLICIT INTEGER          (I-N)
IMPLICIT REAL             S
IMPLICIT DOUBLE PRECISION D
IMPLICIT COMPLEX          C
IMPLICIT DOUBLE COMPLEX   Z

INTEGER                   IX(MX)
REAL                      SX(MX), SY(MY), SZ(MZ),
                          SPARAM(5)
DOUBLE PRECISION          DX(MX), DY(MY), DZ(MZ),
                          DPARAM(5)
DOUBLE PRECISION          DACC(2), DZACC(4)
COMPLEX                   CX(MX), CY(MY)
DOUBLE COMPLEX            ZX(MX), ZY(MY)
```

Since FORTRAN 77 does not include the type `DOUBLE COMPLEX`, subprograms with `DOUBLE COMPLEX` arguments are not available for all systems. Some systems use the declaration `COMPLEX * 16` instead of `DOUBLE COMPLEX`.

In the following descriptions, the original BLAS are marked with an * in the left column.

Table 6 – Level 1 Basic Linear Algebra Subprograms

Operation	Integer	Real	Double	Complex	DoubleComplex	Subprogram
$x_i \leftarrow a$	ISET	SSET	DSET	CSET	ZSET	*Set a Vector to a Constant Value*
$y_i \leftarrow x_i$	ICOPY	SCOPY	DCOPY	CCOPY	ZCOPY	*Copy a Vector*
$x_i \leftarrow ax_i$ $a \in \mathbf{R}$		SSCAL	DSCAL	CSCAL CSSCAL	ZSCAL ZDSCAL	*Scale a Vector*
$y_i \leftarrow ax_i$ $a \in \mathbf{R}$		SVCAL	DVCAL	CVCAL CSVCAL	ZVCAL ZDVCAL	*Multiply a Vector by a Constant*
$x_i \leftarrow x_i + a$	IADD	SADD	DADD	CADD	ZADD	*Add a Constant to a Vector*
$x_i \leftarrow a - x_i$	ISUB	SSUB	DSUB	CSUB	ZSUB	*Subtract a Vector from a Constant*
$y_i \leftarrow ax_i + y_i$		SAXPY	DAXPY	CAXPY	ZAXPY	*Constant Times a Vector Plus a Vector*
$y_i \leftrightarrow x_i$	ISWAP	SSWAP	DSWAP	CSWAP	ZSWAP	*Swap Two Vectors*
$x \cdot y$ $\overline{x} \cdot y$		SDOT	DDOT	CDOTU CDOTC	ZDOTU ZDOTC	*Swap Two Vectors*
$x \cdot y^\dagger$ $\overline{x} \cdot y^\dagger$		DSDOT		CZDOTU CZDOTC	ZQDOTU ZQDOTC	*Dot Product with Higher Precision Accumulation*
$a + x \cdot y^\dagger$ $a + \overline{x} \cdot y^\dagger$		SDSDOT	DQDDOT	CZUDOT CZCDOT	ZQUDOT ZQCDOT	*Constant Plus Dot Product with Higher Precision Accumulation*
$b + x \cdot y^\dagger$ $\mathrm{ACC} + b + x \cdot y^\dagger$		SDDOTI SDDOTA	DQDOTI DQDOTA	CZDOTI CZDOTA	ZQDOTI ZQDOTA	*Dot Product Using the Accumulator*
$z_i \leftarrow x_i y_i$		SHPROD	DHPROD			*Hadamard Product*
$\Sigma x_i y_i z_i$		SXYZ	DXYZ			*Triple Inner Product*
Σx_i	ISUM	SSUM	DSUM			*Sum of the Elements of a Vector*

Table 6 – Level 1 Basic Linear Algebra Subprograms

Operation	Integer	Real	Double	Complex	DoubleComplex	Subprogram
$\Sigma \lvert x_i \rvert$		SASUM	DASUM	SCASUM	DZASUM	*Sum of the Absolute Values of the Elements of a Vector*
$\lVert x \rVert_2$		SNRM2	DNRM2	SCNRM2	DZNRM2	*Euclidean or ℓ_2 Norm of a Vector*
Πx_i		SPRDCT	DPRDCT			*Product of the Elements of a Vector*
$i : x_i = \min_j x_j$	IIMIN	ISMIN	IDMIN			*Index of Element Having Minimum Value*
$i : x_i = \max_j x_j$	IIMAX	ISMAX	IDMAX			*Index of Element Having Maximum Value*
$i : \lvert x_i \rvert = \min_j \lvert x_j \rvert$		ISAMIN	IDAMIN	ICAMIN	IZAMIN	*Index of Element Having Minimum Absolute Value*
$i : \lvert x_i \rvert = \max_j \lvert x_j \rvert$		ISAMAX	IDAMAX	ICAMAX	IZAMAX	*Index of Element Having Maximum Absolute Value*
Construct Givens rotation		SROTG	DROTG	CROTG	ZROTG	*Construct a Givens Plane Rotation*
Apply Givens rotation		SROT	DROT	CROT CSROT	ZROT ZDROT	*Apply a Plane Rotation*
Construct modified Givens transform		SROTMG	DROTMG			*Construct a Modified Givens Transformation*
Apply modified Givens transform		SROTM	DROTM	CSROTM	ZDROTM	*Apply a Modified Givens Transformation*

†Higher precision accumulation used

Set a Vector to a Constant Value

```
CALL ISET (N, IA, IX, INCX)
CALL SSET (N, SA, SX, INCX)
CALL DSET (N, DA, DX, INCX)
CALL CSET (N, CA, CX, INCX)
CALL ZSET (N, ZA, ZX, INCX)
```

These subprograms set $x_i \leftarrow a$ for $i = 1, 2, \ldots, N$. If $N \le 0$, then the subprograms return immediately.

Copy a Vector

```
 CALL ICOPY (N, IX, INCX, IY, INCY)
*CALL SCOPY (N, SX, INCX, SY, INCY)
*CALL DCOPY (N, DX, INCX, DY, INCY)
```

```
*CALL CCOPY (N, CX, INCX, CY, INCY)
 CALL ZCOPY (N, ZX, INCX, ZY, INCY)
```

These subprograms set $y_i \leftarrow x_i$ for $i = 1, 2, \ldots, N$. If $N \le 0$, then the subprograms return immediately.

Scale a Vector

```
*CALL SSCAL (N, SA, SX, INCX)
*CALL DSCAL (N, DA, DX, INCX)
*CALL CSCAL (N, CA, CX, INCX)
 CALL ZSCAL (N, ZA, ZX, INCX)
*CALL CSSCAL (N, SA, CX, INCX)
 CALL ZDSCAL (N, DA, ZX, INCX)
```

These subprograms set $x_i \leftarrow ax_i$ for $i = 1, 2, \ldots, N$. If $N \le 0$, then the subprograms return immediately. CAUTION: For `CSSCAL` and `ZDSCAL`, the scalar quantity a is real and the vector x is complex.

Multiply a Vector by a Constant

```
CALL SVCAL (N, SA, SX, INCX, SY, INCY)
CALL DVCAL (N, DA, DX, INCX, DY, INCY)
CALL CVCAL (N, CA, CX, INCX, CY, INCY)
CALL ZVCAL (N, ZA, ZX, INCX, ZY, INCY)
CALL CSVCAL (N, SA, CX, INCX, CY, INCY)
CALL ZDVCAL (N, DA, ZX, INCX, ZY, INCY)
```

These subprograms set $y_i \leftarrow ax_i$ for $i = 1, 2, \ldots, N$. If $N \le 0$, then the subprograms return immediately. CAUTION: For `CSVCAL` and `ZDVCAL`, the scalar quantity a is real and the vector x is complex.

Add a Constant to a Vector

```
CALL IADD (N, IA, IX, INCX)
CALL SADD (N, SA, SX, INCX)
CALL DADD (N, DA, DX, INCX)
CALL CADD (N, CA, CX, INCX)
CALL ZADD (N, ZA, ZX, INCX)
```

These subprograms set $x_i \leftarrow x_i + a$ for $i = 1, 2, \ldots, N$. If $N \le 0$, then the subprograms return immediately.

Subtract a Vector from a Constant

```
CALL ISUB (N, IA, IX, INCX)
CALL SSUB (N, SA, SX, INCX)
CALL DSUB (N, DA, DX, INCX)
CALL CSUB (N, CA, CX, INCX)
CALL ZSUB (N, ZA, ZX, INCX)
```

These subprograms set $x_i \leftarrow a - x_i$ for $i = 1, 2, \ldots, N$. If $N \le 0$, then the subprograms return immediately.

Constant Times a Vector Plus a Vector

```
*CALL SAXPY (N, SA, SX, INCX, SY, INCY)
```

```
 *CALL DAXPY (N, DA, DX, INCX, DY, INCY)
 *CALL CAXPY (N, CA, CX, INCX, CY, INCY)
  CALL ZAXPY (N, ZA, ZX, INCX, ZY, INCY)
```

These subprograms set $y_i \leftarrow ax_i + y_i$ for $i = 1, 2, \ldots, N$. If $N \le 0$, then the subprograms return immediately.

Swap Two Vectors

```
  CALL ISWAP (N, IX, INCX, IY, INCY)
 *CALL SSWAP (N, SX, INCX, SY, INCY)
 *CALL DSWAP (N, DX, INCX, DY, INCY)
 *CALL CSWAP (N, CX, INCX, CY, INCY)
  CALL ZSWAP (N, ZX, INCX, ZY, INCY)
```

These subprograms perform the exchange $y_i \leftrightarrow x_i$ for $i = 1, 2, \ldots, N$. If $N \le 0$, then the subprograms return immediately.

Dot Product

```
 *SW =  SDOT  (N, SX, INCX, SY, INCY)
 *DW =  DDOT  (N, DX, INCX, DY, INCY)
 *CW =  CDOTU (N, CX, INCX, CY, INCY)
 *CW =  CDOTC (N, CX, INCX, CY, INCY)
  ZW =  ZDOTU (N, ZX, INCX, ZY, INCY)
  ZW =  ZDOTC (N, ZX, INCX, ZY, INCY)
```

The function subprograms `SDOT`, `DDOT`, `CDOTU`, and `ZDOTU` compute

$$\sum_{i=1}^{N} x_i y_i$$

The function subprograms `CDOTC` and `ZDOTC` compute

$$\sum_{i=1}^{N} \bar{x}_i y_i$$

The suffix `C` indicates that the complex conjugates of x_i are used. The suffix `U` indicates that the unconjugated values of x_i are used. If $N \le 0$, then the subprograms return zero.

Dot Product with Higher Precision Accumulation

```
 *DW =  DSDOT  (N, SX, INCX, SY, INCY)
  CW =  CZDOTC (N, CX, INCX, CY, INCY)
  CW =  CZDOTU (N, CX, INCX, CY, INCY)
  ZW =  ZQDOTC (N, ZX, INCX, ZY, INCY)
  ZW =  ZQDOTU (N, ZX, INCX, ZY, INCY)
```

The function subprogram `DSDOT` computes

$$\sum_{i=1}^{N} x_i y_i$$

using double precision accumulation. The function subprograms `CZDOTU` and `ZQDOTU` compute

$$\sum_{i=1}^{N} x_i y_i$$

using double and quadruple complex accumulation, respectively. The function subprograms `CZDOTC` and `ZQDOTC` compute

$$\sum_{i=1}^{N} \bar{x}_i y_i$$

using double and quadruple complex accumulation, respectively. If $N \le 0$, then the subprograms return zero.

Constant Plus Dot Product with Higher Precision Accumulation

```
*SW = SDSDOT (N, SA, SX, INCX, SY, INCY)
 DW = DQDDOT (N, DA, DX, INCX, DY, INCY)
 CW = CZCDOT (N, CA, CX, INCX, CY, INCY)
 CW = CZUDOT (N, CA, CX, INCX, CY, INCY)
 ZW = ZQCDOT (N, ZA, ZX, INCX, ZY, INCY)
 ZW = ZQUDOT (N, ZA, ZX, INCX, ZY, INCY)
```

The function subprograms `SDSDOT`, `DQDDOT`, `CZUDOT`, and `ZQUDOT` compute

$$a + \sum_{i=1}^{N} x_i y_i$$

using higher precision accumulation where `SDSDOT` uses double precision accumulation, `DQDDOT` uses quadruple precision accumulation, `CZUDOT` uses double complex accumulation, and `ZQUDOT` uses quadruple complex accumulation. The function subprograms `CZCDOT` and `ZQCDOT` compute

$$a + \sum_{i=1}^{N} \bar{x}_i y_i$$

using double complex and quadruple complex accumulation, respectively. If $N \le 0$, then the subprograms return zero.

Dot Product Using the Accumulator

```
 SW =  SDDOTI (N, SB,  DACC, SX, INCX, SY, INCY)
 SW =  SDDOTA (N, SB,  DACC, SX, INCX, SY, INCY)
 CW =  CZDOTI (N, CB,  DACC, CX, INCX, CY, INCY)
 CW =  CZDOTA (N, CB,  DACC, CX, INCX, CY, INCY)
*DW =  DQDOTI (N, DB,  DACC, DX, INCX, DY, INCY)
*DW =  DQDOTA (N, DB,  DACC, DX, INCX, DY, INCY)
 ZW =  ZQDOTI (N, ZB, DZACC, ZX, INCX, ZY, INCY)
 ZW =  ZQDOTA (N, ZB, DZACC, ZX, INCX, ZY, INCY)
```

The variable DACC, a double precision array of length two, is used as a quadruple precision accumulator. DZACC, a double precision array of length four, is its complex analog. The function subprograms with a name ending in I initialize DACC to zero. All of the function subprograms then compute

$$DACC + b + \sum_{i=1}^{N} x_i y_i$$

and store the result in DACC. The result, converted to the precision of the function, is also returned as the function value. If $N \le 0$, then the function subprograms return zero.

Hadamard Product

```
CALL SHPROD (N, SX, INCX, SY, INCY, SZ, INCZ)
CALL DHPROD (N, DX, INCX, DY, INCY, DZ, INCZ)
```

These subprograms set $z_i \leftarrow x_i y_i$ for $i = 1, 2, \ldots, N$. If $N \le 0$, then the subprograms return immediately.

Triple Inner Product

```
SW = SXYZ (N, SX, INCX, SY, INCY, SZ, INCZ)
DW = DXYZ (N, DX, INCX, DY, INCY, DZ, INCZ)
```

These function subprograms compute

$$\sum_{i=1}^{N} x_i y_i z_i$$

If $N \le 0$ then the subprograms return zero.

Sum of the Elements of a Vector

```
IW = ISUM (N, IX, INCX)
SW = SSUM (N, SX, INCX)
DW = DSUM (N, DX, INCX)
```

These function subprograms compute

$$\sum_{i=1}^{N} x_i$$

If $N \le 0$, then the subprograms return zero.

Sum of the Absolute Values of the Elements of a Vector

```
*SW = SASUM (N, SX, INCX)
*DW = DASUM (N, DX, INCX)
*SW = SCASUM (N, CX, INCX)
 DW = DZASUM (N, ZX, INCX)
```

The function subprograms `SASUM` and `DASUM` compute

$$\sum_{i=1}^{N} |x_i|$$

The function subprograms `SCASUM` and `DZASUM` compute

$$\sum_{i=1}^{N} \left[|\ \Re\ x_i| + |\ \Im\ x_i| \right]$$

If $N \le 0$, then the subprograms return zero. CAUTION: For `SCASUM` and `DZASUM`, the function subprogram returns a real value.

Euclidean or ℓ_2 Norm of a Vector

```
*SW = SNRM2  (N, SX, INCX)
*DW = DNRM2  (N, DX, INCX)
*SW = SCNRM2 (N, CX, INCX)
 DW = DZNRM2 (N, ZX, INCX)
```

These function subprograms compute

$$\left[\sum_{i=1}^{N} |\ x_i\ |^2 \right]^{1/2}$$

If $N \le 0$, then the subprograms return zero. CAUTION: For `SCNRM2` and `DZNRM2`, the function subprogram returns a real value.

Product of the Elements of a Vector

```
SW = SPRDCT (N, SX, INCX)
DW = DPRDCT (N, DX, INCX)
```

These function subprograms compute

$$\prod_{i=1}^{N} x_i$$

If $N \le 0$, then the subprograms return zero.

Index of Element Having Minimum Value

```
IW = IIMIN (N, IX, INCX)
IW = ISMIN (N, SX, INCX)
IW = IDMIN (N, DX, INCX)
```

These function subprograms compute the smallest index i such that $x_i = \min_{1 \le j \le N} x_j$. If $N \le 0$, then the subprograms return zero.

Index of Element Having Maximum Value

```
IW = IIMAX (N, IX, INCX)
IW = ISMAX (N, SX, INCX)
IW = IDMAX (N, DX, INCX)
```

These function subprograms compute the smallest index *i* such that $x_i = \max_{1 \le j \le N} x_j$. If $N \le 0$, then the subprograms return zero.

Index of Element Having Minimum Absolute Value

```
IW = ISAMIN (N, SX, INCX)
IW = IDAMIN (N, DX, INCX)
IW = ICAMIN (N, CX, INCX)
IW = IZAMIN (N, ZX, INCX)
```

The function subprograms `ISAMIN` and `IDAMIN` compute the smallest index *i* such that $|x_i| = \min_{1 \le j \le N} |x_j|$. The function subprograms `ICAMIN` and `IZAMIN` compute the smallest index *i* such that

$$|\Re x_i| + |\Im x_i| = \min_{1 \le j \le N} \left[|\Re x_j| + |\Im x_j| \right]$$

If $N \le 0$, then the subprograms return zero.

Index of Element Having Maximum Absolute Value

```
*IW = ISAMAX (N, SX, INCX)
*IW = IDAMAX (N, DX, INCX)
*IW = ICAMAX (N, CX, INCX)
 IW = IZAMAX (N, ZX, INCX)
```

The function subprograms `ISAMAX` and `IDAMAX` compute the smallest index *i* such that $|x_i| = \max_{1 \le j \le N} |x_j|$. The function subprograms `ICAMAX` and `IZAMAX` compute the smallest index *i* such that

$$|\Re x_i| + |\Im x_i| = \max_{1 \le j \le N} \left[|\Re x_j| + |\Im x_j| \right]$$

If $N \le 0$, then the subprograms return zero.

Construct a Givens Plane Rotation

```
*CALL SROTG (SA, SB, SC, SS)
*CALL DROTG (SA, SB, SC, SS)
```

Given the values *a* and *b*, these subprograms compute

$$c = \begin{cases} a/r & \text{if } r \ne 0 \\ 1 & \text{if } r = 0 \end{cases}$$

and

$$s = \begin{cases} b/r & \text{if } r \neq 0 \\ 1 & \text{if } r = 0 \end{cases}$$

where $r = \sigma(a^2 + b^2)^{1/2}$ and

$$\sigma = \begin{cases} \text{sign}(a) & \text{if } |a| > |b| \\ \text{sign}(b) & \text{otherwise} \end{cases}$$

Then, the values *c*, *s* and *r* satisfy the matrix equation

$$\begin{bmatrix} c & s \\ -s & c \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} r \\ 0 \end{bmatrix}$$

The introduction of σ is not essential to the computation of the Givens rotation matrix; but its use permits later stable reconstruction of *c* and *s* from just one stored number, an idea due to Stewart (1976). For this purpose, the subprogram also computes

$$z = \begin{cases} s & \text{if } |s| < c \text{ or } c = 0 \\ 1/c & \text{if } 0 < |c| \ \leq s \end{cases}$$

In addition to returning *c* and *s*, the subprograms return *r* overwriting *a*, and *z* overwriting *b*.

Reconstruction of *c* and *s* from *z* can be done as follows:

If $z = 1$, then set $c = 0$ and $s = 1$

If $|z| < 1$, then set

$$c = \sqrt{1 - z^2} \text{ and } s = z$$

If $|z| > 1$, then set

$$c = 1/z \text{ and } s = \sqrt{1 - c^2}$$

Apply a Plane Rotation

```
*CALL SROT (N, SX, INCX, SY, INCY, SC, SS)
*CALL DROT (N, DX, INCX, DY, INCY, DC, DS)
 CALL CSROT (N, CX, INCX, CY, INCY, SC, SS)
 CALL ZDROT (N, ZX, INCX, ZY, INCY, DC, DS)
```

These subprograms compute

$$\begin{bmatrix} x_i \\ y_i \end{bmatrix} \leftarrow \begin{bmatrix} c & s \\ -s & c \end{bmatrix} = \begin{bmatrix} x_i \\ y_i \end{bmatrix} \quad \text{for } i = 1, \ \ldots, N$$

If $N \le 0$, then the subprograms return immediately. CAUTION: For `CSROT` and `ZDROT`, the scalar quantities *c* and *s* are real, and *x* and *y* are complex.

Construct a Modified Givens Transformation

```
*CALL SROTMG (SD1, SD2, SX1, SY1, SPARAM)
*CALL DROTMG (DD1, DD2, DX1, DY1, DPARAM)
```

The input quantities d_1, d_2, x_1 and y_1 define a 2-vector $[w_1, z_1]^T$ by the following:

$$\begin{bmatrix} w_i \\ z_i \end{bmatrix} = \begin{bmatrix} \sqrt{d_1} & 0 \\ 0 & \sqrt{d_2} \end{bmatrix} \begin{bmatrix} x_i \\ y_i \end{bmatrix}$$

The subprograms determine the modified Givens rotation matrix *H* that transforms y_1, and thus, z_1 to zero. They also replace d_1, d_2 and x_1 with

$$\tilde{d}_1, \tilde{d}_2 \text{ and } \tilde{x}_1$$

respectively. That is,

$$\begin{bmatrix} \tilde{w}_1 \\ 0 \end{bmatrix} = \begin{bmatrix} \sqrt{\tilde{d}_1} & 0 \\ 0 & \sqrt{\tilde{d}_2} \end{bmatrix} H \begin{bmatrix} x_1 \\ y_1 \end{bmatrix} = \begin{bmatrix} \sqrt{\tilde{d}_1} & 0 \\ 0 & \sqrt{\tilde{d}_2} \end{bmatrix} \begin{bmatrix} x_1 \\ y_1 \end{bmatrix} = \begin{bmatrix} \tilde{x}_1 \\ 0 \end{bmatrix}$$

A representation of this matrix is stored in the array `SPARAM` or `DPARAM`. The form of the matrix *H* is flagged by `PARAM`(1).

`PARAM`(1) = 1. In this case,

$$|d_1 x_1^2| \le |d_2 y_1^2|$$

and

$$H = \begin{bmatrix} \text{PARAM}(2) & 1 \\ -1 & \text{PARAM}(5) \end{bmatrix}$$

The elements `PARAM`(3) and `PARAM`(4) are not changed.

`PARAM`(1) = 0. In this case,

$$|d_1x_1^2| > |d_2y_1^2|$$

and

$$H = \begin{bmatrix} 1 & \text{PARAM}(4) \\ \text{PARAM}(3) & 1 \end{bmatrix}$$

The elements `PARAM`(2) and `PARAM`(5) are not changed.

`PARAM`(1) = −1. In this case, rescaling was done and

$$H = \begin{bmatrix} PARAM(2) & PARAM(4) \\ PARAM(3) & PARAM(5) \end{bmatrix}$$

`PARAM`(2) = −2. In this case, $H = I$ where I is the identity matrix. The elements `PARAM`(2), `PARAM`(3), `PARAM`(4) and `PARAM`(5) are not changed.

The values of d_1, d_2 and $x_1$are changed to represent the effect of the transformation. The quantity y_1, which would be zeroed by the transformation, is left unchanged.

The input value of d_1 should be nonnegative, but d_2 can be negative for the purpose of removing data from a least-squares problem.

See Lawson et al. (1979) for further details.

Apply a Modified Givens Transformation

```
 *CALL SROTM (N, SX, INCX, SY, INCY, SPARAM)
 *CALL DROTM (N, DX, INCX, DY, INCY, DPARAM)
  CALL CSROTM (N, CX, INCX, CY, INCY, SPARAM)
  CALL ZDROTM (N, ZX, INCX, ZY, INCY, DPARAM)
```

If `PARAM`(1) = 1.0, then these subprograms compute

$$\begin{bmatrix} x_i \\ y_i \end{bmatrix} \leftarrow \begin{bmatrix} \text{PARAM}(2) & 1 \\ -1 & \text{PARAM}(5) \end{bmatrix} \begin{bmatrix} x_i \\ y_i \end{bmatrix} \quad \text{for } i = 1, \ \ldots, N$$

If `PARAM`(1) = 0.0, then the subprograms compute

$$\begin{bmatrix} x_i \\ y_i \end{bmatrix} \leftarrow \begin{bmatrix} 1 & \text{PARAM}(4) \\ \text{PARAM}(3) & 1 \end{bmatrix} \begin{bmatrix} x_i \\ y_i \end{bmatrix} \quad \text{for } i = 1, \ \ldots, N$$

If `PARAM`(1) = 1.0, then the subprograms compute

$$\begin{bmatrix} x_i \\ y_i \end{bmatrix} \leftarrow \begin{bmatrix} \mathrm{PARAM}(2) & \mathrm{PARAM}(4) \\ \mathrm{PARAM}(3) & \mathrm{PARAM}(5) \end{bmatrix} \begin{bmatrix} x_i \\ y_i \end{bmatrix} \quad \text{for } i = 1, \ \ldots, N$$

If $N \le 0$ or if PARAM(1) = −2.0, then the subprograms return immediately. CAUTION: For CSROTM and ZDROTM, the scalar quantities PARAM(*) are real and x and y are complex.

Programming Notes for Level 2 and Level 3 BLAS

For definitions of the matrix data structures used in the discussion below, see *Reference Material*. The Level 2 and Level 3 BLAS, like the Level 1 BLAS, do not follow the IMSL naming conventions. Instead, the names consist of a prefix of one of the letters “S”, “D” , “C” , or “Z”. Next is a root name denoting the kind of matrix. This is followed by a suffix indicating the type of the operation.[1] The prefix denotes the type of operation according to the following table:

S	Real	C	Complex
D	Double	Z	Double Complex

The root names for the kind of matrix:

GE	General	GB	General Band	SP	Symmetric Packed
SY	Symmetric	SB	Symmetric Band	TP	Triangular Packed
HE	Hermitian	HB	Hermitian Band	HP	Hermitian Packed
TR	Triangular	TB	Triangular Band		

The suffixes for the type of operation:

MV	Matrix-Vector Product	SV	Solve for Vector
R	Rank-One Update		
RU	Rank-One Update, Unconjugated	RC	Rank-One Update, Conjugated
R2	Rank-Two Update		
MM	Matrix-Multiply	SM	Symmetric Matrix Multiply
RK	Rank-K Update	R2K	Rank 2K Update

[1]IMSL does not support any extended precision versions of the Level 2 BLAS.

The specifications of the operations are provided by subprogram arguments of CHARACTER*1 data type. Both lower and upper case of the letter have the same meaning:

TRANS, TRANSA, TRANSB	'N'	No Transpose
	'T'	Transpose
	'C'	Conjugage and Transpose
UPLO	'L'	Lower Triangular
	'U'	Upper Triangular
DIAGNL	'N'	Non-unit Triangular
	'U'	Unit Triangular
SIDE	'L'	Multiply "*A*" Matrix on Left side, or
	'R'	Right side of the "*B*" matrix

Note: See the "Triangular Mode" section in the *Reference Material* for definitions of these terms.

Descriptions of the Level 2 and Level 3 BLAS

The subprograms for Level 2 and Level 3 BLAS that perform operations involving the expression βy or βC do not require that the contents of y or C be defined when $\beta = 0$. In that case, the expression βy or βC is defined to be zero. Note that for the _GEMV and _GBMV subprograms, the dimensions of the vectors x and y are implied by the specification of the operation. If TRANS = 'N', the dimension of y is m; if TRANS = 'T' or = 'C', the dimension of y is n. The Level 2 and Level 3 BLAS are summarized in Table 9.2. This table also lists the page numbers where the subprograms are described in more detail.

Specification of the Level 2 BLAS

Type and dimension for variables occurring in the subprogram specifications are

```
INTEGER            INCX, INCY, NCODA, NLCA, NUCA, LDA, M, N
CHARACTER*1        DIAGNL, TRANS, UPLO

REAL               SALPHA, SBETA, SX(*), SY(*), SA(LDA,*)
DOUBLE PRECISION   DALPHA, DBETA, DX(*), DY(*), DA(LDA,*)
COMPLEX            CALPHA, CBETA, CX(*), CY(*), CA(LDA,*)
DOUBLE COMPLEX     ZALPHA, ZBETA, ZX(*), ZY(*), ZA(LDA,*)
```

There is a lower bound on the leading dimension LDA. It must be ≥ the number of rows in the matrix that is contained in this array. Vector arguments have an increment parameter that specifies the storage space or stride between elements. The correspondence between the vector x, y and the arguments SX, SY and INCX, INCY is

$$x_i = \begin{cases} \mathrm{SX}((\mathrm{I}-1) * \mathrm{INCX}+1) & \text{if INCX} > 0 \\ \mathrm{SX}((\mathrm{I}-\mathrm{N}) * \mathrm{INCX}+1) & \text{if INCX} < 0 \end{cases}$$

$$y_i = \begin{cases} \mathrm{SY}((\mathrm{I}-1) * \mathrm{INCY}+1) & \text{if INCY} > 0 \\ \mathrm{SY}((\mathrm{I}-\mathrm{N}) * \mathrm{INCY}+1) & \text{if INCY} < 0 \end{cases}$$

In the Level 2 BLAS, only nonzero values of `INCX`, `INCY` are allowed for operations that have vector arguments. The Level 3 BLAS do not refer to `INCX`, `INCY`.

Specification of the Level 3 BLAS

Type and dimension for variables occurring in the subprogram specifications are

```
INTEGER           K, LDA, LDB, LDC, M, N
CHARACTER*1       DIAGNL, TRANS, TRANSA, TRANSB, SIDE, UPLO
REAL              SALPHA, SBETA, SA(LDA,*), SB(LDB,*), SC(LDC,*)
DOUBLE PRECISION  DALPHA, DBETA, DA(LDA,*), DB(LDB,*), DC(LDC,*)
COMPLEX           CALPHA, CBETA, CA(LDA,*), CB(LDB,*), CC(LDC,*)
DOUBLE COMPLEX    ZALPHA, ZBETA, ZA(LDA,*), ZB(LDB,*), ZC(LDC,*)
```

Each of the integers `K`, `M`, `N` must be ≥ 0. It is an error if any of them are < 0. If any of them are = 0, the subprograms return immediately. There are lower bounds on the leading dimensions `LDA`, `LDB`, `LDC`. Each must be ≥ the number of rows in the matrix that is contained in this array.

describes the Level 2 and 3 BLAS subprograms.

Table 7 – Level 2 and Level 3 Basic Linear Algebra Subprograms –

Operation	Real	Double	Complex	Double-Complex
Matrix–Vector Multiply, General	SGEMV	DGEMV	CGEMV	ZGEMV
Matrix–Vector Multiply, Banded	SGBMV	DGBMV	CGBMV	ZGBMV
Matrix-Vector Multiply, Hermitian			CHEMV	ZHEMV
Matrix-Vector Multiply, Packed Hermitian			CHPMV	ZHPMV
Matrix-Vector Multiply, Hermitian and Banded			CHBMV	ZHBMV
Matrix-Vector Multiply, Symmetric and Real	SSYMV	DSYMV		
Matrix-Vector Multiply, Packed Symmetric and Real	SSPMV	DSPMV		
Matrix-Vector Multiply, Symmetric and Banded	SSBMV	DSBMV		
Matrix-Vector Multiply, Triangular	STRMV	DTRMV	CTRMV	ZTRMV

Table 7 – Level 2 and Level 3 Basic Linear Algebra Subprograms –

Operation	Real	Double	Complex	Double-Complex
Matrix-Vector Multiply, Packed Triangular	STPMV	DTPMV	CTPMV	ZTPMV
Matrix-Vector Multiply, Triangular and Banded	STBMV	DTBMV	CTBMV	ZTBMV
Matrix-Vector Solve, Triangular	STRSV	DTRSV	CTRSV	ZTRSV
Matrix-Vector Solve, Triangular and Banded	STBSV	DTBSV	CTBSV	ZTBSV
Matrix-Vector Solve, Packed Triangular	STPSV	DTPSV	CTPSV	ZTPSV
Rank-One Matrix Update, General and Real	SGER	DGER		
Rank-One Matrix Update, General, Complex, and Transpose			CGERU	ZGERU
Rank-One Matrix Update, General, Complex, and Conjugate Transpose			CGERC	ZGERC
Rank-Two Matrix Update, Hermitian and Conjugate Transpose			CHER	ZHER
Rank-Two Matrix Update, Hermitian and Conjugate Transpose			CHER2	ZHER2
Rank-Two Matrix Update, Packed Hermitian and Conjugate Transpose			CHPR2	ZHPR2
Rank-One Matrix Update, Symmetric and Real	SSYR	DSYR		
Rank-One Matrix Update, Packed Symmetric and Real	SSPR	DSPR		
Rank-One Matrix Update, Packed Hermitian and Conjugate Transpose			CHPR	ZHPR
Rank-Two Matrix Update, Symmetric and Real	SSYR2	DSYR2		
Rank-Two Matrix Update, Packed Symmetric and Real	SSPR2	DSPR2		
Matrix-Matrix Multiply, General	SGEMM	DGEMM	CGEMM	ZGEMM
Matrix-Matrix Multiply, Symmetric	SSYMM	DSYMM	CSYMM	ZSYMM
Matrix-Matrix Multiply, Hermitian			CHEMM	ZHEMM
Rank-k Update, Symmetric	SSYRK	DSYRK	CSYRK	ZSYRK
Rank-k Update, Hermitian			CHERK	ZHERK
Rank-2k, Symmetric	SSYR2K	DSYR2K	CSYR2K	ZSYR2K
Rank-2k, Hermitian			CHER2K	ZHER2K

Table 7 – Level 2 and Level 3 Basic Linear Algebra Subprograms –

Operation	Real	Double	Complex	Double-Complex
Matrix-Matrix Multiply, Triangular	STRMM	DTRMM	CTRMM	ZTRMM
Matrix-Matrix Solve, Triangular	STRSM	DTRSM	CTRSM	ZTRSM

Matrix–Vector Multiply, General

```
CALL SGEMV (TRANS, M, N, SALPHA, SA, LDA, SX, INCX, SBETA, SY, INCY)
CALL DGEMV (TRANS, M, N, DALPHA, DA, LDA, DX, INCX, DBETA, DY, INCY)
CALL CGEMV (TRANS, M, N, CALPHA, CA, LDA, CX, INCX, CBETA, CY, INCY)
CALL ZGEMV (TRANS, M, N, ZALPHA, ZA, LDA, ZX, INCX, ZBETA, ZY, INCY)
```

For all data types, A is an $M \times N$ matrix. These subprograms set y to one of the expressions: $y \leftarrow \alpha Ax + \beta y$, $y \leftarrow \alpha A^T x + \beta y$, or for complex data,

$$y \leftarrow \alpha \overline{A}^T + \beta y$$

The character flag `TRANS` determines the operation.

Matrix–Vector Multiply, Banded

```
CALL SGBMV (TRANS, M, N, NLCA, NUCA SALPHA, SA, LDA, SX, INCX, SBETA, SY, INCY)
CALL DGBMV (TRANS, M, N, NLCA, NUCA DALPHA, DA, LDA, DX, INCX, DBETA, DY, INCY)
CALL CGBMV (TRANS, M, N, NLCA, NUCA CALPHA, CA, LDA, CX, INCX, BETA, CY, INCY)
CALL ZGBMV (TRANS, M, N, NLCA, NUCA ZALPHA, ZA, LDA, ZX, INCX, ZBETA, ZY, INCY)
```

For all data types, A is an $M \times N$ matrix with `NLCA` lower codiagonals and `NUCA` upper codiagonals. The matrix is stored in band storage mode. These subprograms set y to one of the expressions: $y \leftarrow \alpha Ax + \beta y$, $y \leftarrow \alpha A^T x + \beta y$, or for complex data,

$$y \leftarrow \alpha \overline{A}^T x + \beta y$$

The character flag `TRANS` determines the operation.

Matrix-Vector Multiply, Hermitian

```
CALL CHEMV (UPLO, N, CALPHA, CA, LDA, CX, INCX, CBETA, CY, INCY)
CALL ZHEMV (UPLO, N, ZALPHA, ZA, LDA, ZX, INCX, ZBETA, ZY, INCY)
```

For complex types, A is an $N \times N$ matrix. These subprograms set $y \leftarrow \alpha Ax + \beta y$, where A is an Hermitian matrix. The matrix A is either referenced using the upper or lower triangular part. The character flag `UPLO` determines the part used.

Matrix-Vector Multiply, Packed Hermitian

```
CALL CHPMV (UPLO, N, CALPHA, CAP, CX, INCX, CBETA, CY, INCY)
CALL ZHPMV (UPLO, N, ZALPHA, ZAP, ZX, INCX, ZBETA, ZY, INCY)
```

For complex types, A is an $N \times N$ matrix. These subprograms set $y \leftarrow \alpha Ax + \beta y$, where A is an Hermitian matrix. The matrix A is either referenced using the packed upper or lower triangular part. The character flag `UPLO` determines the part used.

Matrix-Vector Multiply, Hermitian and Banded

```
CALL CHBMV (UPLO, N, NCODA, CALPHA, CA, LDA, CX, INCX, CBETA, CY, INCY)
CALL ZHBMV (UPLO, N, NCODA, ZALPHA, ZA, LDA, ZX, INCX, ZBETA, ZY, INCY)
```

For all data types, A is an $N \times N$ matrix with `NCODA` codiagonals. The matrix is stored in band Hermitian storage mode. These subprograms set $y \leftarrow \alpha Ax + \beta y$. The matrix A is either referenced using its upper or lower triangular part. The character flag `UPLO` determines the part used.

Matrix-Vector Multiply, Symmetric and Real

```
CALL SSYMV (UPLO, N, SALPHA, SA, LDA, SX, INCX, SBETA, SY, INCY)
CALL DSYMV (UPLO, N, DALPHA, DA, LDA, DX, INCX, DBETA, DY, INCY)
```

For all data types, A is an $N \times N$ matrix. These subprograms set $y \leftarrow \alpha Ax + \beta y$, where A is a symmetric matrix. The matrix A is either referenced using the upper or lower triangular part. The character flag `UPLO` determines the part used.

Matrix-Vector Multiply, Packed Symmetric and Real

```
CALL SSPMV (UPLO, N, SALPHA, SAP,  SX, INCX, SBETA, SY, INCY)
CALL DSPMV (UPLO, N, DALPHA, DAP,  DX, INCX, DBETA, DY, INCY)
```

For all data types, A is an $N \times N$ matrix. These subprograms set $y \leftarrow \alpha Ax + \beta y$, where A is a *packed triangular matrix*. The matrix A is either referenced using the packed upper or lower triangular part. The character flag `UPLO` determines the part used.

Matrix-Vector Multiply, Symmetric and Banded

```
CALL SSBMV (UPLO, N, NCODA, SALPHA, SA, LDA, SX, INCX, SBETA, SY, INCY)
CALL DSBMV (UPLO, N, NCODA, DALPHA, DA, LDA, DX, INCX, DBETA, DY, INCY)
```

For all data types, A is an $N \times N$ matrix with `NCODA` codiagonals. The matrix is stored in band symmetric storage mode. These subprograms set $y \leftarrow \alpha Ax + \beta y$. The matrix A is either referenced using its upper or lower triangular part. The character flag `UPLO` determines the part used.

Matrix-Vector Multiply, Triangular

```
CALL STRMV (UPLO, TRANS, DIAGNL, N, SA, LDA, SX, INCX)
CALL DTRMV (UPLO, TRANS, DIAGNL, N, DA, LDA, DX, INCX)
CALL CTRMV (UPLO, TRANS, DIAGNL, N, CA, LDA, CX, INCX)
CALL ZTRMV (UPLO, TRANS, DIAGNL, N, ZA, LDA, ZX, INCX)
```

For all data types, A is an $N \times N$ triangular matrix. These subprograms set x to one of the expressions: $x \leftarrow Ax$, $x \leftarrow A^T x$, or for complex data,

$$x \leftarrow \overline{A}^T x$$

The matrix A is either referenced using its upper or lower triangular part and is unit or nonunit triangular. The character flags `UPLO`, `TRANS`, and `DIAGNL` determine the part of the matrix used and the operation performed.

Matrix-Vector Multiply, Packed Triangular

```
CALL STPMV (UPLO, TRANS, DIAGNL, N, SAP, SX, INCX)
CALL DTPMV (UPLO, TRANS, DIAGNL, N, DAP, DX, INCX)
CALL CTPMV (UPLO, TRANS, DIAGNL, N, CAP, CX, INCX)
CALL ZTPMV (UPLO, TRANS, DIAGNL, N, ZAP, ZX, INCX)
```

For all data types, A is an $N \times N$ *packed triangular matrix*. These subprograms set x to one of the expressions: $x \leftarrow Ax$, $x \leftarrow A^T x$, or for complex data,

$$x \leftarrow \overline{A}^T x$$

The matrix A is either referenced using the packed upper or lower triangular part and is unit or nonunit triangular. The character flags `UPLO`, `TRANS`, and `DIAGNL` determine the part of the matrix used and the operation performed.

Matrix-Vector Multiply, Triangular and Banded

```
CALL STBMV (UPLO, TRANS, DIAGNL, N, NCODA, SA, LDA, SX, INCX)
CALL DTBMV (UPLO, TRANS, DIAGNL, N, NCODA, DA, LDA, DX, INCX)
CALL CTBMV (UPLO, TRANS, DIAGNL, N, NCODA, CA, LDA, CX, INCX)
CALL ZTBMV (UPLO, TRANS, DIAGNL, N, NCODA, ZA, LDA, ZX, INCX)
```

For all data types, A is an $N \times N$ matrix with `NCODA` codiagonals. The matrix is stored in band triangular storage mode. These subprograms set x to one of the expressions: $x \leftarrow Ax$, $x \leftarrow A^T x$, or for complex data,

$$x \leftarrow \overline{A}^T x$$

The matrix A is either referenced using its upper or lower triangular part and is unit or nonunit triangular. The character flags `UPLO`, `TRANS`, and `DIAGNL` determine the part of the matrix used and the operation performed.

Matrix-Vector Solve, Triangular

```
CALL STRSV (UPLO, TRANS, DIAGNL, N, SA, LDA, SX, INCX)
CALL DTRSV (UPLO, TRANS, DIAGNL, N, DA, LDA, DX, INCX)
CALL CTRSV (UPLO, TRANS, DIAGNL, N, CA, LDA, CX, INCX)
CALL ZTRSV (UPLO, TRANS, DIAGNL, N, ZA, LDA, ZX, INCX)
```

For all data types, A is an $N \times N$ triangular matrix. These subprograms solve x for one of the expressions: $x \leftarrow A^{-1}x$, $x \leftarrow (A^{-1})^{T}x$, or for complex data,

$$x \leftarrow \left(\overline{A}^{T}\right)^{-1} x \equiv \left(A^{H}\right)^{-1} x$$

The matrix A is either referenced using its upper or lower triangular part and is unit or nonunit triangular. The character flags `UPLO`, `TRANS`, and `DIAGNL` determine the part of the matrix used and the operation performed.

Matrix-Vector Solve, Triangular and Banded

```
CALL STBSV (UPLO, TRANS, DIAGNL, N, NCODA, SA, LDA, SX, INCX)
CALL DTBSV (UPLO, TRANS, DIAGNL, N, NCODA, DA, LDA, DX, INCX)
CALL CTBSV (UPLO, TRANS, DIAGNL, N, NCODA, CA, LDA, CX, INCX)
CALL ZTBSV (UPLO, TRANS, DIAGNL, N, NCODA, ZA, LDA, ZX, INCX)
```

For all data types, A is an $N \times N$ triangular matrix with `NCODA` codiagonals. The matrix is stored in band triangular storage mode. These subprograms solve x for one of the expressions: $x \leftarrow A^{-1}x$, $x \leftarrow (A^{-T})^{-1}x$, or for complex data,

$$x \leftarrow \left(\overline{A}^{T}\right)^{-1} x \equiv \left(A^{H}\right)^{-1} x$$

The matrix A is either referenced using its upper or lower triangular part and is unit or nonunit triangular. The character flags `UPLO`, `TRANS`, and `DIAGNL` determine the part of the matrix used and the operation performed.

Matrix-Vector Solve, Packed Triangular

```
CALL STPSV (UPLO, TRANS, DIAGNL, N, SAP, SX, INCX)
CALL DTPSV (UPLO, TRANS, DIAGNL, N, DAP, DX, INCX)
CALL CTPSV (UPLO, TRANS, DIAGNL, N, CAP, CX, INCX)
CALL ZTPSV (UPLO, TRANS, DIAGNL, N, ZAP, ZX, INCX)
```

For all data types, A is an $N \times N$ *packed triangular matrix*. These subprograms solve x for one of the expressions: $x \leftarrow A^{-1}x$, $x \leftarrow (A^{-1})^{T}x$, or for complex data,

$$x \leftarrow \left(\overline{A}^{T}\right)^{-1} x \equiv \left(A^{H}\right)^{-1} x$$

The matrix A is either referenced using its packed upper or lower triangular part and is unit or nonunit triangular. The character flags `UPLO`, `TRANS`, and `DIAGNL` determine the part of the matrix used and the operation performed.

Rank-One Matrix Update, General and Real

```
CALL SGER (M, N, SALPHA, SX, INCX, SY, INCY, SA, LDA)
CALL DGER (M, N, DALPHA, DX, INCX, DY, INCY, DA, LDA)
```

For all data types, A is an $M \times N$ matrix. These subprograms set $A \leftarrow A + \alpha xy^T$.

Rank-One Matrix Update, General, Complex, and Transpose

```
CALL CGERU (M, N, CALPHA, CX, INCX, CY, INCY, CA, LDA)
CALL ZGERU (M, N, ZALPHA, ZX, INCX, ZY, INCY, ZA, LDA)
```

For all data types, A is an $M \times N$ matrix. These subprograms set $A \leftarrow A + \alpha xy^T$.

Rank-One Matrix Update, General, Complex, and Conjugate Transpose

```
CALL CGERC (M, N, CALPHA, CX, INCX, CY, INCY, CA, LDA)
CALL ZGERC (M, N, ZALPHA, ZX, INCX, ZY, INCY, ZA, LDA)
```

For all data types, A is an $M \times N$ matrix. These subprograms set

$$A \leftarrow A + \alpha x\overline{y}^T$$

Rank-One Matrix Update, Hermitian and Conjugate Transpose

```
CALL CHER (UPLO, N, SALPHA, CX, INCX, CA, LDA)
CALL ZHER (UPLO, N, DALPHA, ZX, INCX, ZA, LDA)
```

For all data types, A is an $N \times N$ matrix. These subprograms set

$$A \leftarrow A + \alpha x\overline{x}^T$$

where A is Hermitian. The matrix A is either referenced by its upper or lower triangular part. The character flag `UPLO` determines the part used. CAUTION: Notice the scalar parameter α is real, and the data in the matrix and vector are complex.

Rank-One Matrix Update, Packed Hermitian and Conjugate Transpose

```
CALL CHPR (UPLO, N, SALPHA, CX, INCX, CAP)
CALL ZHPR (UPLO, N, DALPHA, ZX, INCX, ZAP)
```

For all data types, A is an $N \times N$ matrix. These subprograms set

$$A \leftarrow A + \alpha x\overline{x}^T$$

where A is *packed Hermitian*. The matrix A is either referenced by its upper or lower triangular part. The character flag `UPLO` determines the part used. CAUTION: Notice the scalar parameter α is real, and the data in the matrix and vector are complex.

Rank-Two Matrix Update, Hermitian and Conjugate Transpose

```
CALL CHER2 (UPLO, N, CALPHA, CX, INCX, CY, INCY, CA, LDA)
CALL ZHER2 (UPLO, N, ZALPHA, ZX, INCX, ZY, INCY, ZA, LDA)
```

For all data types, A is an $N \times N$ matrix. These subprograms set

$$A \leftarrow A + \alpha x \overline{y}^T + \overline{\alpha} y \overline{x}^T$$

where A is an Hermitian matrix. The matrix A is either referenced by its upper or lower triangular part. The character flag `UPLO` determines the part used.

Rank-Two Matrix Update, Packed Hermitian and Conjugate Transpose

```
CALL CHPR2 (UPLO, N, CALPHA, CX, INCX, CY, INCY, CAP)
CALL ZHPR2 (UPLO, N, ZALPHA, ZX, INCX, ZY, INCY, ZAP)
```

For all data types, A is an $N \times N$ matrix. These subprograms set

$$A \leftarrow A + \alpha x \overline{y}^T + \overline{\alpha} y \overline{x}^T$$

where A is a packed Hermitian matrix. The matrix A is either referenced by its upper or lower triangular part. The character flag `UPLO` determines the part used.

Rank-One Matrix Update, Symmetric and Real

```
CALL SSYR (UPLO, N, SALPHA, SX, INCX, SA, LDA)
CALL DSYR (UPLO, N, DALPHA, DX, INCX, DA, LDA)
```

For all data types, A is an $N \times N$ matrix. These subprograms set $A \leftarrow A + \alpha x x^T$ where A is a symmetric matrix. The matrix A is either referenced by its upper or lower triangular part. The character flag `UPLO` determines the part used.

Rank-One Matrix Update, Packed Symmetric and Real

```
CALL SSPR (UPLO, N, SALPHA, SX, INCX, SAP)
CALL DSPR (UPLO, N, DALPHA, DX, INCX, DAP)
```

For all data types, A is an $N \times N$ matrix. These subprograms set $A \leftarrow A + \alpha x x^T$ where A is a packed symmetric matrix. The matrix A is either referenced using the packed upper or lower triangular part. The character flag `UPLO` determines the part used.

Rank-One Matrix Update, Packed Hermitian

```
CALL CHPR (UPLO, N, SALPHA, CX, INCX, CAP)
CALL ZHPR (UPLO, N, DALPHA, ZX, INCX, ZAP)
```

For all data types, A is an $N \times N$ matrix. These subprograms set $A \leftarrow A + \alpha x x^T$ where A is a *packed Hermitian* matrix. The matrix A is either referenced using the packed upper or lower triangular part. The character flag `UPLO` determines the part used.

Rank-Two Matrix Update, Symmetric and Real

```
CALL SSYR2 (UPLO, N, SALPHA, SX, INCX, SY, INCY, SA, LDA)
CALL DSYR2 (UPLO, N, DALPHA, DX, INCX, DY, INCY, DA, LDA)
```

For all data types, A is an $N \times N$ matrix. These subprograms set $A \leftarrow A + \alpha x y^T + \alpha y x^T$, where A is a symmetric matrix. The matrix A is referenced by its upper or lower triangular part. The character flag `UPLO` determines the part used.

Rank-Two Matrix Update, Packed Symmetric and Real

```
CALL SSPR2 (UPLO, N, SALPHA, SX, INCX, SY, INCY, SAP)
CALL DSPR2 (UPLO, N, DALPHA, DX, INCX, DY, INCY, DAP)
```

For all data types, A is an $N \times N$ matrix. These subprograms set $A \leftarrow A + \alpha x y^T + \alpha y x^T$, where A is a packed symmetric matrix. The matrix A is referenced by its upper or lower triangular part. The character flag `UPLO` determines the part used.

Matrix-Matrix Multiply, General

```
CALL SGEMM (TRANSA, TRANSB, M, N, K, SALPHA, SA, LDA, SB, LDB, SBETA, SC, LDC)
CALL DGEMM (TRANSA, TRANSB, M, N, K, DALPHA, DA, LDA, DB, LDB, DBETA, DC, LDC)
CALL CGEMM (TRANSA, TRANSB, M, N, K, CALPHA, CA, LDA, CB, LDB, CBETA, CC, LDC)
CALL ZGEMM (TRANSA, TRANSB, M, N, K, ZALPHA, ZA, LDA, ZB, LDB, ZBETA, ZC, LDC)
```

For all data types, these subprograms set $C_{M \times N}$ to one of the expressions:

$$C \leftarrow \alpha AB + \beta C,\ C \leftarrow \alpha A^T B + \beta C,\ C \leftarrow \alpha AB^T + \beta C,\ C \leftarrow \alpha A^T B^T + \beta C,$$
$$\text{or for complex data, } C \leftarrow \alpha A\overline{B}^T + \beta C,\ C \leftarrow \alpha \overline{A}^T B + \beta C,\ C \leftarrow \alpha A^T \overline{B}^T + \beta C,$$
$$C \leftarrow \alpha \overline{A}^T B^T + \beta C,\ C \leftarrow \alpha \overline{A}^T \overline{B}^T + \beta C$$

The character flags `TRANSA` and `TRANSB` determine the operation to be performed. Each matrix product has dimensions that follow from the fact that C has dimension $M \times N$.

Matrix-Matrix Multiply, Symmetric

```
CALL SSYMM (SIDE, UPLO, M, N, SALPHA, SA, LDA, SB, LDB, SBETA, SC, LDC)
CALL DSYMM (SIDE, UPLO, M, N, DALPHA, DA, LDA, DB, LDB, DBETA, DC, LDC)
CALL CSYMM (SIDE, UPLO, M, N, CALPHA, CA, LDA, CB, LDB, CBETA, CC, LDC)
CALL ZSYMM (SIDE, UPLO, M, N, ZALPHA, ZA, LDA, ZB, LDB, ZBETA, ZC, LDC)
```

For all data types, these subprograms set $C_{M \times N}$ to one of the expressions: $C \leftarrow \alpha AB + \beta C$ or $C \leftarrow \alpha BA + \beta C$, where A is a symmetric matrix. The matrix A is referenced either by its upper or lower triangular part. The character flags `SIDE` and `UPLO` determine the part of the matrix used and the operation performed.

Matrix-Matrix Multiply, Hermitian

```
CALL CHEMM  (SIDE, UPLO, M, N, CALPHA, CA, LDA, CB, LDB, CBETA, CC, LDC)
CALL ZHEMM (SIDE, UPLO, M, N, ZALPHA, ZA, LDA, ZB, LDB, ZBETA, ZC, LDC)
```

For all data types, these subprograms set $C_{M \times N}$ to one of the expressions: $C \leftarrow \alpha AB + \beta C$ or $C \leftarrow \alpha BA + \beta C$, where A is an Hermitian matrix. The matrix A is referenced either by its upper or lower triangular part. The character flags `SIDE` and `UPLO` determine the part of the matrix used and the operation performed.

Rank-*k* Update, Symmetric

```
CALL SSYRK (UPLO, TRANS, N, K, SALPHA, SA, LDA, SBETA, SC, LDC)
CALL DSYRK (UPLO, TRANS, N, K, DALPHA, DA, LDA, DBETA, DC, LDC)
CALL CSYRK (UPLO, TRANS, N, K, CALPHA, CA, LDA, CBETA, CC, LDC)
CALL ZSYRK (UPLO, TRANS, N, K, ZALPHA, ZA, LDA, ZBETA, ZC, LDC)
```

For all data types, these subprograms set $C_{M \times N}$ to one of the expressions: $C \leftarrow \alpha AA^T + \beta C$ or $C \leftarrow \alpha A^T A + \beta C$. The matrix C is referenced either by its upper or lower triangular part. The character flags `UPLO` and `TRANS` determine the part of the matrix used and the operation performed. In subprogram `CSYRK` and `ZSYRK`, only values `'N'` or `'T'` are allowed for `TRANS`; `'C'` is not acceptable.

Rank-*k* Update, Hermitian

```
CALL CHERK  (UPLO, TRANS, N, K, SALPHA, CA, LDA, SBETA, CC, LDC)
CALL ZHERK (UPLO, TRANS, N, K, DALPHA, ZA, LDA, DBETA, ZC, LDC)
```

For all data types, these subprograms set $C_{N \times N}$ to one of the expressions:

$$C \leftarrow \alpha A\overline{A}^T + \beta C \text{ or } C \leftarrow \alpha \overline{A}^T A + \beta C$$

The matrix C is referenced either by its upper or lower triangular part. The character flags `UPLO` and `TRANS` determine the part of the matrix used and the operation performed. CAUTION: Notice the scalar parameters α and β are real, and the data in the matrices are complex. Only values `'N'` or `'C'` are allowed for `TRANS`; `'T'` is not acceptable.

Rank-2k, Symmetric

```
CALL SSYR2K  (UPLO, TRANS, N, K, SALPHA, SA, LDA, SB, LDB, SBETA, SC, LDC)
CALL DSYR2K (UPLO, TRANS, N, K, DALPHA, DA, LDA, DB, LDB, DBETA, DC, LDC)
CALL CSYR2K (UPLO, TRANS, N, K, CALPHA, CA, LDA, CB, LDB, CBETA, CC, LDC)
CALL ZSYR2K (UPLO, TRANS, N, K, ZALPHA, ZA, LDA, ZB, LDB, ZBETA, ZC, LDC)
```

For all data types, these subprograms set $C_{N \times N}$ to one of the expressions:

$$C \leftarrow \alpha AB^T + \alpha\beta A^T + \beta C \text{ or } C \leftarrow \alpha A^T B + \alpha B^T A + \beta C$$

The matrix C is referenced either by its upper or lower triangular part. The character flags UPLO and TRANS determine the part of the matrix used and the operation performed. In subprogram CSYR2K and ZSYR2K, only values 'N' or 'T' are allowed for TRANS; 'C' is not acceptable.

Rank-2k, Hermitian

```
CALL CHER2K (UPLO, TRANS, N, K, CALPHA, CA, LDA, CB, LDB, SBETA, CC, LDC)
CALL ZHER2K (UPLO, TRANS, N, K, ZALPHA, ZA, LDA, ZB, LDB, DBETA, ZC, LDC)
```

For all data types, these subprograms set $C_{N \times N}$ to one of the expressions:

$$C \leftarrow \alpha A\overline{B}^T + \overline{\alpha} B\overline{A}^T + \beta C \text{ or } C \leftarrow \alpha \overline{A}^T B + \overline{\alpha}\overline{B}^T A + \beta C$$

The matrix C is referenced either by its upper or lower triangular part. The character flags UPLO and TRANS determine the part of the matrix used and the operation performed. CAUTION: Notice the scalar parameter β is real, and the data in the matrices are complex. In subprogram CHER2K and ZHER2K, only values 'N' or 'C' are allowed for TRANS; 'T' is not acceptable.

Matrix-Matrix Multiply, Triangular

```
CALL STRMM  (SIDE, UPLO, TRANSA, DIAGNL, M, N, SALPHA, SA, LDA, SB, LDB)
CALL DTRMM (SIDE, UPLO, TRANSA, DIAGNL, M, N, DALPHA, DA, LDA, DB, LDB)
CALL CTRMM (SIDE, UPLO, TRANSA, DIAGNL, M, N, CALPHA, CA, LDA, CB,LDB)
CALL ZTRMM (SIDE, UPLO, TRANSA, DIAGNL, M, N, ZALPHA, ZA, LDA, ZB, LDB)
```

For all data types, these subprograms set $B_{M \times N}$ to one of the_expressions:

$$B \leftarrow \alpha AB,\ B \leftarrow \alpha A^T B,\ B \leftarrow \alpha BA,\ B \leftarrow \alpha BA^T,$$

or for complex data,

$$B \leftarrow \alpha \overline{A}^T B, \text{ or } B \leftarrow \alpha B\overline{A}^T$$

where A is a triangular matrix. The matrix A is either referenced using its upper or lower triangular part and is unit or nonunit triangular. The character flags SIDE, UPLO, TRANSA, and DIAGNL determine the part of the matrix used and the operation performed.

Matrix-Matrix Solve, Triangular

```
CALL STRSM  (SIDE, UPLO, TRANSA, DIAGNL, M, N, SALPHA, SA, LDA, SB, LDB)
CALL DTRSM (SIDE, UPLO, TRANSA, DIAGNL, M, N, DALPHA, DA, LDA, DB, LDB)
CALL CTRSM (SIDE, UPLO, TRANSA, DIAGNL, M, N, CALPHA, CA, LDA, CB, LDB)
CALL ZTRSM (SIDE, UPLO, TRANSA, DIAGNL, M, N, ZALPHA, ZA, LDA, ZB, LDB)
```

For all data types, these subprograms set $B_{\boldsymbol{M}\times\boldsymbol{N}}$ to one of the expressions:

$$B \leftarrow \alpha A^{-1}B,\ B \leftarrow \alpha BA^{-1},\ B \leftarrow \alpha\left(A^{-1}\right)^{T}B,\ B \leftarrow \alpha B\left(A^{-1}\right)^{T},$$

or for complex data,

$$B \leftarrow \alpha\left(\overline{A}^{T}\right)^{-1}B, \text{ or } B \leftarrow \alpha B\left(\overline{A}^{T}\right)^{-1}$$

where A is a triangular matrix. The matrix A is either referenced using its upper or lower triangular part and is unit or nonunit triangular. The character flags `SIDE`, `UPLO`, `TRANSA`, and `DIAGNL` determine the part of the matrix used and the operation performed.

Other Matrix/Vector Operations

This section describes a set of routines for matrix/vector operations. The matrix copy and conversion routines are summarized by the following table:

	To			
From	**Real General**	**Complex General**	**Real Band**	**Complex Band**
Real General	CRGRG	CRGCG	CRGRB	
Complex General		CCGCG		CCGCB
Real Band	CRBRG		CRBRB	CRBCB
Complex Band		CCBCG		CCBCB
Symmetric Full	CSFRG			
Hermitian Full		CHFCG		
Symmetric Band			CSBRB	
Hermitian Band				CHBCB

The matrix multiplication routines are summarized as follows:

AB	***A***			
B	**Real Rectangular**	**Complex Rectangular**	**Real Band**	**Complex Band**
Real Rectangular	MRRRR			
Complex Rect.		MCRCR		
Vector	MURRV	MUCRV	MURBV	MUCBV

The matrix norm routines are summarized as follows:

$\|\|A\|\|$	**Real Rectangular**	**Real Band**	**Complex Band**
∞-norm	NRIRR		
1-norm	NR1RR	NR1RB	NR1CB
Frobenius	NR2RR		

CRGRG

Copies a real general matrix.

Required Arguments

A — Matrix of order `N`. (Input)

B — Matrix of order `N` containing a copy of `A`. (Output)

Optional Arguments

N — Order of the matrices. (Input)
Default: `N` = `SIZE` (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = `SIZE` (`A`,1).

LDB — Leading dimension of `B` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDB` = `SIZE` (`B`,1).

FORTRAN 90 Interface

Generic: `CALL CRGRG (A, B [, …])`

Specific: The specific interface names are `S_CRGRG` and `D_CRGRG`.

FORTRAN 77 Interface

Single: `CALL CRGRG (N, A, LDA, B, LDB)`

Double: The double precision name is `DCRGRG`.

Description

The routine `CRGRG` copies the real $N \times N$ general matrix A into the real $N \times N$ general matrix B.

Example

A real 3 × 3 general matrix is copied into another real 3 × 3 general matrix.

```
      USE CRGRG_INT
      USE WRRRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    LDA, LDB, N
      PARAMETER  (LDA=3, LDB=3, N=3)
!
      REAL       A(LDA,N), B(LDB,N)
!                                 Set values for  A
!                                 A = (   0.0   1.0   1.0  )
!                                     (  -1.0   0.0   1.0  )
!                                     (  -1.0  -1.0   0.0  )
!
      DATA A/0.0, 2* - 1.0, 1.0, 0.0, -1.0, 2*1.0, 0.0/
!                                 Copy real matrix A to real matrix B
      CALL CRGRG (A, B)
!                                 Print results
      CALL WRRRN ('B', B)
      END
```

Output

```
            B
        1        2        3
1   0.000    1.000    1.000
2  -1.000    0.000    1.000
3  -1.000   -1.000    0.000
```

CCGCG

Copies a complex general matrix.

Required Arguments

A — Complex matrix of order `N`. (Input)

B — Complex matrix of order `N` containing a copy of `A`. (Output)

Optional Arguments

N — Order of the matrices `A` and `B`. (Input)
Default: `N` = `SIZE` (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = `SIZE` (`A`,1).

LDB — Leading dimension of `B` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDB` = `SIZE` (`B`,1).

FORTRAN 90 Interface

Generic: `CALL CCGCG (A, B [, …])`

Specific: The specific interface names are `S_CCGCG` and `D_CCGCG`.

FORTRAN 77 Interface

Single: `CALL CCGCG (N, A, LDA, B, LDB)`

Double: The double precision name is `DCCGCG`.

Description

The routine `CCGCG` copies the complex $N \times N$ general matrix A into the complex $N \times N$ general matrix B.

Example

A complex 3 × 3 general matrix is copied into another complex 3 × 3 general matrix.

```
      USE CCGCG_INT
      USE WRCRN_INT

      IMPLICIT   NONE
!                                   Declare variables
      INTEGER    LDA, LDB, N
      PARAMETER  (LDA=3, LDB=3, N=3)
!
      COMPLEX    A(LDA,N), B(LDB,N)
!                             Set values for  A
!                             A = (  0.0+0.0i  1.0+1.0i  1.0+1.0i  )
!                                 ( -1.0-1.0i  0.0+0.0i  1.0+1.0i  )
!                                 ( -1.0-1.0i -1.0-1.0i  0.0+0.0i  )
!
      DATA A/(0.0,0.0), 2*(-1.0,-1.0), (1.0,1.0), (0.0,0.0), &
          (-1.0,-1.0), 2*(1.0,1.0), (0.0,0.0)/
!                                   Copy matrix A to matrix B
      CALL CCGCG (A, B)
!                                   Print results
      CALL WRCRN ('B', B)
      END
```

Output

```
                         B
              1                 2                 3
1  ( 0.000, 0.000)  ( 1.000, 1.000)  ( 1.000, 1.000)
2  (-1.000,-1.000)  ( 0.000, 0.000)  ( 1.000, 1.000)
3  (-1.000,-1.000)  (-1.000,-1.000)  ( 0.000, 0.000)
```

CRBRB

Copies a real band matrix stored in band storage mode.

Required Arguments

A — Real band matrix of order N. (Input)

NLCA — Number of lower codiagonals in A. (Input)

NUCA — Number of upper codiagonals in A. (Input)

B — Real band matrix of order N containing a copy of A. (Output)

NLCB — Number of lower codiagonals in B. (Input)
NLCB must be at least as large as NLCA.

NUCB — Number of upper codiagonals in B. (Input)
NUCB must be at least as large as NUCA.

Optional Arguments

N — Order of the matrices A and B. (Input)
Default: N = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = SIZE (A,1).

LDB — Leading dimension of B exactly as specified in the dimension statement of the calling program. (Input)
Default: LDB = SIZE (B,1).

FORTRAN 90 Interface

Generic: CALL CRBRB (A, NLCA, NUCA, B, NLCB, NUCB [, …])

Specific: The specific interface names are S_CRBRB and D_CRBRB.

FORTRAN 77 Interface

Single: CALL CRBRB (N, A, LDA, NLCA, NUCA, B, LDB, NLCB, NUCB)

Double: The double precision name is DCRBRB.

Description

The routine CRBRB copies the real band matrix *A* in band storage mode into the real band matrix *B* in band storage mode.

Example

A real band matrix of order 3, in band storage mode with one upper codiagonal, and one lower codiagonal is copied into another real band matrix also in band storage mode.

```
      USE CRBRB_INT
      USE WRRRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    LDA, LDB, N, NLCA, NLCB, NUCA, NUCB
      PARAMETER  (LDA=3, LDB=3, N=3, NLCA=1, NLCB=1, NUCA=1, NUCB=1)
!
      REAL       A(LDA,N), B(LDB,N)
!                                 Set values for  A (in band mode)
!                                 A = (  0.0  1.0   1.0  )
!                                     (  1.0  1.0   1.0  )
!                                     (  1.0  1.0   0.0  )
!
      DATA A/0.0, 7*1.0, 0.0/
!                                 Copy A to B
      CALL CRBRB (A, NLCA, NUCA, B, NLCB, NUCB)
!                                 Print results
      CALL WRRRN ('B', B)
      END
```

Output

```
            B
        1       2       3
1   0.000   1.000   1.000
2   1.000   1.000   1.000
3   1.000   1.000   0.000
```

CCBCB

Copies a complex band matrix stored in complex band storage mode.

Required Arguments

A — Complex band matrix of order `N`. (Input)

NLCA — Number of lower codiagonals in `A`. (Input)

NUCA — Number of upper codiagonals in `A`. (Input)

B — Complex matrix of order `N` containing a copy of `A`. (Output)

NLCB — Number of lower codiagonals in `B`. (Input)
`NLCB` must be at least as large as `NLCA`.

NUCB — Number of upper codiagonals in `B`. (Input)
`NUCB` must be at least as large as `NUCA`.

Optional Arguments

N — Order of the matrices `A` and `B`. (Input)
Default: `N` = `SIZE` (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = `SIZE` (`A`,1).

LDB — Leading dimension of `B` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDB` = `SIZE` (`B`,1).

FORTRAN 90 Interface

Generic: `CALL CCBCB (A, NLCA, NUCA, B, NLCB, NUCB [, …])`

Specific: The specific interface names are `S_CCBCB` and `D_CCBCB`.

FORTRAN 77 Interface

Single: CALL CCBCB (N, A, LDA, NLCA, NUCA, B, LDB, NLCB, NUCB)

Double: The double precision name is DCCBCB.

Description

The routine CCBCB copies the complex band matrix *A* in band storage mode into the complex band matrix *B* in band storage mode.

Example

A complex band matrix of order 3 in band storage mode with one upper codiagonal and one lower codiagonal is copied into another complex band matrix in band storage mode.

```
      USE CCBCB_INT
      USE WRCRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    LDA, LDB, N, NLCA, NLCB, NUCA, NUCB
      PARAMETER  (LDA=3, LDB=3, N=3, NLCA=1, NLCB=1, NUCA=1, NUCB=1)
!
      COMPLEX    A(LDA,N), B(LDB,N)
!                        Set values for  A (in band mode)
!                        A = (  0.0+0.0i  1.0+1.0i  1.0+1.0i  )
!                            (  1.0+1.0i  1.0+1.0i  1.0+1.0i  )
!                            (  1.0+1.0i  1.0+1.0i  0.0+0.0i  )
!
      DATA A/(0.0,0.0), 7*(1.0,1.0), (0.0,0.0)/
!                                 Copy A to B
      CALL CCBCB (A, NLCA, NUCA, B, NLCB, NUCB)
!                                 Print results
      CALL WRCRN ('B', B)
      END
```

Output

```
                          B
                1                 2                 3
1  ( 0.000, 0.000)  ( 1.000, 1.000)  ( 1.000, 1.000)
2  ( 1.000, 1.000)  ( 1.000, 1.000)  ( 1.000, 1.000)
3  ( 1.000, 1.000)  ( 1.000, 1.000)  ( 0.000, 0.000)
```

CRGRB

Converts a real general matrix to a matrix in band storage mode.

Required Arguments

A — Real N by N matrix. (Input)

NLC — Number of lower codiagonals in B. (Input)

NUC — Number of upper codiagonals in B. (Input)

B — Real (NUC + 1 + NLC) by N array containing the band matrix in band storage mode. (Output)

Optional Arguments

N — Order of the matrices A and B. (Input)
Default: N = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = SIZE (A,1).

LDB — Leading dimension of B exactly as specified in the dimension statement of the calling program. (Input)
Default: LDB = SIZE (B,1).

FORTRAN 90 Interface

Generic: CALL CRGRB (A, NLC, NUC, B [, …])

Specific: The specific interface names are S_CRGRB and D_CRGRB.

FORTRAN 77 Interface

Single: CALL CRGRB (N, A, LDA, NLC, NUC, B, LDB)

Double: The double precision name is DCRGRB.

Description

The routine CRGRB converts the real general $N \times N$ matrix A with m_u = NUC upper codiagonals and m_l = NLC lower codiagonals into the real band matrix B of order N. The first m_u rows of B then contain the upper codiagonals of A, the next row contains the main diagonal of A, and the last m_l rows of B contain the lower codiagonals of A.

Example

A real 4 × 4 matrix with one upper codiagonal and three lower codiagonals is copied to a real band matrix of order 4 in band storage mode.

```
      USE CRGRB_INT
      USE WRRRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    LDA, LDB, N, NLC, NUC
      PARAMETER  (LDA=4, LDB=5, N=4, NLC=3, NUC=1)
!
      REAL       A(LDA,N), B(LDB,N)
!                                 Set values for  A
!                                 A = (  1.0     2.0    0.0    0.0)
!                                     ( -2.0     1.0    3.0    0.0)
!                                     (  0.0    -3.0    1.0    4.0)
!                                     ( -7.0     0.0   -4.0    1.0)
!
      DATA A/1.0, -2.0, 0.0, -7.0, 2.0, 1.0, -3.0, 0.0, 0.0, 3.0, 1.0, &
          -4.0, 0.0, 0.0, 4.0, 1.0/
!                                 Convert A to band matrix B
      CALL CRGRB (A, NLC, NUC, B)
!                                 Print results
      CALL WRRRN ('B', B)
      END
```

Output

```
                 B
         1        2        3        4
1    0.000    2.000    3.000    4.000
2    1.000    1.000    1.000    1.000
3   -2.000   -3.000   -4.000    0.000
4    0.000    0.000    0.000    0.000
5   -7.000    0.000    0.000    0.000
```

CRBRG

Converts a real matrix in band storage mode to a real general matrix.

Required Arguments

A — Real (`NUC` + 1 + `NLC`) by `N` array containing the band matrix in band storage mode. (Input)

NLC — Number of lower codiagonals in `A`. (Input)

NUC — Number of upper codiagonals in `A`. (Input)

B — Real `N` by `N` array containing the matrix. (Output)

Optional Arguments

N — Order of the matrices `A` and `B`. (Input)
Default: `N` = `SIZE` (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = `SIZE` (`A`,1).

LDB — Leading dimension of `B` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDB` = `SIZE` (`B`,1).

FORTRAN 90 Interface

Generic: `CALL CRBRG (A, NLC, NUC, B [, …])`

Specific: The specific interface names are `S_CRBRG` and `D_CRBRG`.

FORTRAN 77 Interface

Single: `CALL CRBRG (N, A, LDA, NLC, NUC, B, LDB)`

Double: The double precision name is `DCRBRG`.

Description

The routine CRBRG converts the real band matrix *A* of order *N* in band storage mode into the real $N \times N$ general matrix *B* with m_u = NUC upper codiagonals and m_l = NLC lower codiagonals. The first m_u rows of *A* are copied to the upper codiagonals of *B*, the next row of *A* is copied to the diagonal of *B*, and the last m_l rows of *A* are copied to the lower codiagonals of *B*.

Example

A real band matrix of order 3 in band storage mode with one upper codiagonal and one lower codiagonal is copied to a 3×3 real general matrix.

```
      USE CRBRG_INT
      USE WRRRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    LDA, LDB, N, NLC, NUC
      PARAMETER  (LDA=3, LDB=3, N=3, NLC=1, NUC=1)
!
      REAL       A(LDA,N), B(LDB,N)
!                                 Set values for  A (in band mode)
!                                 A = (  0.0     1.0    1.0)
!                                     (  4.0     3.0    2.0)
!                                     (  2.0     2.0    0.0)
!
      DATA A/0.0, 4.0, 2.0, 1.0, 3.0, 2.0, 1.0, 2.0, 0.0/
!                                 Convert band matrix A to matrix B
      CALL CRBRG (A, NLC, NUC, B)
!                                 Print results
      CALL WRRRN ('B', B)
      END
```

Output

```
             B
        1        2        3
1   4.000    1.000    0.000
2   2.000    3.000    1.000
3   0.000    2.000    2.000
```

CCGCB

Converts a complex general matrix to a matrix in complex band storage mode.

Required Arguments

A — Complex N by N array containing the matrix. (Input)

NLC — Number of lower codiagonals in B. (Input)

NUC — Number of upper codiagonals in B. (Input)

B — Complex (NUC + 1 + NLC) by N array containing the band matrix in band storage mode. (Output)

Optional Arguments

N — Order of the matrices A and B. (Input)
Default: N = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = SIZE (A,1).

LDB — Leading dimension of B exactly as specified in the dimension statement of the calling program. (Input)
Default: LDB = SIZE (B,1).

FORTRAN 90 Interface

Generic: CALL CCGCB (A, NLC, NUC, B [, …])

Specific: The specific interface names are S_CCGCB and D_CCGCB.

FORTRAN 77 Interface

Single: CALL CCGCB (N, A, LDA, NLC, NUC, B, LDB)

Double: The double precision name is DCCGCB.

Description

The routine CCGCB converts the complex general matrix *A* of order *N* with m_u = NUC upper codiagonals and m_l = NLC lower codiagonals into the complex band matrix *B* of order *N* in band storage mode. The first m_u rows of *B* then contain the upper codiagonals of *A*, the next row contains the main diagonal of *A*, and the last m_l rows of *B* contain the lower codiagonals of *A*.

Example

A complex general matrix of order 4 with one upper codiagonal and three lower codiagonals is copied to a complex band matrix of order 4 in band storage mode.

```
      USE CCGCB_INT
      USE WRCRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    LDA, LDB, N, NLC, NUC
      PARAMETER  (LDA=4, LDB=5, N=4, NLC=3, NUC=1)
!
      COMPLEX    A(LDA,N), B(LDB,N)
!                     Set values for  A
!                     A = (  1.0+0.0i   2.0+1.0i  0.0+0.0i  0.0+0.0i )
!                         ( -2.0+1.0i   1.0+0.0i  3.0+2.0i  0.0+0.0i )
!                         (  0.0+0.0i  -3.0+2.0i  1.0+0.0i  4.0+3.0i )
!                         ( -7.0+1.0i   0.0+0.0i -4.0+3.0i  1.0+0.0i )
!
      DATA A/(1.0,0.0), (-2.0,1.0), (0.0,0.0), (-7.0,1.0), (2.0,1.0), &
          (1.0,0.0), (-3.0,2.0), (0.0,0.0), (0.0,0.0), (3.0,2.0), &
          (1.0,0.0), (-4.0,3.0), (0.0,0.0), (0.0,0.0), (4.0,3.0), &
          (1.0,0.0)/
!                                 Convert A to band matrix B
      CALL CCGCB (A, NLC, NUC, B)
!                                 Print results
      CALL WRCRN ('B', B)
      END
```

Output

```
                                B
                 1                 2                 3                 4
1  ( 0.000, 0.000)  ( 2.000, 1.000)  ( 3.000, 2.000)  ( 4.000, 3.000)
2  ( 1.000, 0.000)  ( 1.000, 0.000)  ( 1.000, 0.000)  ( 1.000, 0.000)
3  (-2.000, 1.000)  (-3.000, 2.000)  (-4.000, 3.000)  ( 0.000, 0.000)
4  ( 0.000, 0.000)  ( 0.000, 0.000)  ( 0.000, 0.000)  ( 0.000, 0.000)
5  (-7.000, 1.000)  ( 0.000, 0.000)  ( 0.000, 0.000)  ( 0.000, 0.000)
```

CCBCG

Converts a complex matrix in band storage mode to a complex matrix in full storage mode.

Required Arguments

A — Complex (NUC + 1 + NLC) by N matrix containing the band matrix in band mode. (Input)

NLC — Number of lower codiagonals in A. (Input)

NUC — Number of upper codiagonals in A. (Input)

B — Complex N by N matrix containing the band matrix in full mode. (Output)

Optional Arguments

N — Order of the matrices A and B. (Input)
Default: N = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = SIZE (A,1).

LDB — Leading dimension of B exactly as specified in the dimension statement of the calling program. (Input)
Default: LDB = SIZE (B,1).

FORTRAN 90 Interface

Generic: CALL CCBCG (A, NLC, NUC, B [, …])

Specific: The specific interface names are S_CCBCG and D_CCBCG.

FORTRAN 77 Interface

Single: CALL CCBCG (N, A, LDA, NLC, NUC, B, LDB)

Double: The double precision name is DCCBCG.

Description

The routine CCBCG converts the complex band matrix A of order N with m_u = NUC upper codiagonals and m_l = NLC lower codiagonals into the $N \times N$ complex general matrix B. The first m_u rows of A are copied to the upper codiagonals of B, the next row of A is copied to the diagonal of B, and the last m_l rows of A are copied to the lower codiagonals of B.

Example

A complex band matrix of order 4 in band storage mode with one upper codiagonal and three lower codiagonals is copied into a 4×4 complex general matrix.

```
      USE CCBCG_INT
      USE WRCRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    LDA, LDB, N, NLC, NUC
      PARAMETER  (LDA=5, LDB=4, N=4, NLC=3, NUC=1)
!
      COMPLEX    A(LDA,N), B(LDB,N)
!                     Set values for  A (in band mode)
!                     A = (  0.0+0.0i  2.0+1.0i  3.0+2.0i  4.0+3.0i  )
!                         (  1.0+0.0i  1.0+0.0i  1.0+0.0i  1.0+0.0i  )
!                         ( -2.0+1.0i -3.0+2.0i -4.0+3.0i  0.0+0.0i  )
!                         (  0.0+0.0i  0.0+0.0i  0.0+0.0i  0.0+0.0i  )
!                         ( -7.0+1.0i  0.0+0.0i  0.0+0.0i  0.0+0.0i  )
!
      DATA A/(0.0,0.0), (1.0,0.0), (-2.0,1.0), (0.0,0.0), (-7.0,1.0), &
          (2.0,1.0), (1.0,0.0), (-3.0,2.0), 2*(0.0,0.0), (3.0,2.0), &
          (1.0,0.0), (-4.0,3.0), 2*(0.0,0.0), (4.0,3.0), (1.0,0.0), &
          3*(0.0,0.0)/
!                                 Convert band matrix A to matrix B
      CALL CCBCG (A, NLC, NUC, B)
!                                 Print results
      CALL WRCRN ('B', B)
      END
```

Output

```
                                B
                 1                 2                 3                 4
1  ( 1.000, 0.000)  ( 2.000, 1.000)  ( 0.000, 0.000)  ( 0.000, 0.000)
2  (-2.000, 1.000)  ( 1.000, 0.000)  ( 3.000, 2.000)  ( 0.000, 0.000)
3  ( 0.000, 0.000)  (-3.000, 2.000)  ( 1.000, 0.000)  ( 4.000, 3.000)
4  (-7.000, 1.000)  ( 0.000, 0.000)  (-4.000, 3.000)  ( 1.000, 0.000)
```

CRGCG

Copies a real general matrix to a complex general matrix.

Required Arguments

A — Real matrix of order N. (Input)

B — Complex matrix of order N containing a copy of A. (Output)

Optional Arguments

N — Order of the matrices A and B. (Input)
Default: N = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = SIZE (A,1).

LDB — Leading dimension of B exactly as specified in the dimension statement of the calling program. (Input)
Default: LDB = SIZE (B,1).

FORTRAN 90 Interface

Generic: CALL CRGCG (A, B [, …])

Specific: The specific interface names are S_CRGCG and D_CRGCG.

FORTRAN 77 Interface

Single: CALL CRGCG (N, A, LDA, B, LDB)

Double: The double precision name is DCRGCG.

Description

The routine CRGCG copies a real $N \times N$ matrix to a complex $N \times N$ matrix.

Example

A 3 × 3 real matrix is copied to a 3 × 3 complex matrix.

```
      USE CRGCG_INT
      USE WRCRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    LDA, LDB, N
      PARAMETER  (LDA=3, LDB=3, N=3)
!
      REAL       A(LDA,N)
      COMPLEX    B(LDB,N)
!                                 Set values for  A
!                                 A = (  2.0     1.0    3.0 )
!                                     (  4.0     1.0    0.0 )
!                                     ( -1.0     2.0    0.0 )
!
      DATA A/2.0, 4.0, -1.0, 1.0, 1.0, 2.0, 3.0, 0.0, 0.0/
!                                 Convert real A to complex B
      CALL CRGCG (A, B)
!                                 Print results
      CALL WRCRN ('B', B)
      END
```

Output

```
                           B
                 1                 2                 3
1  ( 2.000, 0.000)  ( 1.000, 0.000)  ( 3.000, 0.000)
2  ( 4.000, 0.000)  ( 1.000, 0.000)  ( 0.000, 0.000)
3  (-1.000, 0.000)  ( 2.000, 0.000)  ( 0.000, 0.000)
```

CRRCR

Copies a real rectangular matrix to a complex rectangular matrix.

Required Arguments

A — Real NRA by NCA rectangular matrix. (Input)

B — Complex NRB by NCB rectangular matrix containing a copy of A. (Output)

Optional Arguments

NRA — Number of rows in A. (Input)
Default: NRA = SIZE (A,1).

NCA — Number of columns in A. (Input)
Default: NCA = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = SIZE (A,1).

NRB — Number of rows in B. (Input)
It must be the same as NRA.
Default: NRB = SIZE (B,1).

NCB — Number of columns in B. (Input)
It must be the same as NCA.
Default: NCB = SIZE (B,2).

LDB — Leading dimension of B exactly as specified in the dimension statement of the calling program. (Input)
Default: LDB = SIZE (B,1).

FORTRAN 90 Interface

Generic: CALL CRRCR (A, B [, …])

Specific: The specific interface names are S_CRRCR and D_CRRCR.

FORTRAN 77 Interface

Single: CALL CRRCR (NRA, NCA, A, LDA, NRB, NCB, B, LDB)

Double: The double precision name is DCRRCR.

Description

The routine CRRCR copies a real rectangular matrix to a complex rectangular matrix.

Example

A 3 × 2 real matrix is copied to a 3 × 2 complex matrix.

```
      USE CRRCR_INT
      USE WRCRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    LDA, LDB, NCA, NCB, NRA, NRB
      PARAMETER  (LDA=3, LDB=3, NCA=2, NCB=2, NRA=3, NRB=3)
!
      REAL       A(LDA,NCA)
      COMPLEX    B(LDB,NCB)
!                                 Set values for  A
!                                 A = (  1.0     4.0  )
!                                     (  2.0     5.0  )
!                                     (  3.0     6.0  )
!
      DATA A/1.0, 2.0, 3.0, 4.0, 5.0, 6.0/
!                                 Convert real A to complex B
      CALL CRRCR (A, B)
!                                 Print results
      CALL WRCRN ('B', B)
      END
```

Output

```
                  B
                   1                 2
1   ( 1.000, 0.000)   ( 4.000, 0.000)
2   ( 2.000, 0.000)   ( 5.000, 0.000)
3   ( 3.000, 0.000)   ( 6.000, 0.000)
```

CRBCB

Converts a real matrix in band storage mode to a complex matrix in band storage mode.

Required Arguments

A — Real band matrix of order `N`. (Input)

NLCA — Number of lower codiagonals in `A`. (Input)

NUCA — Number of upper codiagonals in `A`. (Input)

B — Complex matrix of order `N` containing a copy of `A`. (Output)

NLCB — Number of lower codiagonals in `B`. (Input)
`NLCB` must be at least as large as `NLCA`.

NUCB — Number of upper codiagonals in `B`. (Input)
`NUCB` must be at least as large as `NUCA`.

Optional Arguments

N — Order of the matrices `A` and `B`. (Input)
Default: `N` = `SIZE` (A,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = `SIZE` (A,1).

LDB — Leading dimension of `B` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDB` = `SIZE` (B,1).

FORTRAN 90 Interface

Generic: `CALL CRBCB (A, NLCA, NUCA, B, NLCB, NUCB [, …])`

Specific: The specific interface names are `S_CRBCB` and `D_CRBCB`.

FORTRAN 77 Interface

Single: CALL CRBCB (N, A, LDA, NLCA, NUCA, B, LDB, NLCB, NUCB)

Double: The double precision name is DCRBCB.

Description

The routine CRBCB converts a real band matrix in band storage mode with NUCA upper codiagonals and NLCA lower codiagonals into a complex band matrix in band storage mode with NUCB upper codiagonals and NLCB lower codiagonals.

Example

A real band matrix of order 3 in band storage mode with one upper codiagonal and one lower codiagonal is copied into another complex band matrix in band storage mode.

```
      USE CRBCB_INT
      USE WRCRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    LDA, LDB, N, NLCA, NLCB, NUCA, NUCB
      PARAMETER  (LDA=3, LDB=3, N=3, NLCA=1, NLCB=1, NUCA=1, NUCB=1)
!
      REAL       A(LDA,N)
      COMPLEX    B(LDB,N)
!                                 Set values for  A (in band mode)
!                                 A = (  0.0     1.0    1.0)
!                                     (  1.0     1.0    1.0)
!                                     (  1.0     1.0    0.0)
!
      DATA A/0.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 0.0/
!                                 Convert real band matrix A
!                                 to complex band matrix B
      CALL CRBCB (A, NLCA, NUCA, B, NLCB, NUCB)
!                                 Print results
      CALL WRCRN ('B', B)
      END
```

Output

```
                            B
                 1                 2                 3
1  ( 0.000, 0.000)  ( 1.000, 0.000)  ( 1.000, 0.000)
2  ( 1.000, 0.000)  ( 1.000, 0.000)  ( 1.000, 0.000)
3  ( 1.000, 0.000)  ( 1.000, 0.000)  ( 0.000, 0.000)
```

CSFRG

Extends a real symmetric matrix defined in its upper triangle to its lower triangle.

Required Arguments

A — `N` by `N` symmetric matrix of order `N` to be filled out. (Input/Output)

Optional Arguments

N – Order of the matrix `A`. (Input)
Default: `N` = `SIZE` (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = `SIZE` (`A`,1).

FORTRAN 90 Interface

Generic: `CALL CSFRG (A [, …])`

Specific: The specific interface names are `S_CSFRG` and `D_CSFRG`.

FORTRAN 77 Interface

Single: `CALL CSFRG (N, A, LDA)`

Double: The double precision name is `DCSFRG`.

Description

The routine `CSFRG` converts an $N \times N$ matrix A in symmetric mode into a general matrix by filling in the lower triangular portion of A using the values defined in its upper triangular portion.

Example

The lower triangular portion of a real 3 3 symmetric matrix is filled with the values defined in its upper triangular portion.

```
      USE CSFRG_INT
      USE WRRRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    LDA, N
      PARAMETER  (LDA=3, N=3)
!
      REAL       A(LDA,N)
!                                 Set values for  A
!                                 A = (   0.0   3.0   4.0  )
!                                     (         1.0   5.0  )
!                                     (               2.0  )
!
      DATA A/3*0.0, 3.0, 1.0, 0.0, 4.0, 5.0, 2.0/
!                                 Fill the lower portion of A
      CALL CSFRG (A)
!                                 Print results
      CALL WRRRN ('A', A)
      END
```

Output

```
            A
        1       2       3
1   0.000   3.000   4.000
2   3.000   1.000   5.000
3   4.000   5.000   2.000
```

CHFCG

Extends a complex Hermitian matrix defined in its upper triangle to its lower triangle.

Required Arguments

A — Complex Hermitian matrix of order `N`. (Input/Output)
On input, the upper triangle of `A` defines a Hermitian matrix. On output, the lower triangle of `A` is defined so that `A` is Hermitian.

Optional Arguments

N — Order of the matrix. (Input)
Default: `N` = `SIZE` (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = `SIZE` (`A`,1).

FORTRAN 90 Interface

Generic: `CALL CHFCG (A [, …])`

Specific: The specific interface names are `S_CHFCG` and `D_CHFCG`.

FORTRAN 77 Interface

Single: `CALL CHFCG (N, A, LDA)`

Double: The double precision name is `DCHFCG`.

Description

The routine `CHFCG` converts an $N \times N$ complex matrix A in Hermitian mode into a complex general matrix by filling in the lower triangular portion of A using the values defined in its upper triangular portion.

Comments

Informational errors

Type	Code	Description
3	1	The matrix is not Hermitian. It has a diagonal entry with a small imaginary part.
4	2	The matrix is not Hermitian. It has a diagonal entry with an imaginary part.

Example

A complex 3 × 3 Hermitian matrix defined in its upper triangle is extended to its lower triangle.

```
      USE CHFCG_INT
      USE WRCRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    LDA, N
      PARAMETER  (LDA=3, N=3)
!
      COMPLEX    A(LDA,N)
!                                 Set values for  A
!                           A = (  1.0+0.0i  1.0+1.0i  1.0+2.0i  )
!                               (            2.0+0.0i  2.0+2.0i  )
!                               (                      3.0+0.0i  )
!
      DATA A/(1.0,0.0), 2*(0.0,0.0), (1.0,1.0), (2.0,0.0), (0.0,0.0), &
          (1.0,2.0), (2.0,2.0), (3.0,0.0)/
!                                 Fill in lower Hermitian matrix
      CALL CHFCG (A)
!                                 Print results
      CALL WRCRN ('A', A)
      END
```

Output

```
                            A
                 1                 2                 3
1  ( 1.000, 0.000)  ( 1.000, 1.000)  ( 1.000, 2.000)
2  ( 1.000,-1.000)  ( 2.000, 0.000)  ( 2.000, 2.000)
3  ( 1.000,-2.000)  ( 2.000,-2.000)  ( 3.000, 0.000)
```

CSBRB

Copies a real symmetric band matrix stored in band symmetric storage mode to a real band matrix stored in band storage mode.

Required Arguments

A — Real band symmetric matrix of order N. (Input)

NUCA — Number of codiagonals in A. (Input)

B — Real band matrix of order N containing a copy of A. (Output)

NLCB — Number of lower codiagonals in B. (Input)
NLCB must be at least as large as NUCA.

NUCB — Number of upper codiagonals in B. (Input)
NUCB must be at least as large as NUCA.

Optional Arguments

N — Order of the matrices A and B. (Input)
Default: N = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = SIZE (A,1).

LDB — Leading dimension of B exactly as specified in the dimension statement of the calling program. (Input)
Default: LDB = SIZE (B,1).

FORTRAN 90 Interface

Generic: CALL CSBRB (A, NUCA, B, NLCB, NUCB [, …])

Specific: The specific interface names are S_CSBRB and D_CSBRB.

FORTRAN 77 Interface

Single: CALL CSBRB (N, A, LDA, NUCA, B, LDB, NLCB, NUCB)

Double: The double precision name is DCSBRB.

Description

The routine CSBRB copies a real matrix *A* stored in symmetric band mode to a matrix B stored in band mode. The lower codiagonals of *B* are set using the values from the upper codiagonals of *A*.

Example

A real matrix of order 4 in band symmetric storage mode with 2 upper codiagonals is copied to a real matrix in band storage mode with 2 upper codiagonals and 2 lower codiagonals.

```
      USE CSBRB_INT
      USE WRRRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    LDA, LDB, N, NLCB, NUCA, NUCB
      PARAMETER  (N=4, NUCA=2, LDA=NUCA+1, NLCB=NUCA, NUCB=NUCA, &
                LDB=NLCB+NUCB+1)
!
      REAL       A(LDA,N), B(LDB,N)
!                         Set values for  A, in band mode
!                         A = (  0.0  0.0  2.0  1.0 )
!                             (  0.0  2.0  3.0  1.0 )
!                             (  1.0  2.0  3.0  4.0 )
!
      DATA A/2*0.0, 1.0, 0.0, 2.0, 2.0, 2.0, 3.0, 3.0, 1.0, 1.0, 4.0/
!                                 Copy A to B
      CALL CSBRB (A, NUCA, B, NLCB, NUCB)
!                                 Print results
      CALL WRRRN ('B', B)
      END
```

Output

```
               B
         1        2        3        4
1    0.000    0.000    2.000    1.000
2    0.000    2.000    3.000    1.000
3    1.000    2.000    3.000    4.000
4    2.000    3.000    1.000    0.000
5    2.000    1.000    0.000    0.000
```

CHBCB

Copies a complex Hermitian band matrix stored in band Hermitian storage mode to a complex band matrix stored in band storage mode.

Required Arguments

A — Complex band Hermitian matrix of order N. (Input)

NUCA — Number of codiagonals in A. (Input)

B — Complex band matrix of order N containing a copy of A. (Output)

NLCB — Number of lower codiagonals in B. (Input)
NLCB must be at least as large as NUCA.

NUCB — Number of upper codiagonals in B. (Input)
NUCB must be at least as large as NUCA.

Optional Arguments

N — Order of the matrices A and B. (Input)
Default: N = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = SIZE (A,1).

LDB — Leading dimension of B exactly as specified in the dimension statement of the calling program. (Input)
Default: LDB = SIZE (B,1).

FORTRAN 90 Interface

Generic: CALL CHBCB (A, NUCA, B, NLCB, NUCB [, …])

Specific: The specific interface names are S_CHBCB and D_CHBCB.

FORTRAN 77 Interface

Single: CALL CHBCB (N, A, LDA, NUCA, B, LDB, NLCB, NUCB)

Double: The double precision name is DCHBCB.

Description

The routine CSBRB copies a complex matrix *A* stored in Hermitian band mode to a matrix *B* stored in complex band mode. The lower codiagonals of *B* are filled using the values in the upper codiagonals of *A*.

Comments

Informational errors

Type	Code	Description
3	1	An element on the diagonal has a complex part that is near zero, the complex part is set to zero.
4	1	An element on the diagonal has a complex part that is not zero.

Example

A complex Hermitian matrix of order 3 in band Hermitian storage mode with one upper codiagonal is copied to a complex matrix in band storage mode.

```
      USE CHBCB_INT
      USE WRCRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    LDA, LDB, N, NLCB, NUCA, NUCB
      PARAMETER  (N=3, NUCA=1, LDA=NUCA+1, NLCB=NUCA, NUCB=NUCA, &
                LDB=NLCB+NUCB+1)
!
      COMPLEX    A(LDA,N), B(LDB,N)
!                                 Set values for  A (in band mode)
!                           A = (  0.0+0.0i -1.0+1.0i -2.0+2.0i  )
!                               (  1.0+0.0i  1.0+0.0i  1.0+0.0i  )
!
      DATA A/(0.0,0.0), (1.0,0.0), (-1.0,1.0), (1.0,0.0), (-2.0,2.0), &
          (1.0,0.0)/
!                                 Copy a complex Hermitian band matrix
!                                 to a complex band matrix
      CALL CHBCB (A, NUCA, B, NLCB, NUCB)
!                                 Print results
      CALL WRCRN ('B', B)
      END
```

Output

```
                            B
                  1                 2                 3
1  ( 0.000, 0.000)  (-1.000, 1.000)  (-2.000, 2.000)
2  ( 1.000, 0.000)  ( 1.000, 0.000)  ( 1.000, 0.000)
```

```
 3  (-1.000,-1.000)  (-2.000,-2.000)  ( 0.000, 0.000)
```

TRNRR

Transposes a rectangular matrix.

Required Arguments

A — Real NRA by NCA matrix in full storage mode. (Input)

B — Real NRB by NCB matrix in full storage mode containing the transpose of A. (Output)

Optional Arguments

NRA — Number of rows of A. (Input)
Default: NRA = SIZE (A,1).

NCA — Number of columns of A. (Input)
Default: NCA = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = SIZE (A,1).

NRB — Number of rows of B. (Input)
NRB must be equal to NCA.
Default: NRB = SIZE (B,1).

NCB — Number of columns of B. (Input)
NCB must be equal to NRA.
Default: NCB = SIZE (B,2).

LDB — Leading dimension of B exactly as specified in the dimension statement of the calling program. (Input)
Default: LDB = SIZE (B,1).

FORTRAN 90 Interface

Generic: CALL TRNRR (A, B [, …])

Specific: The specific interface names are S_TRNRR and D_TRNRR.

FORTRAN 77 Interface

Single: CALL TRNRR (NRA, NCA, A, LDA, NRB, NCB, B, LDB)

Double: The double precision name is DTRNRR.

Description

The routine TRNRR computes the transpose $B = A^T$ of a real rectangular matrix A.

Comments

If LDA = LDB and NRA = NCA, then A and B can occupy the same storage locations; otherwise, A and B must be stored separately.

Example

Transpose the 5 × 3 real rectangular matrix A into the 3 × 5 real rectangular matrix B.

```
      USE TRNRR_INT
      USE WRRRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    NCA, NCB, NRA, NRB
      PARAMETER  (NCA=3, NCB=5, NRA=5, NRB=3)
!
      REAL       A(NRA,NCA), B(NRB,NCB)
!                                 Set values for A
!                                 A = ( 11.0  12.0  13.0 )
!                                     ( 21.0  22.0  23.0 )
!                                     ( 31.0  32.0  33.0 )
!                                     ( 41.0  42.0  43.0 )
!                                     ( 51.0  52.0  53.0 )
!
      DATA A/11.0, 21.0, 31.0, 41.0, 51.0, 12.0, 22.0, 32.0, 42.0,&
          52.0, 13.0, 23.0, 33.0, 43.0, 53.0/
!                                 B = transpose(A)
      CALL TRNRR (A, B)
!                                 Print results
      CALL WRRRN ('B = trans(A)', B)
      END
```

Output

```
                B = trans(A)
          1        2        3        4        5
1     11.00    21.00    31.00    41.00    51.00
2     12.00    22.00    32.00    42.00    52.00
3     13.00    23.00    33.00    43.00    53.00
```

MXTXF

more...

Computes the transpose product of a matrix, $A^T A$.

Required Arguments

A — Real NRA by NCA rectangular matrix. (Input)
The transpose product of A is to be computed.

B — Real NB by NB symmetric matrix containing the transpose product $A^T A$. (Output)

Optional Arguments

NRA — Number of rows in A. (Input)
Default: NRA = SIZE (A,1).

NCA — Number of columns in A. (Input)
Default: NCA = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = SIZE (A,1).

NB — Order of the matrix B. (Input)
NB must be equal to NCA.
Default: NB = SIZE (B,1).

LDB — Leading dimension of *B* exactly as specified in the dimension statement of the calling program. (Input)
Default: LDB = SIZE (B,1).

FORTRAN 90 Interface

Generic: CALL MXTXF (A, B [, …])

Specific: The specific interface names are S_MXTXF and D_MXTXF.

FORTRAN 77 Interface

Single: CALL MXTXF (NRA, NCA, A, LDA, NB, B, LDB)

Double: The double precision name is DMXTXF.

Description

The routine MXTXF computes the real general matrix $B = A^T A$ given the real rectangular matrix A.

Example

Multiply the transpose of a 3 × 4 real matrix by itself. The output matrix will be a 4 × 4 real symmetric matrix.

```
      USE MXTXF_INT
      USE WRRRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    NB, NCA, NRA
      PARAMETER  (NB=4, NCA=4, NRA=3)
!
      REAL       A(NRA,NCA), B(NB,NB)
!                                 Set values for A
!                                 A = ( 3.0  1.0  4.0  2.0 )
!                                     ( 0.0  2.0  1.0 -1.0 )
!                                     ( 6.0  1.0  3.0  2.0 )
!
      DATA A/3.0, 0.0, 6.0, 1.0, 2.0, 1.0, 4.0, 1.0, 3.0, 2.0, -1.0, &
          2.0/
!                                 Compute B = trans(A)*A
      CALL MXTXF (A, B)
!                                 Print results
      CALL WRRRN ('B = trans(A)*A', B)
      END
```

Output

```
         B = trans(A)*A
        1        2        3        4
1   45.00     9.00    30.00    18.00
2    9.00     6.00     9.00     2.00
3   30.00     9.00    26.00    13.00
4   18.00     2.00    13.00     9.00
```

MXTYF

more...

Multiplies the transpose of matrix *A* by matrix *B*, $A^T B$.

Required Arguments

A — Real `NRA` by `NCA` matrix. (Input)

B — Real `NRB` by `NCB` matrix. (Input)

C — Real `NCA` by `NCB` matrix containing the transpose product $A^T B$. (Output)

Optional Arguments

NRA — Number of rows in `A`. (Input)
Default: NRA = `SIZE` (A,1).

NCA — Number of columns in `A`. (Input)
Default: `NCA` = `SIZE` (A,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = `SIZE` (A,1).

NRB — Number of rows in `B`. (Input)
`NRB` must be the same as `NRA`.
Default: `NRB` = `SIZE` (B,1).

NCB — Number of columns in `B`. (Input)
Default: `NCB` = `SIZE` (B,2).

LDB — Leading dimension of `B` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDB` = `SIZE` (B,1).

NRC — Number of rows of C. (Input)
NRC must be equal to NCA.
Default: NRC = SIZE (C,1).

NCC — Number of columns of C. (Input)
NCC must be equal to NCB.
Default: NCC = SIZE (C,2).

LDC — Leading dimension of C exactly as specified in the dimension statement of the calling program. (Input)
Default: LDC = SIZE (C,1).

FORTRAN 90 Interface

Generic: CALL MXTYF (A, B, C [, …])

Specific: The specific interface names are S_MXTYF and D_MXTYF.

FORTRAN 77 Interface

Single: CALL MXTYF (NRA, NCA, A, LDA, NRB, NCB, B, LDB, NRC, NCC, C, LDC)

Double: The double precision name is DMXTYF.

Description

The routine MXTYF computes the real general matrix $C = A^T B$ given the real rectangular matrices A and B.

Example

Multiply the transpose of a 3 × 4 real matrix by a 3 × 3 real matrix. The output matrix will be a 4 × 3 real matrix.

```
      USE MXTYF_INT
      USE WRRRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    NCA, NCB, NCC, NRA, NRB, NRC
      PARAMETER  (NCA=4, NCB=3, NCC=3, NRA=3, NRB=3, NRC=4)
!
      REAL       A(NRA,NCA), B(NRB,NCB), C(NRC,NCC)
!                                 Set values for A
!                                 A = ( 1.0  0.0  2.0  0.0 )
!                                     ( 3.0  4.0 -1.0  0.0 )
!                                     ( 2.0  1.0  2.0  1.0 )
!
!                                 Set values for B
```

```
!                                  B = ( -1.0  2.0  0.0 )
!                                      (  3.0  0.0 -1.0 )
!                                      (  0.0  5.0  2.0 )
!
      DATA A/1.0, 3.0, 2.0, 0.0, 4.0, 1.0, 2.0, -1.0, 2.0, 0.0, 0.0, &
          1.0/
      DATA B/-1.0, 3.0, 0.0, 2.0, 0.0, 5.0, 0.0, -1.0, 2.0/
!                                  Compute C = trans(A)*B
      CALL MXTYF (A, B, C)
!                                  Print results
      CALL WRRRN ('C = trans(A)*B', C)
      END
```

Output

```
      C = trans(A)*B
        1       2       3
1    8.00   12.00    1.00
2   12.00    5.00   -2.00
3   -5.00   14.00    5.00
4    0.00    5.00    2.00
```

MXYTF

Multiplies a matrix *A* by the transpose of a matrix *B*, AB^T.

Required Arguments

A — Real NRA by NCA rectangular matrix. (Input)

B — Real NRB by NCB rectangular matrix. (Input)

C — Real NRC by NCC rectangular matrix containing the transpose product AB^T. (Output)

Optional Arguments

NRA — Number of rows in A. (Input)
Default: NRA = SIZE (A,1).

NCA — Number of columns in A. (Input)
Default: NCA = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = SIZE (A,1).

NRB — Number of rows in B. (Input)
Default: NRB = SIZE (B,1).

NCB — Number of columns in B. (Input)
NCB must be the same as NCA.
Default: NCB = SIZE (B,2).

LDB — Leading dimension of B exactly as specified in the dimension statement of the calling program. (Input)
Default: LDB = SIZE (B,1).

NRC — Number of rows of C. (Input)
NRC must be equal to NRA.
Default: NRC = SIZE (C,1).

NCC — Number of columns of `C`. (Input)
`NCC` must be equal to `NRB`.
Default: `NCC` = `SIZE` (C,2).

LDC — Leading dimension of `C` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDC` = `SIZE` (C,1).

FORTRAN 90 Interface

Generic: `CALL MXYTF` (A, B, C [, …])

Specific: The specific interface names are `S_MXYTF` and `D_MXYTF`.

FORTRAN 77 Interface

Single: `CALL MXYTF` (NRA, NCA, A, LDA, NRB, NCB, B, LDB, NRC, NCC, C, LDC)

Double: The double precision name is `DMXYTF`.

Description

The routine `MXYTF` computes the real general matrix $C = AB^T$ given the real rectangular matrices A and B.

Example

Multiply a 3 × 4 real matrix by the transpose of a 3 × 4 real matrix. The output matrix will be a 3 × 3 real matrix.

```
      USE MXYTF_INT
      USE WRRRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    NCA, NCB, NCC, NRA, NRB, NRC
      PARAMETER  (NCA=4, NCB=4, NCC=3, NRA=3, NRB=3, NRC=3)
!
      REAL       A(NRA,NCA), B(NRB,NCB), C(NRC,NCC)
!                                 Set values for A
!                                 A = ( 1.0  0.0  2.0  0.0 )
!                                     ( 3.0  4.0 -1.0  0.0 )
!                                     ( 2.0  1.0  2.0  1.0 )
!
!                                 Set values for B
!                                 B = ( -1.0  2.0  0.0  2.0 )
!                                     (  3.0  0.0 -1.0 -1.0 )
!                                     (  0.0  5.0  2.0  5.0 )
!
      DATA A/1.0, 3.0, 2.0, 0.0, 4.0, 1.0, 2.0, -1.0, 2.0, 0.0, 0.0, &
          1.0/
      DATA B/-1.0, 3.0, 0.0, 2.0, 0.0, 5.0, 0.0, -1.0, 2.0, 2.0, -1.0, &
```

```
          5.0/
!                                   Compute C = A*trans(B)
      CALL MXYTF (A, B, C)
!                                   Print results
      CALL WRRRN ('C = A*trans(B)', C)
      END
```

Output

```
      C = A*trans(B)
        1       2       3
1   -1.00    1.00    4.00
2    5.00   10.00   18.00
3    2.00    3.00   14.00
```

MRRRR

more...

Multiplies two real rectangular matrices, *AB*.

Required Arguments

A — Real `NRA` by `NCA` matrix in full storage mode. (Input)

B — Real `NRB` by `NCB` matrix in full storage mode. (Input)

C — Real `NRC` by `NCC` matrix containing the product *AB* in full storage mode. (Output)

Optional Arguments

NRA — Number of rows of `A`. (Input)
Default: `NRA` = `SIZE` (A,1).

NCA — Number of columns of `A`. (Input)
Default: `NCA` = `SIZE` (A,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = `SIZE` (A,1).

NRB — Number of rows of `B`. (Input)
`NRB` must be equal to `NCA`.
Default: `NRB` = `SIZE` (B,1).

NCB — Number of columns of `B`. (Input)
Default: `NCB` = `SIZE` (B,2).

LDB — Leading dimension of `B` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDB` = `SIZE` (B,1).

NRC — Number of rows of C. (Input)
NRC must be equal to NRA.
Default: NRC = SIZE (C,1).

NCC — Number of columns of C. (Input)
NCC must be equal to NCB.
Default: NCC = SIZE (C,2).

LDC — Leading dimension of C exactly as specified in the dimension statement of the calling program. (Input)
Default: LDC = SIZE (C,1).

FORTRAN 90 Interface

Generic: CALL MRRRR (A, B, C [, …])

Specific: The specific interface names are S_MRRRR and D_MRRRR.

FORTRAN 77 Interface

Single: CALL MRRRR (NRA, NCA, A, LDA, NRB, NCB, B, LDB, NRC, NCC, C, LDC)

Double: The double precision name is DMRRRR.

Description

Given the real rectangular matrices A and B, MRRRR computes the real rectangular matrix $C = AB$.

Example

Multiply a 3 × 4 real matrix by a 4 × 3 real matrix. The output matrix will be a 3 × 3 real matrix.

```
      USE MRRRR_INT

      USE WRRRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    NCA, NCB, NCC, NRA, NRB, NRC
      PARAMETER  (NCA=4, NCB=3, NCC=3, NRA=3, NRB=4, NRC=3)
!
      REAL       A(NRA,NCA), B(NRB,NCB), C(NRC,NCC)
!                                 Set values for A
!                                 A = ( 1.0  0.0  2.0  0.0 )
!                                     ( 3.0  4.0 -1.0  0.0 )
!                                     ( 2.0  1.0  2.0  1.0 )
!
!                                 Set values for B
!                                 B = ( -1.0  0.0  2.0 )
```

```
!                                     (  3.0  5.0  2.0 )
!                                     (  0.0  0.0 -1.0 )
!                                     (  2.0 -1.0  5.0 )
!
      DATA A/1.0, 3.0, 2.0, 0.0, 4.0, 1.0, 2.0, -1.0, 2.0, 0.0, 0.0, &
          1.0/
      DATA B/-1.0, 3.0, 0.0, 2.0, 0.0, 5.0, 0.0, -1.0, 2.0, 2.0, -1.0, &
          5.0/
!                                 Compute C = A*B
      CALL MRRRR (A, B, C)
!                                 Print results
      CALL WRRRN ('C = A*B', C)
      END
```

Output

```
          C = A*B
        1       2       3
1   -1.00    0.00    0.00
2    9.00   20.00   15.00
3    3.00    4.00    9.00
```

MCRCR

Multiplies two complex rectangular matrices, *AB*.

Required Arguments

A — Complex NRA by NCA rectangular matrix. (Input)

B — Complex NRB by NCB rectangular matrix. (Input)

C — Complex NRC by NCC rectangular matrix containing the product A * B. (Output)

Optional Arguments

NRA — Number of rows of A. (Input)
Default: NRA = SIZE (A,1).

NCA — Number of columns of A. (Input)
Default: NCA = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = SIZE (A,1).

NRB — Number of rows of B. (Input)
NRB must be equal to NCA.
Default: NRB = SIZE (B,1).

NCB — Number of columns of B. (Input)
Default: NCB = SIZE (B,2).

LDB — Leading dimension of B exactly as specified in the dimension statement of the calling program. (Input)
Default: LDB = SIZE (B,1).

NRC — Number of rows of C. (Input)
NRC must be equal to NRA.
Default: NRC = SIZE (C,1).

NCC — Number of columns of C. (Input)
NCC must be equal to NCB.
Default: NCC = SIZE (C,2).

LDC — Leading dimension of C exactly as specified in the dimension statement of the calling program. (Input)
Default: LDC = SIZE (C,1).

FORTRAN 90 Interface

Generic: CALL MCRCR (A, B, C [, …])

Specific: The specific interface names are S_MCRCR and D_MCRCR.

FORTRAN 77 Interface

Single: CALL MCRCR (NRA, NCA, A, LDA, NRB, NCB, B, LDB, NRC, NCC, C, LDC)

Double: The double precision name is DMCRCR.

Description

Given the complex rectangular matrices *A* and *B*, MCRCR computes the complex rectangular matrix *C* = *AB*.

Example

Multiply a 3 × 4 complex matrix by a 4 × 3 complex matrix. The output matrix will be a 3 × 3 complex matrix.

```
      USE MCRCR_INT
      USE WRCRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    NCA, NCB, NCC, NRA, NRB, NRC
      PARAMETER  (NCA=4, NCB=3, NCC=3, NRA=3, NRB=4, NRC=3)
!
      COMPLEX    A(NRA,NCA), B(NRB,NCB), C(NRC,NCC)
!                                 Set values for A
!             A = ( 1.0 + 1.0i  -1.0+ 2.0i  0.0 + 1.0i  0.0 - 2.0i )
!                 ( 3.0 + 7.0i  6.0 - 4.0i  2.0 - 1.0i  0.0 + 1.0i )
!                 ( 1.0 + 0.0i  1.0 - 2.0i  -2.0+ 0.0i  0.0 + 0.0i )
!
!                                 Set values for B
!             B = ( 2.0 + 1.0i  3.0 + 2.0i  3.0 + 1.0i )
!                 ( 2.0 - 1.0i  4.0 - 2.0i  5.0 - 3.0i )
!                 ( 1.0 + 0.0i  0.0 - 1.0i  0.0 + 1.0i )
!                 ( 2.0 + 1.0i  1.0 + 2.0i  0.0 - 1.0i )
!
      DATA A/(1.0,1.0), (3.0,7.0), (1.0,0.0), (-1.0,2.0), (6.0,-4.0), &
          (1.0,-2.0), (0.0,1.0), (2.0,-1.0), (-2.0,0.0), (0.0,-2.0), &
          (0.0,1.0), (0.0,0.0)/
```

```
      DATA B/(2.0,1.0), (2.0,-1.0), (1.0,0.0), (2.0,1.0), (3.0,2.0), &
          (4.0,-2.0), (0.0,-1.0), (1.0,2.0), (3.0,1.0), (5.0,-3.0), &
          (0.0,1.0), (0.0,-1.0)/
!                                Compute C = A*B
      CALL MCRCR (A, B, C)
!                                Print results
      CALL WRCRN ('C = A*B', C)
      END
```

Output

```
                      C = A*B
                  1                2                3
1  (  3.00,  5.00)  (  6.00, 13.00)  (  0.00, 17.00)
2  (  8.00,  4.00)  (  8.00, -2.00)  ( 22.00,-12.00)
3  (  0.00, -4.00)  (  3.00, -6.00)  (  2.00,-14.00)
```

HRRRR

Computes the Hadamard product of two real rectangular matrices.

Required Arguments

A — Real NRA by NCA rectangular matrix. (Input)

B — Real NRB by NCB rectangular matrix. (Input)

C — Real NRC by NCC rectangular matrix containing the Hadamard product of A and B. (Output)
If A is not needed, then C can share the same storage locations as A. Similarly, if B is not needed, then C can share the same storage locations as B.

Optional Arguments

NRA — Number of rows of A. (Input)
Default: NRA = SIZE (A,1).

NCA — Number of columns of A. (Input)
Default: NCA = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = SIZE (A,1).

NRB — Number of rows of B. (Input)
NRB must be equal to NRA.
Default: NRB = SIZE (B,1).

NCB — Number of columns of B. (Input)
NCB must be equal to NCA.
Default: NCB = SIZE (B,2).

LDB — Leading dimension of B exactly as specified in the dimension statement of the calling program. (Input)
Default: LDB = SIZE (B,1).

NRC — Number of rows of C. (Input)
NRC must be equal to NRA.
Default: NRC = SIZE (C,1).

NCC — Number of columns of `C`. (Input)
`NCC` must be equal to `NCA`.
Default: `NCC` = `SIZE` (C,2).

LDC — Leading dimension of `C` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDC` = `SIZE` (C,1).

FORTRAN 90 Interface

Generic: `CALL HRRRR (A, B, C [, …])`

Specific: The specific interface names are `S_HRRRR` and `D_HRRRR`.

FORTRAN 77 Interface

Single: `CALL HRRRR (NRA, NCA, A, LDA, NRB, NCB, B, LDB, NRC, NCC, C, LDC)`

Double: The double precision name is `DHRRRR`.

Description

The routine `HRRRR` computes the Hadamard product of two real matrices A and B and returns a real matrix C, where $C_{ij} = A_{ij}B_{ij}$.

Example

Compute the Hadamard product of two 4 × 4 real matrices. The output matrix will be a 4 × 4 real matrix.

```
      USE HRRRR_INT
      USE WRRRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    NCA, NCB, NCC, NRA, NRB, NRC
      PARAMETER  (NCA=4, NCB=4, NCC=4, NRA=4, NRB=4, NRC=4)
!
      REAL       A(NRA,NCA), B(NRB,NCB), C(NRC,NCC)
!                                 Set values for A
!                                 A = ( -1.0  0.0 -3.0  8.0 )
!                                     (  2.0  1.0  7.0  2.0 )
!                                     (  3.0 -2.0  2.0 -6.0 )
!                                     (  4.0  1.0 -5.0 -8.0 )
!
!                                 Set values for B
!                                 B = (  2.0  3.0  0.0 -10.0 )
!                                     (  1.0 -1.0  4.0   2.0 )
!                                     ( -1.0 -2.0  7.0   1.0 )
!                                     (  2.0  1.0  9.0   0.0 )
!
      DATA A/-1.0, 2.0, 3.0, 4.0, 0.0, 1.0, -2.0, 1.0, -3.0, 7.0, 2.0, &
```

```
          -5.0, 8.0, 2.0, -6.0, -8.0/
      DATA B/2.0, 1.0, -1.0, 2.0, 3.0, -1.0, -2.0, 1.0, 0.0, 4.0, 7.0, &
          9.0, -10.0, 2.0, 1.0, 0.0/
!                                Compute Hadamard product of A and B
      CALL HRRRR (A, B, C)
!                                Print results
      CALL WRRRN ('C = A (*) B', C)
      END
```

Output

```
             C = A (*) B
         1        2        3        4
1    -2.00     0.00     0.00   -80.00
2     2.00    -1.00    28.00     4.00
3    -3.00     4.00    14.00    -6.00
4     8.00     1.00   -45.00     0.00
```

BLINF

This function computes the bilinear form $x^T Ay$.

Function Return Value

BLINF — The value of $x^T Ay$ is returned in `BLINF`. (Output)

Required Arguments

A — Real `NRA` by `NCA` matrix. (Input)

X — Real vector of length `NRA`. (Input)

Y — Real vector of length `NCA`. (Input)

Optional Arguments

NRA — Number of rows of `A`. (Input)
Default: `NRA` = `SIZE` (`A`,1).

NCA — Number of columns of `A`. (Input)
Default: `NCA` = `SIZE` (`A`,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement of the calling program. (Input)
Default: `LDA` = `SIZE` (`A`,1).

FORTRAN 90 Interface

Generic: `BLINF (A, X, Y [, …])`

Specific: The specific interface names are `S_BLINF` and `D_BLINF`.

FORTRAN 77 Interface

Single: BLINF(`NRA, NCA, A, LDA, X, Y`)

Double: The double precision name is `DBLINF`.

Description

Given the real rectangular matrix A and two vectors x and y, BLINF computes the bilinear form $x^T Ay$.

Comments

The quadratic form can be computed by calling BLINF with the vector X in place of the vector Y.

Example

Compute the bilinear form $x^T Ay$, where x is a vector of length 5, A is a 5×2 matrix and y is a vector of length 2.

```
      USE BLINF_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    NCA, NRA
      PARAMETER  (NCA=2, NRA=5)
!
      INTEGER    NOUT
      REAL       A(NRA,NCA), VALUE, X(NRA), Y(NCA)
!                                 Set values for A
!                                 A = ( -2.0  2.0 )
!                                     (  3.0 -6.0 )
!                                     ( -4.0  7.0 )
!                                     (  1.0 -8.0 )
!                                     (  0.0 10.0 )
!                                 Set values for X
!                                 X = (  1.0 -2.0  3.0 -4.0 -5.0 )
!                                 Set values for Y
!                                 Y = ( -6.0  3.0 )
!
      DATA A/-2.0, 3.0, -4.0, 1.0, 0.0, 2.0, -6.0, 7.0, -8.0, 10.0/
      DATA X/1.0, -2.0, 3.0, -4.0, -5.0/
      DATA Y/-6.0, 3.0/
!                                 Compute bilinear form
      VALUE = BLINF(A,X,Y)
!                                 Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,*) ' The bilinear form trans(x)*A*y = ', VALUE
      END
```

Output

```
The bilinear form trans(x)*A*y =     195.000
```

POLRG

more...

Evaluates a real general matrix polynomial.

Required Arguments

A — N by N matrix for which the polynomial is to be computed. (Input)

COEF — Vector of length NCOEF containing the coefficients of the polynomial in order of increasing power. (Input)

B — N by N matrix containing the value of the polynomial evaluated at A. (Output)

Optional Arguments

N — Order of the matrix A. (Input)
Default: N = SIZE (A,1).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = SIZE (A,1).

NCOEF — Number of coefficients. (Input)
Default: NCOEF = SIZE (COEF,1).

LDB — Leading dimension of B exactly as specified in the dimension statement of the calling program. (Input)
Default: LDB = SIZE (B,1).

FORTRAN 90 Interface

Generic: CALL POLRG (A, COEF, B [, …])

Specific: The specific interface names are S_POLRG and D_POLRG.

FORTRAN 77 Interface

Single: CALL POLRG (N, A, LDA, NCOEF, COEF, B, LDB)

Double: The double precision name is DPOLRG.

Description

Let m = NCOEF and c = COEF.

The routine POLRG computes the matrix polynomial

$$B = \sum_{k=1}^{m} c_k A^{k-1}$$

using Horner's scheme

$$B = \left(\ldots \left(\left(c_m A + c_{m-1} I \right) A + c_{m-2} I \right) A + \ldots + c_1 I \right)$$

where I is the $N \times N$ identity matrix.

Comments

Workspace may be explicitly provided, if desired, by use of P2LRG/DP2LRG. The reference is

CALL P2LRG (N, A, LDA, NCOEF, COEF, B, LDB, WORK)

The additional argument is

WORK — Work vector of length N * N.

Example

This example evaluates the matrix polynomial $3I + A + 2A^2$, where A is a 3×3 matrix.

```
      USE POLRG_INT
      USE WRRRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    LDA, LDB, N, NCOEF
      PARAMETER  (N=3, NCOEF=3, LDA=N, LDB=N)
!
      REAL       A(LDA,N), B(LDB,N), COEF(NCOEF)
!                                 Set values of A and COEF
!
!                                 A = (  1.0    3.0    2.0  )
!                                     ( -5.0    1.0    7.0  )
!                                     (  1.0    5.0   -4.0  )
!
```

```
!                                    COEF = (3.0, 1.0, 2.0)
!
      DATA A/1.0, -5.0, 1.0, 3.0, 1.0, 5.0, 2.0, 7.0, -4.0/
      DATA COEF/3.0, 1.0, 2.0/
!
!                                    Evaluate B = 3I + A + 2*A**2
      CALL POLRG (A, COEF, B)
!                                    Print B
      CALL WRRRN ('B = 3I + A + 2*A**2', B)
      END
```

Output

```
    B = 3I + A + 2*A**2
        1        2        3
1   -20.0     35.0     32.0
2   -11.0     46.0    -55.0
3   -55.0    -19.0    105.0
```

MURRV

Multiplies a real rectangular matrix by a vector.

Required Arguments

A — Real NRA by NCA rectangular matrix. (Input)

X — Real vector of length NX. (Input)

Y — Real vector of length NY containing the product A * X if IPATH is equal to 1 and the product trans(A) * X if IPATH is equal to 2. (Output)

Optional Arguments

NRA — Number of rows of A. (Input)
Default: NRA = SIZE (A,1).

NCA — Number of columns of A. (Input)
Default: NCA = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = SIZE (A,1).

NX — Length of the vector X. (Input)
NX must be equal to NCA if IPATH is equal to 1. NX must be equal to NRA if IPATH is equal to 2.
Default: NX = SIZE (X,1).

IPATH — Integer flag. (Input)
IPATH = 1 means the product Y = A * X is computed. IPATH = 2 means the product Y = trans(A) * X is computed, where trans(A) is the transpose of A.
Default: IPATH =1.

NY — Length of the vector Y. (Input)
NY must be equal to NRA if IPATH is equal to 1. NY must be equal to NCA if IPATH is equal to 2.
Default: NY = SIZE (Y,1).

FORTRAN 90 Interface

Generic: CALL MURRV (A, X, Y [, …])

Specific: The specific interface names are S_MURRV and D_MURRV.

FORTRAN 77 Interface

Single: CALL MURRV (NRA, NCA, A, LDA, NX, X, IPATH, NY, Y)

Double: The double precision name is DMURRV.

Description

If IPATH = 1, MURRV computes $y = Ax$, where A is a real general matrix and x and y are real vectors. If IPATH = 2, MURRV computes $y = A^T x$.

Example

Multiply a 3 × 3 real matrix by a real vector of length 3. The output vector will be a real vector of length 3.

```
      USE MURRV_INT
      USE WRRRN_INT

      IMPLICIT   NONE
!                                  Declare variables
      INTEGER    LDA, NCA, NRA, NX, NY
      PARAMETER  (NCA=3, NRA=3, NX=3, NY=3)
!
      INTEGER    IPATH
      REAL       A(NRA,NCA), X(NX), Y(NY)
!                                  Set values for A and X
!                                  A = ( 1.0  0.0  2.0 )
!                                      ( 0.0  3.0  0.0 )
!                                      ( 4.0  1.0  2.0 )
!
!                                  X = ( 1.0  2.0  1.0 )
!
!
      DATA A/1.0, 0.0, 4.0, 0.0, 3.0, 1.0, 2.0, 0.0, 2.0/
      DATA X/1.0, 2.0, 1.0/
!                                  Compute y = Ax
      IPATH = 1
      CALL MURRV (A, X, Y)
!                                  Print results
      CALL WRRRN ('y = Ax', Y, 1, NY, 1)
      END
```

Output

```
        y = Ax
    1        2        3
3.000    6.000    8.000
```

MURBV

Multiplies a real band matrix in band storage mode by a real vector.

Required Arguments

A — Real NLCA + NUCA + 1 by N band matrix stored in band mode. (Input)

NLCA — Number of lower codiagonals in A. (Input)

NUCA — Number of upper codiagonals in A. (Input)

X — Real vector of length NX. (Input)

Y — Real vector of length NY containing the product A * X if IPATH is equal to 1 and the product trans(A) * X if IPATH is equal to 2. (Output)

Optional Arguments

N — Order of the matrix. (Input)
Default: N = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = SIZE (A,1).

NX — Length of the vector X. (Input)
NX must be equal to N.
Default: NX = SIZE (X,1).

IPATH — Integer flag. (Input)
IPATH = 1 means the product Y = A * X is computed. IPATH = 2 means the product Y = trans(A) * X is computed, where trans(A) is the transpose of A.
Default: IPATH = 1.

NY — Length of vector Y. (Input)
NY must be equal to N.
Default: NY = SIZE (Y,1).

FORTRAN 90 Interface

Generic: CALL MURBV (A, NLCA, NUCA, X, Y [, …])

Specific: The specific interface names are S_MURBV and D_MURBV.

FORTRAN 77 Interface

Single: CALL MURBV (N, A, LDA, NLCA, NUCA, NX, X, IPATH, NY, Y)

Double: The double precision name is DMURBV.

Description

If IPATH = 1, MURBV computes $y = Ax$, where A is a real band matrix and x and y are real vectors. If IPATH = 2, MURBV computes $y = A^T x$.

Example

Multiply a real band matrix of order 6, with two upper codiagonals and two lower codiagonals stored in band mode, by a real vector of length 6. The output vector will be a real vector of length 6.

```
      USE MURBV_INT
      USE WRRRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    LDA, N, NLCA, NUCA, NX, NY
      PARAMETER  (LDA=5, N=6, NLCA=2, NUCA=2, NX=6, NY=6)
!
      INTEGER    IPATH
      REAL       A(LDA,N), X(NX), Y(NY)
!                                 Set values for A (in band mode)
!                                 A = ( 0.0  0.0  1.0  2.0  3.0  4.0 )
!                                     ( 0.0  1.0  2.0  3.0  4.0  5.0 )
!                                     ( 1.0  2.0  3.0  4.0  5.0  6.0 )
!                                     (-1.0 -2.0 -3.0 -4.0 -5.0  0.0 )
!                                     (-5.0 -6.0 -7.0 -8.0  0.0  0.0 )
!
!                                 Set values for X
!                                 X = (-1.0  2.0 -3.0  4.0 -5.0  6.0 )
!
      DATA A/0.0, 0.0, 1.0, -1.0, -5.0, 0.0, 1.0, 2.0, -2.0, -6.0, &
          1.0, 2.0, 3.0, -3.0, -7.0, 2.0, 3.0, 4.0, -4.0, -8.0, 3.0, &
          4.0, 5.0, -5.0, 0.0, 4.0, 5.0, 6.0, 0.0, 0.0/
      DATA X/-1.0, 2.0, -3.0, 4.0, -5.0, 6.0/
!                                 Compute y = Ax
      IPATH = 1
      CALL MURBV (A, NLCA, NUCA, X, Y)
!                                 Print results
      CALL WRRRN ('y = Ax', Y, 1, NY, 1)
      END
```

Output

```
                      y = Ax
     1        2        3        4        5        6
 -2.00     7.00   -11.00    17.00    10.00    29.00
```

MUCRV

Multiplies a complex rectangular matrix by a complex vector.

Required Arguments

A — Complex NRA by NCA rectangular matrix. (Input)

X — Complex vector of length NX. (Input)

Y — Complex vector of length NY containing the product A * X if IPATH is equal to 1 and the product trans(A) * X if IPATH is equal to 2. (Output)

Optional Arguments

NRA — Number of rows of A. (Input)
Default: NRA = SIZE (A,1).

NCA — Number of columns of A. (Input)
Default: NCA = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = SIZE (A,1).

NX — Length of the vector X. (Input)
NX must be equal to NCA if IPATH is equal to 1. NX must be equal to NRA if IPATH is equal to 2.
Default: NX = SIZE (X,1).

IPATH — Integer flag. (Input)
IPATH = 1 means the product Y = A * X is computed. IPATH = 2 means the product Y = trans(A) * X is computed, where trans(A) is the transpose of A.
Default: IPATH =1.

NY — Length of the vector Y. (Input)
NY must be equal to NRA if IPATH is equal to 1. NY must be equal to NCA if IPATH is equal to 2.
Default: NY = SIZE (Y,1).

FORTRAN 90 Interface

Generic: `CALL MUCRV (A, X, Y [, …])`

Specific: The specific interface names are `S_MUCRV` and `D_MUCRV`.

FORTRAN 77 Interface

Single: `CALL MUCRV (NRA, NCA, A, LDA, NX, X, IPATH, NY, Y)`

Double: The double precision name is `DMUCRV`.

Description

If `IPATH` = 1, `MUCRV` computes $y = Ax$, where A is a complex general matrix and x and y are complex vectors. If `IPATH` = 2, `MUCRV` computes $y = A^T x$.

Example

Multiply a 3 × 3 complex matrix by a complex vector of length 3. The output vector will be a complex vector of length 3.

```
      USE MUCRV_INT
      USE WRCRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    NCA, NRA, NX, NY
      PARAMETER  (NCA=3, NRA=3, NX=3, NY=3)
!
      INTEGER    IPATH
      COMPLEX    A(NRA,NCA), X(NX), Y(NY)
!
!                                 Set values for A and X
!             A = ( 1.0 + 2.0i  3.0 + 4.0i  1.0 + 0.0i )
!                 ( 2.0 + 1.0i  3.0 + 2.0i  0.0 - 1.0i )
!                 ( 2.0 - 1.0i  1.0 + 0.0i  0.0 + 1.0i )
!
!             X = ( 1.0 - 1.0i  2.0 - 2.0i  0.0 - 1.0i )
!
      DATA A/(1.0,2.0), (2.0,1.0), (2.0,-1.0), (3.0,4.0), (3.0,2.0), &
          (1.0,0.0), (1.0,0.0), (0.0,-1.0), (0.0,1.0)/
      DATA X/(1.0,-1.0), (2.0,-2.0), (0.0,-1.0)/
!                                 Compute y = Ax
      IPATH = 1
      CALL MUCRV (A, X, Y)
!                                 Print results
      CALL WRCRN ('y = Ax', Y, 1, NY, 1)
      END
```

Output

```
                              y = Ax
```

```
                 1                   2                   3
  ( 17.00,   2.00)  ( 12.00, -3.00)  (  4.00, -5.00)
```

MUCBV

Multiplies a complex band matrix in band storage mode by a complex vector.

Required Arguments

A — Complex NLCA + NUCA + 1 by N band matrix stored in band mode. (Input)

NLCA — Number of lower codiagonals in A. (Input)

NUCA — Number of upper codiagonals in A. (Input)

X — Complex vector of length NX. (Input)

Y — Complex vector of length NY containing the product A * X if IPATH is equal to 1 and the product trans(A) * X if IPATH is equal to 2. (Output)

Optional Arguments

N — Order of the matrix. (Input)
Default: N = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = SIZE (A,1).

NX — Length of the vector X. (Input)
NX must be equal to N.
Default: NX = SIZE (X,1).

IPATH — Integer flag. (Input)
IPATH = 1 means the product Y = A * X is computed. IPATH = 2 means the product Y = trans(A) * X is computed, where trans(A) is the transpose of A.
Default: IPATH = 1.

NY — Length of vector Y. (Input)
NY must be equal to N.
Default: NY = SIZE (Y,1).

FORTRAN 90 Interface

Generic: CALL MUCBV (A, NLCA, NUCA, X, Y [, …])

Specific: The specific interface names are S_MUCBV and D_MUCBV.

FORTRAN 77 Interface

Single: CALL MUCBV (N, A, LDA, NLCA, NUCA, NX, X, IPATH, NY, Y)

Double: The double precision name is DMUCBV.

Description

If IPATH = 1, MUCBV computes $y = Ax$, where A is a complex band matrix and x and y are complex vectors. If IPATH = 2, MUCBV computes $y = A^T x$.

Example

Multiply the transpose of a complex band matrix of order 4, with one upper codiagonal and two lower codiagonals stored in band mode, by a complex vector of length 3. The output vector will be a complex vector of length 3.

```
      USE MUCBV_INT
      USE WRCRN_INT

      IMPLICIT   NONE
!                                  Declare variables
      INTEGER    LDA, N, NLCA, NUCA, NX, NY
      PARAMETER  (LDA=4, N=4, NLCA=2, NUCA=1, NX=4, NY=4)
!
      INTEGER    IPATH
      COMPLEX    A(LDA,N), X(NX), Y(NY)
!                                  Set values for A (in band mode)
!             A = (  0.0+ 0.0i   1.0+ 2.0i   3.0+ 4.0i   5.0+ 6.0i )
!                 ( -1.0- 1.0i  -1.0- 1.0i  -1.0- 1.0i  -1.0- 1.0i )
!                 ( -1.0+ 2.0i  -1.0+ 3.0i  -2.0+ 1.0i   0.0+ 0.0i )
!                 (  2.0+ 0.0i   0.0+ 2.0i   0.0+ 0.0i   0.0+ 0.0i )
!
!                                  Set values for X
!             X = ( 3.0 + 4.0i  0.0 + 0.0i  1.0 + 2.0i  -2.0 - 1.0i )
!
      DATA A/(0.0,0.0), (-1.0,-1.0), (-1.0,2.0), (2.0,0.0), (1.0,2.0), &
          (-1.0,-1.0), (-1.0,3.0), (0.0,2.0), (3.0,4.0), (-1.0,-1.0), &
          (-2.0,1.0), (0.0,0.0), (5.0,6.0), (-1.0,-1.0), (0.0,0.0), &
          (0.0,0.0)/
      DATA X/(3.0,4.0), (0.0,0.0), (1.0,2.0), (-2.0,-1.0)/
!                                  Compute y = Ax
      IPATH = 2
      CALL MUCBV (A, NLCA, NUCA, X, Y, IPATH=IPATH)
!                                  Print results
      CALL WRCRN ('y = Ax', Y, 1, NY, 1)
      END
```

Output

```
                              y = Ax
                1                 2                 3                 4
 (  3.00, -3.00)  (-10.00,  7.00)  (  6.00, -3.00)  ( -6.00, 19.00)
```

ARBRB

Adds two band matrices, both in band storage mode.

Required Arguments

A — N by N band matrix with NLCA lower codiagonals and NUCA upper codiagonals stored in band mode with dimension (NLCA + NUCA + 1) by N. (Input)

NLCA — Number of lower codiagonals of A. (Input)

NUCA — Number of upper codiagonals of A. (Input)

B — N by N band matrix with NLCB lower codiagonals and NUCB upper codiagonals stored in band mode with dimension (NLCB + NUCB + 1) by N. (Input)

NLCB — Number of lower codiagonals of B. (Input)

NUCB — Number of upper codiagonals of B. (Input)

C — N by N band matrix with NLCC lower codiagonals and NUCC upper codiagonals containing the sum A + B in band mode with dimension (NLCC + NUCC + 1) by N. (Output)

NLCC — Number of lower codiagonals of C. (Input)
NLCC must be at least as large as max(NLCA, NLCB).

NUCC — Number of upper codiagonals of C. (Input)
NUCC must be at least as large as max(NUCA, NUCB).

Optional Arguments

N — Order of the matrices A, B and C. (Input)
Default: N = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = SIZE (A,1).

LDB — Leading dimension of B exactly as specified in the dimension statement of the calling program. (Input)
Default: LDB = SIZE (B,1).

LDC — Leading dimension of C exactly as specified in the dimension statement of the calling program. (Input)
Default: LDC = SIZE (C,1).

FORTRAN 90 Interface

Generic: CALL ARBRB (A, NLCA, NUCA, B, NLCB, NUCB, C, NLCC, NUCC [, …])

Specific: The specific interface names are S_ARBRB and D_ARBRB.

FORTRAN 77 Interface

Single: CALL ARBRB (N, A, LDA, NLCA, NUCA, B, LDB, NLCB, NUCB, C, LDC, NLCC, NUCC)

Double: The double precision name is DARBRB.

Description

The routine ARBRB adds two real matrices stored in band mode, returning a real matrix stored in band mode.

Example

Add two real matrices of order 4 stored in band mode. Matrix *A* has one upper codiagonal and one lower codiagonal. Matrix *B* has no upper codiagonals and two lower codiagonals. The output matrix *C*, has one upper codiagonal and two lower codiagonals.

```
      USE ARBRB_INT
      USE WRRRN_INT

      IMPLICIT   NONE
!                                  Declare variables
      INTEGER    LDA, LDB, LDC, N, NLCA, NLCB, NLCC, NUCA, NUCB, NUCC
      PARAMETER  (LDA=3, LDB=3, LDC=4, N=4, NLCA=1, NLCB=2, NLCC=2, &
                NUCA=1, NUCB=0, NUCC=1)
!
      REAL       A(LDA,N), B(LDB,N), C(LDC,N)
!                                  Set values for  A (in band mode)
!                                  A = (  0.0     2.0    3.0   -1.0)
!                                      (  1.0     1.0    1.0    1.0)
!                                      (  0.0     3.0    4.0    0.0)
!
!                                  Set values for  B (in band mode)
!                                  B = (  3.0     3.0    3.0    3.0)
!                                      (  1.0    -2.0    1.0    0.0)
!                                      ( -1.0     2.0    0.0    0.0)
!
      DATA A/0.0, 1.0, 0.0, 2.0, 1.0, 3.0, 3.0, 1.0, 4.0, -1.0, 1.0, &
          0.0/
      DATA B/3.0, 1.0, -1.0, 3.0, -2.0, 2.0, 3.0, 1.0, 0.0, 3.0, 0.0, &
          0.0/
!                                  Add A and B to obtain C (in band
```

```
!                                                                   mode)
      CALL ARBRB (A, NLCA, NUCA, B, NLCB, NUCB, C, NLCC, NUCC)
!                                   Print results
      CALL WRRRN ('C = A+B', C)
      END
```

Output

```
              C = A+B
        1        2        3        4
1   0.000    2.000    3.000   -1.000
2   4.000    4.000    4.000    4.000
3   1.000    1.000    5.000    0.000
4  -1.000    2.000    0.000    0.000
```

ACBCB

Adds two complex band matrices, both in band storage mode.

Required Arguments

A — N by N complex band matrix with NLCA lower codiagonals and NUCA upper codiagonals stored in band mode with dimension (NLCA + NUCA + 1) by N. (Input)

NLCA — Number of lower codiagonals of A. (Input)

NUCA — Number of upper codiagonals of A. (Input)

B — N by N complex band matrix with NLCB lower codiagonals and NUCB upper codiagonals stored in band mode with dimension (NLCB + NUCB + 1) by N. (Input)

NLCB — Number of lower codiagonals of B. (Input)

NUCB — Number of upper codiagonals of B. (Input)

C — N by N complex band matrix with NLCC lower codiagonals and NUCC upper codiagonals containing the sum A + B in band mode with dimension (NLCC + NUCC + 1) by N. (Output)

NLCC — Number of lower codiagonals of C. (Input)
NLCC must be at least as large as max(NLCA, NLCB).

NUCC — Number of upper codiagonals of C. (Input)
NUCC must be at least as large as max(NUCA, NUCB).

Optional Arguments

N — Order of the matrices A, B and C. (Input)
Default: N = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = SIZE (A,1).

LDB — Leading dimension of B exactly as specified in the dimension statement of the calling program. (Input)
Default: LDB = SIZE (B,1).

LDC — Leading dimension of C exactly as specified in the dimension statement of the calling program. (Input)
Default: LDC = SIZE (C,1).

FORTRAN 90 Interface

Generic: CALL ACBCB (A, NLCA, NUCA, B, NLCB, NUCB, C, NLCC, NUCC [, …])

Specific: The specific interface names are S_ACBCB and D_ACBCB.

FORTRAN 77 Interface

Single: CALL ACBCB (N, A, LDA, NLCA, NUCA, B, LDB, NLCB, NUCB, C, LDC, NLCC, NUCC)

Double: The double precision name is DACBCB.

Description

The routine ACBCB adds two complex matrices stored in band mode, returning a complex matrix stored in band mode.

Example

Add two complex matrices of order 4 stored in band mode. Matrix *A* has two upper codiagonals and no lower codiagonals. Matrix *B* has no upper codiagonals and two lower codiagonals. The output matrix *C* has two upper codiagonals and two lower codiagonals.

```
      USE ACBCB_INT
      USE WRCRN_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    LDA, LDB, LDC, N, NLCA, NLCB, NLCC, NUCA, NUCB, NUCC
      PARAMETER  (LDA=3, LDB=3, LDC=5, N=3, NLCA=0, NLCB=2, NLCC=2, &
                NUCA=2, NUCB=0, NUCC=2)
!
      COMPLEX    A(LDA,N), B(LDB,N), C(LDC,N)
!                                 Set values for A (in band mode)
!                 A = ( 0.0 + 0.0i  0.0 + 0.0i  3.0 - 2.0i )
!                     ( 0.0 + 0.0i  -1.0+ 3.0i  6.0 + 0.0i )
!                     ( 1.0 + 4.0i  5.0 - 2.0i  3.0 + 1.0i )
!
!                                 Set values for B (in band mode)
!                 B = ( 3.0 + 1.0i  4.0 + 1.0i  7.0 - 1.0i )
!                     ( -1.0- 4.0i  9.0 + 3.0i  0.0 + 0.0i )
!                     ( 2.0 - 1.0i  0.0 + 0.0i  0.0 + 0.0i )
!
      DATA A/(0.0,0.0), (0.0,0.0), (1.0,4.0), (0.0,0.0), (-1.0,3.0), &
          (5.0,-2.0), (3.0,-2.0), (6.0,0.0), (3.0,1.0)/
      DATA B/(3.0,1.0), (-1.0,-4.0), (2.0,-1.0), (4.0,1.0), (9.0,3.0), &
```

```
          (0.0,0.0), (7.0,-1.0), (0.0,0.0), (0.0,0.0)/
!                                 Compute C = A+B
      CALL ACBCB (A, NLCA, NUCA, B, NLCB, NUCB, C, NLCC, NUCC)
!                                 Print results
      CALL WRCRN ('C = A+B', C)
      END
```

Output

```
                           C = A+B
                    1                 2                 3
1  (  0.00,  0.00)  (  0.00,  0.00)  (  3.00, -2.00)
2  (  0.00,  0.00)  ( -1.00,  3.00)  (  6.00,  0.00)
3  (  4.00,  5.00)  (  9.00, -1.00)  ( 10.00,  0.00)
4  ( -1.00, -4.00)  (  9.00,  3.00)  (  0.00,  0.00)
5  (  2.00, -1.00)  (  0.00,  0.00)  (  0.00,  0.00)
```

NRIRR

Computes the infinity norm of a real matrix.

Required Arguments

A — Real NRA by NCA matrix whose infinity norm is to be computed. (Input)

ANORM — Real scalar containing the infinity norm of A. (Output)

Optional Arguments

NRA — Number of rows of A. (Input)
Default: NRA = SIZE (A,1).

NCA — Number of columns of A. (Input)
Default: NCA = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = SIZE (A,1).

FORTRAN 90 Interface

Generic: CALL NRIRR (A, ANORM [, …])

Specific: The specific interface names are S_NRIRR and D_NRIRR.

FORTRAN 77 Interface

Single: CALL NRIRR (NRA, NCA, A, LDA, ANORM)

Double: The double precision name is DNRIRR.

Description

The routine NRIRR computes the infinity norm of a real rectangular matrix A. If m = NRA and n = NCA, then the ∞-norm of A is

$$\|A\|_\infty = \max_{1 \le i \le m} \sum_{j=1}^{n} |A_{ij}|$$

This is the maximum of the sums of the absolute values of the row elements.

Example

Compute the infinity norm of a 3 × 4 real rectangular matrix.

```
      USE NRIRR_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    NCA, NRA
      PARAMETER  (NCA=4, NRA=3)
!
      INTEGER    NOUT
      REAL       A(NRA,NCA), ANORM
!
!                                 Set values for A
!                                 A = ( 1.0  0.0  2.0  0.0 )
!                                     ( 3.0  4.0 -1.0  0.0 )
!                                     ( 2.0  1.0  2.0  1.0 )
!
      DATA A/1.0, 3.0, 2.0, 0.0, 4.0, 1.0, 2.0, -1.0, 2.0, 0.0, 0.0, &
          1.0/
!                                 Compute the infinity norm of A
      CALL NRIRR (A, ANORM)
!                                 Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,*) ' The infinity norm of A is ', ANORM
      END
```

Output

```
 The infinity norm of A is     8.00000
```

NR1RR

Computes the 1-norm of a real matrix.

Required Arguments

A — Real NRA by NCA matrix whose 1-norm is to be computed. (Input)

ANORM — Real scalar containing the 1-norm of A. (Output)

Optional Arguments

NRA — Number of rows of A. (Input)
Default: NRA = SIZE (A,1).

NCA — Number of columns of A. (Input)
Default: NCA = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = SIZE (A,1).

FORTRAN 90 Interface

Generic: CALL NR1RR (A, ANORM [, …])

Specific: The specific interface names are S_NR1RR and D_NR1RR.

FORTRAN 77 Interface

Single: CALL NR1RR (NRA, NCA, A, LDA, ANORM)

Double: The double precision name is DNR1RR.

Description

The routine NR1RR computes the 1-norm of a real rectangular matrix *A*. If *m* = NRA and *n* = NCA, then the 1-norm of *A* is

$$\|A\|_1 = \max_{1 \le j \le n} \sum_{i=1}^{m} |A_{ij}|$$

This is the maximum of the sums of the absolute values of the column elements.

Example

Compute the 1-norm of a 3 × 4 real rectangular matrix.

```
      USE NR1RR_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    NCA, NRA
      PARAMETER  (NCA=4, NRA=3)
!
      INTEGER    NOUT
      REAL       A(NRA,NCA), ANORM
!
!                 Set values for A
!                         A = ( 1.0  0.0  2.0  0.0 )
!                             ( 3.0  4.0 -1.0  0.0 )
!                             ( 2.0  1.0  2.0  1.0 )
!
      DATA A/1.0, 3.0, 2.0, 0.0, 4.0, 1.0, 2.0, -1.0, 2.0, 0.0, 0.0, &
          1.0/
!                                     Compute the L1 norm of A
      CALL NR1RR (A, ANORM)
!                                     Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,*) ' The 1-norm of A is ', ANORM
      END
```

Output

```
The 1-norm of A is     6.00000
```

NR2RR

Computes the Frobenius norm of a real rectangular matrix.

Required Arguments

A — Real NRA by NCA rectangular matrix. (Input)

ANORM — Frobenius norm of A. (Output)

Optional Arguments

NRA — Number of rows of A. (Input)
Default: NRA = SIZE (A,1).

NCA — Number of columns of A. (Input)
Default: NCA = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = SIZE (A,1).

FORTRAN 90 Interface

Generic: CALL NR2RR (A, ANORM [, …])

Specific: The specific interface names are S_NR2RR and D_NR2RR.

FORTRAN 77 Interface

Single: CALL NR2RR (NRA, NCA, A, LDA, ANORM)

Double: The double precision name is DNR2RR.

Description

The routine NR2RR computes the Frobenius norm of a real rectangular matrix *A*. If *m* = NRA and *n* = NCA, then the Frobenius norm of *A* is

$$\|A\|_2 = \left[\sum_{i=1}^{m} \sum_{j=1}^{n} A_{ij}^{\,2} \right]^{1/2}$$

Example

Compute the Frobenius norm of a 3 × 4 real rectangular matrix.

```
      USE NR2RR_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    LDA, NCA, NRA
      PARAMETER  (LDA=3, NCA=4, NRA=3)
!
      INTEGER    NOUT
      REAL       A(LDA,NCA), ANORM
!
!                                 Set values for A
!                                 A = ( 1.0  0.0  2.0  0.0 )
!                                     ( 3.0  4.0 -1.0  0.0 )
!                                     ( 2.0  1.0  2.0  1.0 )
!
      DATA A/1.0, 3.0, 2.0, 0.0, 4.0, 1.0, 2.0, -1.0, 2.0, 0.0, 0.0, &
          1.0/
!
!                                 Compute Frobenius norm of A
      CALL NR2RR (A, ANORM)
!                                 Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,*) ' The Frobenius norm of A is ', ANORM
      END
```

Output

```
 The Frobenius norm of A is     6.40312
```

NR1RB

Computes the 1-norm of a real band matrix in band storage mode.

Required Arguments

A — Real (NUCA + NLCA + 1) by N array containing the N by N band matrix in band storage mode. (Input)

NLCA — Number of lower codiagonals of A. (Input)

NUCA — Number of upper codiagonals of A. (Input)

ANORM — Real scalar containing the 1-norm of A. (Output)

Optional Arguments

N — Order of the matrix. (Input)
Default: N = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = SIZE (A,1).

FORTRAN 90 Interface

Generic: CALL NR1RB (A, NLCA, NUCA, ANORM [, …])

Specific: The specific interface names are S_NR1RB and D_NR1RB.

FORTRAN 77 Interface

Single: CALL NR1RB (N, A, LDA, NLCA, NUCA, ANORM)

Double: The double precision name is DNR1RB.

Description

The routine NR1RB computes the 1-norm of a real band matrix *A*. The 1-norm of a matrix *A* is

$$\|A\|_1 = \max_{1 \le j \le N} \sum_{i=1}^{N} |A_{ij}|$$

This is the maximum of the sums of the absolute values of the column elements.

Example

Compute the 1-norm of a 4 × 4 real band matrix stored in band mode.

```
      USE NR1RB_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    LDA, N, NLCA, NUCA
      PARAMETER  (LDA=4, N=4, NLCA=2, NUCA=1)
!
      INTEGER    NOUT
      REAL       A(LDA,N), ANORM
!
!                                 Set values for A (in band mode)
!                                 A = (  0.0  2.0  2.0  3.0  )
!                                     ( -2.0 -3.0 -4.0 -1.0  )
!                                     (  2.0  1.0  0.0  0.0  )
!                                     (  0.0  1.0  0.0  0.0  )
!
      DATA A/0.0, -2.0, 2.0, 0.0, 2.0, -3.0, 1.0, 1.0, 2.0, -4.0, 0.0, &
          0.0, 3.0, -1.0, 2*0.0/
!                                 Compute the L1 norm of A
      CALL NR1RB (A, NLCA, NUCA, ANORM)
!                                 Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,*) ' The 1-norm of A is ', ANORM
      END
```

Output

```
The 1-norm of A is     7.00000
```

NR1CB

Computes the 1-norm of a complex band matrix in band storage mode.

Required Arguments

A — Complex (NUCA + NLCA + 1) by N array containing the N by N band matrix in band storage mode. (Input)

NLCA — Number of lower codiagonals of A. (Input)

NUCA — Number of upper codiagonals of A. (Input)

ANORM — Real scalar containing the 1-norm of A. (Output)

Optional Arguments

N — Order of the matrix. (Input)
Default: N = SIZE (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = SIZE (A,1).

FORTRAN 90 Interface

Generic: CALL NR1CB (A, NLCA, NUCA, ANORM [, …])

Specific: The specific interface names are S_NR1CB and D_NR1CB.

FORTRAN 77 Interface

Single: CALL NR1CB (N, A, LDA, NLCA, NUCA, ANORM)

Double: The double precision name is DNR1CB.

Description

The routine NR1CB computes the 1-norm of a complex band matrix *A*. The 1-norm of a complex matrix *A* is

$$\|A\|_1 = \max_{1 \le j \le N} \sum_{i=1}^{N} \left[|\Re A_{ij}| + |\Im A_{ij}| \right]$$

Example

Compute the 1-norm of a complex matrix of order 4 in band storage mode.

```
      USE NR1CB_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    LDA, N, NLCA, NUCA
      PARAMETER  (LDA=4, N=4, NLCA=2, NUCA=1)
!
      INTEGER    NOUT
      REAL       ANORM
      COMPLEX    A(LDA,N)
!
!                                 Set values for A (in band mode)
!                     A = (  0.0+0.0i  2.0+3.0i -1.0+1.0i -2.0-1.0i )
!                         ( -2.0+3.0i  1.0+0.0i -4.0-1.0i  0.0-4.0i )
!                         (  2.0+2.0i  4.0+6.0i  3.0+2.0i  0.0+0.0i )
!                         (  0.0-1.0i  2.0+1.0i  0.0+0.0i  0.0+0.0i )
!
      DATA A/(0.0,0.0), (-2.0,3.0), (2.0,2.0), (0.0,-1.0), (2.0,3.0), &
          (1.0,0.0), (4.0,6.0), (2.0,1.0), (-1.0,1.0), (-4.0,-1.0), &
          (3.0,2.0), (0.0,0.0), (-2.0,-1.0), (0.0,-4.0), (0.0,0.0), &
          (0.0,0.0)/
!                                 Compute the L1 norm of A
      CALL NR1CB (A, NLCA, NUCA, ANORM)
!                                 Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,*) ' The 1-norm of A is ', ANORM
      END
```

Output

```
 The 1-norm of A is     19.0000
```

DISL2

This function computes the Euclidean (2-norm) distance between two points.

Function Return Value

DISL2 — Euclidean (2-norm) distance between the points X and Y. (Output)

Required Arguments

X — Vector of length max(N * |INCX|, 1). (Input)

Y — Vector of length max(N * |INCY|, 1). (Input)

Optional Arguments

N — Length of the vectors X and Y. (Input)
Default: N = SIZE (X,1).

INCX — Displacement between elements of X. (Input)
The I-th element of X is X(1 + (I − 1) * INCX) if INCX is greater than or equal to zero, or X(1 + (I − N) * INCX) if INCX is less than zero.
Default: INCX = 1.

INCY — Displacement between elements of Y. (Input)
The I-th element of Y is Y(1 + (I − 1) * INCY) if INCY is greater than or equal to zero, or Y(1 + (I − N) * INCY) if INCY is less than zero.
Default: INCY = 1.

FORTRAN 90 Interface

Generic: DISL2 (X, Y [, …])

Specific: The specific interface names are S_DISL2 and D_DISL2.

FORTRAN 77 Interface

Single: DISL2(N, X, INCX, Y, INCY)

Double: The double precision function name is DDISL2.

Description

The function `DISL2` computes the Euclidean (2-norm) distance between two points *x* and *y*. The Euclidean distance is defined to be

$$\left[\sum_{i=1}^{N}(x_i - y_i)^2\right]^{1/2}$$

Example

Compute the Euclidean (2-norm) distance between two vectors of length 4.

```
      USE DISL2_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                  Declare variables
      INTEGER    INCX, INCY, N
      PARAMETER  (N=4)
!
      INTEGER    NOUT
      REAL       VAL, X(N), Y(N)
!
!                                  Set values for X and Y
!                                  X = ( 1.0 -1.0  0.0  2.0 )
!
!                                  Y = ( 4.0  2.0  1.0 -3.0 )
!
      DATA X/1.0, -1.0, 0.0, 2.0/
      DATA Y/4.0, 2.0, 1.0, -3.0/
!                                  Compute L2 distance
      VAL = DISL2(X,Y)
!                                  Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,*) ' The 2-norm distance is ', VAL
      END
```

Output

```
 The 2-norm distance is     6.63325
```

DISL1

This function computes the 1-norm distance between two points.

Function Return Value

DISL1 — 1-norm distance between the points X and Y. (Output)

Required Arguments

X — Vector of length max(N * |INCX|, 1). (Input)

Y — Vector of length max(N * |INCY|, 1). (Input)

Optional Arguments

N — Length of the vectors X and Y. (Input)
Default: N = SIZE (X,1).

INCX — Displacement between elements of X. (Input)
The I-th element of X is X(1 + (I − 1) * INCX) if INCX is greater than or equal to zero, or X(1 + (I − N) * INCX) if INCX is less than zero.
Default: INCX = 1.

INCY — Displacement between elements of Y. (Input)
The I-th element of Y is Y(1 + (I − 1) * INCY) if INCY is greater than or equal to zero, or Y(1 + (I − N) * INCY) if INCY is less than zero.
Default: INCY = 1.

FORTRAN 90 Interface

Generic: DISL1 (X, Y [, …])

Specific: The specific interface names are S_DISL1 and D_DISL1.

FORTRAN 77 Interface

Single: DISL1(N, X, INCX, Y, INCY)

Double: The double precision function name is DDISL1.

Description

The function `DISL1` computes the 1-norm distance between two points *x* and *y*. The 1-norm distance is defined to be

$$\sum_{i=1}^{N} |x_i - y_i|$$

Example

Compute the 1-norm distance between two vectors of length 4.

```
      USE DISL1_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                  Declare variables
      INTEGER    INCX, INCY, N
      PARAMETER  (N=4)
!
      INTEGER    NOUT
      REAL       VAL, X(N), Y(N)
!
!                                  Set values for X and Y
!                                  X = ( 1.0 -1.0  0.0  2.0 )
!
!                                  Y = ( 4.0  2.0  1.0 -3.0 )
!
      DATA X/1.0, -1.0, 0.0, 2.0/
      DATA Y/4.0, 2.0, 1.0, -3.0/
!                                  Compute L1 distance
      VAL = DISL1(X,Y)
!                                  Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,*) ' The 1-norm distance is ', VAL
      END
```

Output

```
The 1-norm distance is     12.0000
```

DISLI

This function computes the infinity norm distance between two points.

Function Return Value

DISLI — Infinity norm distance between the points X and Y. (Output)

Required Arguments

X — Vector of length max(N * |INCX|, 1). (Input)

Y — Vector of length max(N * |INCY|, 1). (Input)

Optional Arguments

N — Length of the vectors X and Y. (Input)
Default: N = SIZE (X,1).

INCX — Displacement between elements of X. (Input)
The I-th element of X is X(1 + (I − 1) * INCX) if INCX is greater than or equal to zero, or X(1 + (I − N) * INCX) if INCX is less than zero.
Default: INCX = 1.

INCY — Displacement between elements of Y. (Input)
The I-th element of Y is Y(1 + (I − 1) * INCY) if INCY is greater than or equal to zero, or Y(1 + (I − N) * INCY) if INCY is less than zero.
Default: INCY = 1.

FORTRAN 90 Interface

Generic: DISLI (X, Y [, …])

Specific: The specific interface names are S_DISLI and D_DISLI.

FORTRAN 77 Interface

Single: DISLI(N, X, INCX, Y, INCY)

Double: The double precision function function name is DDISLI.

Description

The function `DISLI` computes the ∞-norm distance between two points *x* and *y*. The ∞-norm distance is defined to be

$$\max_{1 \le i \le N} |x_i - y_i|$$

Example

Compute the ∞-norm distance between two vectors of length 4.

```
      USE DISLI_INT
      USE UMACH_INT

      IMPLICIT    NONE
!                                 Declare variables
      INTEGER    INCX, INCY, N
      PARAMETER  (N=4)
!
      INTEGER    NOUT
      REAL       VAL, X(N), Y(N)
!
!                                 Set values for X and Y
!                                 X = ( 1.0 -1.0  0.0  2.0 )
!
!                                 Y = ( 4.0  2.0  1.0 -3.0 )
!
      DATA X/1.0, -1.0, 0.0, 2.0/
      DATA Y/4.0, 2.0, 1.0, -3.0/
!                                 Compute L-infinity distance
      VAL = DISLI(X,Y)
!                                 Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,*) ' The infinity-norm distance is ', VAL
      END
```

Output

```
The infinity-norm distance is     5.00000
```

VCONR

more...

Computes the convolution of two real vectors.

Required Arguments

X — Vector of length `NX`. (Input)

Y — Vector of length `NY`. (Input)

Z — Vector of length `NZ` containing the convolution `Z` = `X * Y`. (Output)

Optional Arguments

NX — Length of the vector `X`. (Input)
Default: `NX` = `SIZE` (`X`,1).

NY — Length of the vector `Y`. (Input)
Default: `NY` = `SIZE` (`Y`,1).

NZ — Length of the vector `Z`. (Input)
`NZ` must be at least `NX` + `NY` 1.
Default: `NZ` = `SIZE` (`Z`,1).

FORTRAN 90 Interface

Generic: `CALL VCONR (X, Y, Z [, …])`

Specific: The specific interface names are `S_VCONR` and `D_VCONR`.

FORTRAN 77 Interface

Single: `CALL VCONR (NX, X, NY, Y, NZ, Z)`

Double: The double precision name is `DVCONR`.

Description

The routine VCONR computes the convolution z of two real vectors x and y. Let n_x = NX, n_y = NY and n_z = NZ. The vector z is defined to be

$$z_j = \sum_{k=1}^{n_x} x_{j-k+1} y_k \quad \text{for } j = 1, 2, \ \ldots \ , n_z$$

where $n_z = n_x + n_y - 1$. If the index $j - k + 1$ is outside the range 1, 2, …, n_x, then x_{j-k+1} is taken to be zero.

The fast Fourier transform is used to compute the convolution. Define the complex vector u of length $n_z = n_x + n_y - 1$ to be

$$u = \left(x_1, x_2, \ \ldots \ , x_{n_x}, 0, \ \ldots \ , 0\right)$$

The complex vector v, also of length n_z, is defined similarly using y. Then, by the Fourier convolution theorem,

$$\hat{w}_i = \hat{u}_i \hat{v}_i \quad \text{for } i = 1, 2, \ \ldots \ , n_z$$

where the $\hat{u}$ indicates the Fourier transform of u computed via IMSL routines FFTCF and FFTCB (see *Chapter 6, "Transforms"*) is used to compute the complex vector w from $\hat{w}$. The vector z is then found by taking the real part of the vector w.

Comments

Workspace may be explicitly provided, if desired, by use of V2ONR/DV2ONR. The reference is

CALL V2ONR (NX, X, NY, Y, NZ, Z, XWK, YWK, ZWK, WK)

The additional arguments are as follows:

XWK — Complex work array of length NX + NY − 1.

YWK — Complex work array of length NX + NY − 1.

ZWK — Complex work array of length NX + NY − 1.

WK — Real work array of length 6 * (NX + NY − 1) + 15.

Example

In this example, the convolution of a vector x of length 8 and a vector y of length 3 is computed. The resulting vector z is of length 8 + 3 − 1 = 10. (The vector y is sometimes called a *filter*.)

```
      USE VCONR_INT
      USE WRRRN_INT
```

```
      IMPLICIT   NONE
      INTEGER    NX, NY, NZ
      PARAMETER  (NX=8, NY=3, NZ=NX+NY-1)
!
      REAL       X(NX), Y(NY), Z(NZ)
!                               Set values for X
!                     X = (1.0  2.0  3.0  4.0  5.0  6.0  7.0  8.0)
!                               Set values for Y
!                     Y = (0.0  0.0  1.0)
!
      DATA X/1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0/
      DATA Y/0.0, 0.0, 1.0/
!                               Compute vector convolution
!                               Z = X * Y
      CALL VCONR (X,Y,Z)
!                               Print results
      CALL WRRRN ('Z = X (*) Y', Z, 1, NZ, 1)
      END
```

Output

```
                                Z = X (*) Y
     1      2      3       4       5       6       7       8       9      10
 0.000  0.000  1.000   2.000   3.000   4.000   5.000   6.000   7.000   8.000
```

VCONC

more...

Computes the convolution of two complex vectors.

Required Arguments

X — Complex vector of length NX. (Input)

Y — Complex vector of length NY. (Input)

Z — Complex vector of length NZ containing the convolution Z = X * Y. (Output)

Optional Arguments

NX — Length of the vector X. (Input)
Default: NX = SIZE (X,1).

NY — Length of the vector Y. (Input)
Default: NY = SIZE (Y,1).

NZ — Length of the vector Z. (Input)
NZ must be at least NX + NY 1.
Default: NZ = SIZE (Z,1).

FORTRAN 90 Interface

Generic: CALL VCONC (X, Y, Z [, …])

Specific: The specific interface names are S_VCONC and D_VCONC.

FORTRAN 77 Interface

Single: CALL VCONC (NX, X, NY, Y, NZ, Z)

Double: The double precision name is DVCONC.

Description

The routine VCONC computes the convolution z of two complex vectors x and y. Let n_x = NX, then n_y = NY and n_z = NZ. The vector z is defined to be

$$z_j = \sum_{k=1}^{n_x} x_{j-k+1} y_k \quad \text{for } j = 1, 2, \ldots, n_z$$

where $n_z = n_x + n_y - 1$. If the index $j - k + 1$ is outside the range 1, 2, …, n_x, then x_{j-k+1} is taken to be zero.

The fast Fourier transform is used to compute the convolution. Define the complex vector u of length $n_z = n_x + n_y - 1$ to be

$$u = \left(x_1, x_2, \ldots, x_{n_z}, 0, \ldots, 0\right)$$

The complex vector v, also of length n_z, is defined similarly using y. Then, by the Fourier convolution theorem,

$$\hat{z}_i = \hat{u}_i \hat{v}_i \quad \text{for } i = 1, 2, \ldots, n_z$$

where the $\hat{u}$ indicates the Fourier transform of u computed using IMSL routine FFTCF. The complex vector z is computed from $\hat{w}$ via IMSL routine FFTCB. See *Chapter 6, "Transforms"* for more information on these functions.

Comments

Workspace may be explicitly provided, if desired, by use of V2ONC/DV2ONC. The reference is

```
CALL V2ONC (NX, X, NY, Y, NZ, Z, XWK, YWK, WK)
```

The additional arguments are as follows:

XWK — Complex work array of length NX + NY 1.

YWK — Complex work array of length NX + NY 1.

WK — Real work array of length 6 * (NX + NY − 1) + 15.

Example

In this example, the convolution of a vector x of length 4 and a vector y of length 3 is computed. The resulting vector z is of length 4 + 3 − 1. (y is sometimes called a *filter*.)

```
      USE VCONC_INT
      USE WRCRN_INT

      IMPLICIT   NONE
      INTEGER    NX, NY, NZ
```

```
      PARAMETER  (NX=4, NY=3, NZ=NX+NY-1)
!
      COMPLEX    X(NX), Y(NY), Z(NZ)
!                                Set values for X
!               X = ( 1.0+2.0i 3.0+4.0i 5.0+6.0i 7.0+8.0i )
!                                Set values for Y
!               Y = (0.0+0i 0.0+0i 1.0+0i )
!
      DATA X/(1.0,2.0), (3.0,4.0), (5.0,6.0), (7.0,8.0)/
      DATA Y/(0.0,0.0), (0.0,0.0), (1.0,1.0)/
!                                Compute vector convolution
!                                Z = X * Y
      CALL VCONC (X,Y,Z)
!                                Print results
      CALL WRCRN ('Z = X (*) Y', Z, 1, NZ, 1)
      END
```

Output

```
                            Z = X (*) Y
              1                 2                 3                 4
(  0.00,  0.00)  (  0.00,  0.00)  ( -1.00,  3.00)  ( -1.00,  7.00)

              5                 6
( -1.00, 11.00)  ( -1.00, 15.00)
```

Extended Precision Arithmetic

This section describes a set of routines for mixed precision arithmetic. The routines are designed to allow the computation and use of the full quadruple precision result from the multiplication of two double precision numbers. An array called the accumulator stores the result of this multiplication. The result of the multiplication is added to the current contents of the accumulator. It is also possible to add a double precision number to the accumulator or to store a double precision approximation in the accumulator.

The mixed double precision arithmetic routines are described below. The accumulator array, `QACC`, is a double precision array of length 2. Double precision variables are denoted by `DA` and `DB`. Available operations are:

Initialize a real accumulator, `QACC` ← `DA`.

`CALL DQINI (DA, QACC)`

Store a real accumulator, `DA` ← `QACC`.

`CALL DQSTO (QACC, DA)`

Add to a real accumulator, `QACC` ← `QACC` + `DA`.

`CALL DQADD (DA, QACC)`

Add a product to a real accumulator, `QACC` ← `QACC` + `DA*DB`.

`CALL DQMUL (DA, DB, QACC)`

There are also mixed double complex arithmetic versions of the above routines. The accumulator, `ZACC`, is a double precision array of length 4. Double complex variables are denoted by `ZA` and `ZB`. Available operations are:

Initialize a complex accumulator, `ZACC` ← `ZA`.

`CALL ZQINI (ZA, ZACC)`

Store a complex accumulator, `ZA` ← `ZACC`.

`CALL ZQSTO (ZACC, ZA)`

Add to a complex accumulator, `ZACC` ← `ZACC` + `ZA`.

`CALL ZQADD (ZA, ZACC)`

Add a product to a complex accumulator, `ZACC` ← `ZACC` + `ZA * ZB`.

CALL ZQMUL (ZA, ZB, ZACC)

Example

In this example, the value of 1.0D0/3.0D0 is computed in quadruple precision using Newton's method. Four iterations of

$$x_{k+1} = x_k + \left(x_k - a x_k^2\right)$$

with $a = 3$ are taken. The error $ax - 1$ is then computed. The results are accurate to approximately twice the usual double precision accuracy, as given by the IMSL routine DMACH(4), in the Reference Material section of this manual;. Since DMACH is machine dependent, the actual accuracy obtained is also machine dependent.

```
      USE IMSL_LIBRARIES

      IMPLICIT   NONE
      INTEGER    I, NOUT
      DOUBLE PRECISION A, DACC(2), DMACH, ERROR, SACC(2), X(2), X1, X2, EPSQ
!
      CALL UMACH (2, NOUT)
      A = 3.0D0
      CALL DQINI (1.0001D0/A, X)
!                                  Compute X(K+1) = X(K) - A*X(K)*X(K)
!                                  + X(K)
      DO 10  I=1, 4
         X1 = X(1)
         X2 = X(2)
!                                  Compute X + X
         CALL DQADD (X1, X)
         CALL DQADD (X2, X)
!                                  Compute X*X
         CALL DQINI (0.0D0, DACC)
         CALL DQMUL (X1, X1, DACC)
         CALL DQMUL (X1, X2, DACC)
         CALL DQMUL (X1, X2, DACC)
         CALL DQMUL (X2, X2, DACC)
!                                  Compute -A*(X*X)
         CALL DQINI (0.0D0, SACC)
         CALL DQMUL (-A, DACC(1), SACC)
         CALL DQMUL (-A, DACC(2), SACC)
!                                  Compute -A*(X*X) + (X + X)
         CALL DQADD (SACC(1), X)
         CALL DQADD (SACC(2), X)
   10 CONTINUE
!                                  Compute A*X - 1
      CALL DQINI (0.0D0, SACC)
      CALL DQMUL (A, X(1), SACC)
      CALL DQMUL (A, X(2), SACC)
      CALL DQADD (-1.0D0, SACC)
      CALL DQSTO (SACC, ERROR)
!                                  ERROR should be less than MACHEPS**2
      EPSQ = AMACH(4)
      EPSQ = EPSQ * EPSQ
      WRITE (NOUT,99999) ERROR, ERROR/EPSQ
!
99999 FORMAT ('  A*X - 1 = ', D15.7, ' = ', F10.5, '*MACHEPS**2')
      END
```

Output

```
A*X - 1 =   0.6162976D-32 =    0.12500*MACHEPS**2
```

Linear Algebra Operators and Generic Functions

Routines

Usage Notes

This chapter describes numerical linear algebra, Fourier transforms, random number generation, and other utility software packaged as *defined operations* that are executed with a function notation similar to standard mathematics. The resulting interface alters the way libraries are presented to the user. Many computations of numerical linear algebra are documented here as operators and generic functions. A notation is developed reminiscent of matrix algebra. This allows the Fortran user to express mathematical formulas in terms of operators. The operators can be used with both dense and sparse matrices.

A comprehensive Fortran module, *linear_operators*, defines the operators and functions. Its use provides this simplification. Subroutine calls and the use of type-dependent procedure names are largely avoided. This makes a rapid development cycle possible, at least for the purposes of experiments and proof-of-concept. The goal is to provide the Fortran programmer with an interface, operators, and functions that are useful and succinct. The modules can be used with or added to existing Fortran programs, but the operators provide a more readable program whenever they apply. This approach may require more hidden working storage. The size of the executable program may be larger than alternatives using subroutines. There are applications wherein the operator and function interface does not have the functionality that is available using subroutine libraries. To retain greater flexibility, some users will continue to require the techniques of calling subroutines.

A parallel computation for many of the defined operators and functions has been implemented. The type of problem solved is a simple one: several independent problems of the same data type and size. Most of the detailed communication for parallel computation is hidden from the user. Those functions having this data type computed in parallel are designated by the “MPI Capable” logo. The section *Dense Matrix Parallelism Using MPI* gives an introduction on how users should write their codes to use machines on a network.

A number of examples, in addition to those shown in this document, are supplied in the product examples directory. The name of the example code is shown in parentheses in the example heading, for those examples that are included with the product.

Matrix Optional Data Changes

To reset tolerances for determining singularity and to allow for other data changes, non-allocated "hidden" variables are defined within the modules. These variables can be allocated first, then assigned values which result in the use of different tolerances or greater efficiency in the executable program. The non-allocated variables, whose scope is limited to the module, are hidden from the casual user. Default values or rules are applied if these arrays are not allocated. In more detail, the inverse matrix operator **".i."** applied to a square matrix first uses the *LU* factorization code LIN_SOL_GEN and row pivoting. The default value for a small diagonal term is defined to be:

sqrt(epsilon(A))*sum(abs(A))/(n*n+1)

If the system is singular, a generalized matrix inverse is computed with the *QR* factorization code LIN_SOL_LSQ using this same tolerance. Both row and column pivoting are used. If the system is singular, an error message will be printed and a Fortran 90 STOP is executed. Users may want to change this rule. This is illustrated by continuing and not printing the error message. The following is a additional source to accomplish this, for all following invocations of the operator **".i."**:

allocate(s_inv_options(1))

s_inv_options (1) = skip_error_processing

B = .i. A

There are additional self-documenting integer parameters, packaged in the module *linear_operators*, that allow users other choices, such as changing the value of the tolerance, as noted above. Included is the ability to have the option apply for just the next invocation of the operator. Options are available that allow optional data to be passed to supporting Fortran 90 subroutines. This is illustrated in the following example:

Operator_ex36.f90

```
      use linear_operators

      implicit none

! This is the equivalent of Example 4 for LIN_GEIG_GEN (using operators).

      integer, parameter :: n=32
      real(kind(1d0)), parameter :: one=1d0, zero=0d0
      real(kind(1d0)) a(n,n), b(n,n), bta(n), err
      complex(kind(1d0)) alpha(n), v(n,n)

! Generate random matrices for both A and B.
      A = rand(A); B = rand(B)

! Set the option, a larger tolerance than default for lin_sol_lsq.
      allocate(d_eig_options(6))
```

```
       d_eig_options(1) = options_for_lin_geig_gen
       d_eig_options(2) = 4
       d_eig_options(3) = d_lin_geig_gen_for_lin_sol_lsq
       d_eig_options(4) = 2
       d_eig_options(5) = d_options(d_lin_sol_lsq_set_small,&
                          sqrt(epsilon(one))*norm(B,1))
       d_eig_options(6) = d_lin_sol_lsq_no_sing_mess

 ! Compute the generalized eigenvalues.
       alpha = EIG(A, B=B, D=bta, W=V)

 ! Check the residuals.
       err = norm((A .x. V .x. diag(bta)) - (B .x. V .x. diag(alpha)),1)/&
             (norm(A,1)*norm(bta,1)+norm(B,1)*norm(alpha,1))

       if (err  <= sqrt(epsilon(one))) then
          write (*,*) 'Example 4 for LIN_GEIG_GEN (operators) is correct.'
       end if
 ! Clean up the allocated array.  This is good housekeeping.
       deallocate(d_eig_options)
       end
```

Note that in this example one first allocates the array by which the user will pass the new options for `EIG` to use. This array is named `d_eig_options` in accordance with the name of the unallocated option array specified in the documentation for `EIG`. A size of 6 is specified because a total of six options must be passed to `EIG` to accomplish the resetting of the singular value tolerance and to turn off the printing of the error message when the matrix is singular. The first entry of `d_eig_options` specifies which of the options for `EIG` will be set. The next entry designates the number of entries which follows that apply to "`options_for_lin_geig_gen`". The third entry specifies the option value of `LIN_GEIG_GEN` to be set, `d_lin_geig_gen_for_lin_sol_lsq`. The fourth entry specifies the number of entries that follow which apply to `LIN_SOL_LSQ`. Finally, the fifth and sixth entries set the two `LIN_SOL_LSQ` options that we desire.

Dense Matrix Computations

MPI CAPABLE

For a detailed description of MPI Capability see *Dense Matrix Parallelism Using MPI*.

This section is concerned with methods for computing with dense matrices. Consider a Fortran 90 code fragment that solves a linear system of algebraic equations, $Ay = b$, then computes the residual $r = b - Ay$. A standard mathematical notation is often used to write the solution,

$$y = A^{-1}b$$

A user thinks: "matrix and right-hand side yields solution." The code shows the computation of this mathematical solution using a defined Fortran operator "**.ix.**", and random data obtained with the function, *rand*. This operator is read "inverse matrix times." The residuals are computed with another defined Fortran operator "**.x.**", read "matrix times vector." Once a user understands the equivalence of a mathematical formula with the corresponding Fortran operator, it is possible to write this program with little effort. The last line of the example before `end` is discussed below.

```
USE linear_operators
   integer,parameter :: n=3; real A(n,n), y(n), b(n), r(n)
   A=rand(A); b=rand(b); y = A .ix. b
   r = b - (A .x. y ) ! Parentheses are needed
end
```

The IMSL Fortran Numerical Library provides additional lower-level software that implements the operation "**.ix.**", the function *rand*, matrix multiply "**.x.**", and others not used in this example. Standard matrix products and inverse operations of matrix algebra are shown in the following table:

Defined Array Operation	**Matrix Operation**	**Alternative in Fortran 90**
A .x. B	AB	matmul(A, B)
.i. A	A^{-1}	lin_sol_gen lin_sol_lsq
.t. A, .h. A	A^T, A^H	transpose(A) conjg(transpose(A))

Defined Array Operation	Matrix Operation	Alternative in Fortran 90
A .ix. B	$A^{-1}B$	lin_sol_gen lin_sol_lsq
B .xi. A	BA^{-1}	lin_sol_gen lin_sol_lsq
A .tx. B, or (.t. A) .x. B A .hx. B, or (.h. A) .x. B	$A^TB,\ A^HB$	matmul(transpose (A), B) matmul(conjg(transpose(A)), B)
B .xt. A, or B .x. (.t. A) B .xh. A, or B .x. (.h. A)	$BA^T,\ BA^H$	matmul(B, transpose(A)) matmul(B, conjg(transpose(A)))

The IMSL operators apply generically to all standard precisions and floating-point data types – real and complex – and to objects that are broader in scope than arrays with a fixed number of dimensions. For example, the matrix product "**.x**." applies to matrix times vector and matrix times matrix represented as Fortran 90 arrays. It also applies to "independent matrix products." For this, use the notion: *a box of problems* to refer to independent linear algebra computations, of the same kind and dimension, but different data. The *racks* of the box are the distinct problems. In terms of Fortran 90 arrays, a rank-3, assumed-shape array is the data structure used for a box. The first two dimensions are the data for a matrix; the third dimension is the rack number. Each problem is independent of other problems in consecutive racks of the box. We use parallelism of an underlying network of processors, and MPI, when computing these disjoint problems.

In addition to the operators **.ix.**, **.xi.**, **.i.**, and **.x.**, additional operators **.t.**, **.h.**, **.tx.**, **.hx.**, **.xt.**, and **.xh.** are provided for complex matrices. Since the transpose matrix is defined for complex matrices, this meaning is kept for the defined operations. In order to write one defined operation for both real and complex matrices, use the conjugate-transpose in all cases. This will result in only real operations when the data arrays are real.

For sums and differences of vectors and matrices, the intrinsic array operations "+" and "−" are available. It is not necessary to have separate defined operations. A parsing rule in Fortran 90 states that the result of a defined operation involving two quantities has *a lower precedence* than any intrinsic operation. This explains the parentheses around the next-to-last line containing the sub-expression "`A .x. y`" found in the example. Users are advised to always include parentheses around array expressions that are mixed with defined operations, or whenever there is possible confusion without them. The next-to-last line of the example results in computing the residual associated with the solution, namely $r = b - Ay$. Ideally, this residual is zero when the system has a unique solution. It will be computed as a non-zero vector due to rounding errors and conditioning of the problem.

Dense Matrix Functions

MPI CAPABLE

For a detailed description of MPI Capability see *Dense Matrix Parallelism Using MPI*.

Several decompositions and functions required for numerical linear algebra follow. The convention of enclosing optional quantities in brackets, "[ ]" is used.

Defined Array Functions	**Matrix Operation**
S=SVD(A [,U=U, V=V])	$A = USV^T$
E=EIG(A [[,B=B, D=D], V=V, W=W])	$(AV = VE), AVD = BVE$ $(AW = WE), AWD = BWE$
R=CHOL(A)	$A = R^T R$
Q=ORTH(A [,R=R])	$(A = QR), Q^TQ = I$
U=UNIT(A)	$[u_1, \ldots] = [a_1/\|a_1\|, \ldots]$
F=DET(A)	Det(A) = determinant
K=RANK(A)	rank(A) = rank
P=NORM(A[,[type=]i])	$\left\Vert A \right\Vert_1 = \max_j(\sum_{i=1}^{m} \vert a_{ij} \vert)$ $\Vert A \Vert_2 = s_1 = \text{largest singular value}$ $\left\Vert A \right\Vert_{\infty \leftrightarrow \text{huge}(1)} = \max_i(\sum_{j=1}^{n} \vert a_{ij} \vert)$
C=COND(A)	$s_1 / s_{\text{rank}(A)}$
Z=EYE(N)	$Z = I_N$
A=DIAG(X)	$A = diag(x_1, \ldots)$
X=DIAGONALS(A)	$x = (a_{11}, \ldots)$
Y=FFT (X,[WORK=W]); X=IFFT(Y,[WORK=W])	Discrete Fourier Transform, Inverse
Y=FFT_BOX (X,[WORK=W]); X=IFFT_BOX(Y,[WORK=W])	Discrete Fourier Transform for Boxes, Inverse

Defined Array Functions	Matrix Operation
A=RAND(A)	Random numbers, $0 < A < 1$
L=isNaN(A)	Test for `NaN`, *if (l) then…*

In certain functions, the optional arguments are inputs while other optional arguments are outputs. To illustrate the example of the box **SVD** function, a code is given that computes the singular value decomposition and the reconstruction of the random matrix box, A, using the computed factors, $R = USV^T$. Mathematically $R = A$, but this will be true, only approximately, due to rounding errors. The value $units\_of\_error = \|A - R\|/(\|A\|\varepsilon)$, shows the merit of this approximation.

Dense Matrix Parallelism Using MPI

more...

General Remarks

The central theme we use for the computing functions of the box data type is that of delivering results to a distinguished node of the machine. One of the design goals was to shield much of the complexity of distributed computing from the user.

The nodes are numbered by their "ranks." Each node has *rank value* `MP_RANK`. There are `MP_NPROCS` nodes, so `MP_RANK = 0, 1,...,MP_NPROCS-1`. The root node has `MP_RANK = 0`. Most of the elementary MPI material is found in Gropp, Lusk, and Skjellum (1994) and Snir, Otto, Huss-Lederman, Walker, and Dongarra (1996). Although IMSL Fortran Numerical Library users are for the most part shielded from the complexity of MPI, it is desirable for some users to learn this important topic. Users should become familiar with any referenced MPI routines and the documentation of their usage. MPI routines are not discussed here, because that is best found in the above references.

The IMSL Fortran Numerical Library algorithm for allocating the racks of the box to the processors consists of creating a schedule for the processors, followed by communication and execution of this schedule. The efficiency may be improved by using the nodes according to a specific *priority order*. This order can reflect information such as a powerful machine on the network other than the user's work station, or even transient network behavior.

The IMSL Fortran Numerical Library allows users to define this order, but a default order is provided. A setup function establishes an order based on timing matrix products of a size given by the user. See *Parallel Example 4* for an illustration of this usage.

Getting Started with Modules MPI_setup_int and MPI_node_int

The `MPI_setup_int` and `MPI_node_int` modules are part of the IMSL Fortran Numerical Library and not part of MPI itself. Following a call to the function `MP_SETUP()`, the module `MPI_node_int` will contain information about the number of processors, the rank of a processor, the communicator for IMSL Fortran Numerical Library, and the usage priority order of the node machines. Since `MPI_node_int` is used by `MPI_setup_int`, it is not necessary to explicitly use this module. If neither `MP_SETUP()` nor `MPI_Init()` is called, then the box data type will compute entirely on one node. No routine from MPI will be called.

```
MODULE MPI_NODE_INT
  INTEGER, ALLOCATABLE :: MPI_NODE_PRIORITY(:)
  INTEGER, SAVE :: MP_LIBRARY_WORLD = huge(1)
  LOGICAL, SAVE :: MPI_ROOT_WORKS = .TRUE.
  INTEGER, SAVE :: MP_RANK = 0, MP_NPROCS = 1
END MODULE
```

When the function `MP_SETUP()` is called with no arguments, the following events occur:

- If MPI has not been initialized, it is first initialized. This step uses the routines `MPI_Initialized()` and possibly `MPI_Init()`. Users who choose not to call `MP_SETUP()` must make the required initialization call before using any IMSL Fortran Numerical Library code that relies on MPI for its execution. If the user's code calls an IMSL Fortran Numerical Library function utilizing the box data type and MPI has not been initialized, then the computations are performed on the root node. The only MPI routine always called in this context is `MPI_Initialized()`. The name `MP_SETUP` is pushed onto the subprogram or call stack.
- If `MP_LIBRARY_WORLD` equals its initial value `(=huge(1))` then `MPI_COMM_WORLD`, the default MPI communicator, is duplicated and becomes its handle. This uses the routine `MPI_Comm_dup()`. Users can change the handle of `MP_LIBRARY_WORLD` as required by their application code. Often this issue can be ignored.
- The integers `MP_RANK` and `MP_NPROCS` are respectively the node's rank and the number of nodes in the communicator, `MP_LIBRARY_WORLD`. Their values require the routines `MPI_Comm_size()` and `MPI_Comm_rank()`. The default values are important when MPI is not initialized and a box data type is computed. In this case the root node is the only node and it will do all the work. No calls to MPI communication routines are made when `MP_NPROCS = 1` when computing the box data type functions. A program can temporarily assign this value to force box data type computation entirely at the root node. This is desirable for problems where using many nodes would be less efficient than using the root node exclusively.

- The array MPI_NODE_PRIORITY(:) is unallocated unless the user allocates it. The IMSL Fortran Numerical Library codes use this array for assigning tasks to processors, if it is allocated. If it is not allocated, the default priority of the nodes is (0,1,...,MP_NPROCS-1). Use of the function call MP_SETUP(N) allocates the array, as explained below. Once the array is allocated its size is MP_NPROCS. The contents of the array is a permutation of the integers 0,...,MP_NPROCS-1. Nodes appearing at the start of the list are used first for parallel computing. A node other than the root can avoid any computing, except receiving the schedule, by setting the value MPI_NODE_PRIORITY(I) < 0. This means that node |MPI_NODE_PRIORITY(I)| will be sent the task schedule but will not perform any significant work as part of box data type function evaluations.
- The LOGICAL flag MPI_ROOT_WORKS designates whether or not the root node participates in the major computation of the tasks. The root node communicates with the other nodes to complete the tasks but can be designated to do no other work. Since there may be only one processor, this flag has the default value .TRUE., assuring that one node exists to do work. When more than one processor is available users can consider assigning MPI_ROOT_WORKS=.FALSE.. This is desirable when the alternate nodes have equal or greater computational resources compared with the root node. *Parallel Example 4* illustrates this usage. A single problem is given a box data type, with one rack. The computing is done at the node, other than the root, with highest priority. This example requires more than one processor since the root does no work.

When the generic function MP_SETUP(N) is called, where N is a positive integer, a call to MP_SETUP() is first made, using no argument. Use just one of these calls to MP_SETUP(). This initializes the MPI system and the other parameters described above. The array MPI_NODE_PRIORITY(:) is allocated with size MP_NPROCS. Then DOUBLE PRECISION matrix products $C = AB$, where A and B are N by N matrices, are computed at each node and the elapsed time is recorded. These elapsed times are sorted and the contents of MPI_NODE_PRIORITY(:) are permuted in accordance with the shortest times yielding the highest priority. All the nodes in the communicator MP_LIBRARY_WORLD are timed. The array MPI_NODE_PRIORITY(:) is then broadcast from the root to the remaining nodes of MP_LIBRARY_WORLD using the routine MPI_Bcast(). Timing matrix products to define the node priority is relevant because the effort to compute C is comparable to that of many linear algebra computations of similar size. Users are free to define their own node priority and broadcast the array MPI_NODE_PRIORITY(:) to the alternate nodes in the communicator.

To print any IMSL Fortran Numerical Library error messages that have occurred at any node, and to finalize MPI, use the function call MP_SETUP('Final'). Case of the string 'Final' is not important. Any error messages pending will be discarded after printing on the root node. This is triggered by popping the name 'MP_SETUP' from the subprogram stack or returning to Level 1 in the stack. Users can obtain error messages by popping the stack to Level 1 and still continuing with MPI calls. This requires executing `call e1pop ('MP_SETUP')`. To continue on after summarizing errors execute `call e1psh ('MP_SETUP')`. More details about the error processor are found in *Reference Material* chapter of this manual.

Messages are printed by nodes from largest rank to smallest, which is the root node. Use of the routine `MPI_Finalize()` is made within `MP_SETUP('Final')`, which shuts down MPI. After `MPI_Finalize()` is called, the value of `MP_NPROCS = 0`. This flags that MPI has been initialized and terminated. It cannot be initialized again in the same program unit execution. No MPI routine is defined when `MP_NPROCS` has this value.

Using Processors

There are certain pitfalls to avoid when using IMSL Fortran Numerical Library and box data types as implemented with MPI. A fundamental requirement is to allow all processors to participate in parts of the program where their presence is needed for correctness. It is incorrect to have a program unit that restricts nodes from executing a block of code required when computing with the box data type. On the other hand it is appropriate to restrict computations with rank-2 arrays to the root node. This is not required, but the results for the alternate nodes are normally discarded. This will avoid gratuitous error messages that may appear at alternate nodes.

Observe that only the root has a correct result for a box data type function. Alternate nodes have the constant value one as the result. The reason for this is that during the computation of the functions, sub-problems are allocated to the alternate nodes by the root, but for only the root to utilize the result. If a user needs a value at the other nodes, then the root must send it to the nodes. See *Parallel Example 3* for an illustration of this usage. Convergence information is computed at the root node and broadcast to the others. Without this step some nodes would not terminate the loop even when corrections at the root become small. This would cause the program to be incorrect.

Sparse Matrix Computations

Introduction

This section is concerned with methods for computing with sparse matrices. Our primary goal is to give the appearance of simplicity and allow ease-of-use in dealing with these calculations. The underlying principle in our design is to use Fortran 2003 standard support for derived types with initialized and allocatable components. To perform data storage and conversions we use overloaded assignment to hide complexity. The operations currently supported are:

- defining entries of the matrices,
- adding sparse matrices,
- forming products of sparse matrices and dense vectors or matrices,
- solving linear systems of algebraic equations
- condition number computation
- conversion of sparse matrices or dense arrays to the converse
- storage management operations

The definition of the sparse matrices starts with a *triplet* consisting of the row and column indices and a value at that entry. By setting a flag in the derived type `SLU_Options`, repeated values may be accumulated to yield a value that is the sum of all triplets for that matrix entry. A diagram for constructing a single precision sparse 10000 × 10000 matrix, `H`, is illustrated with the pseudocode fragment:

```
Use linear_operators
Integer I, J; Real(Kind(1.e0)) value, x(10000)
Type(s_sparse) A
Type(s_hbc_sparse) H
```

Define non-zero values of A with repeated overloaded assignments

`A = s_entry(I, J, value)`.

Convert to computational Harwell-Boeing form with the overloaded assignment `H = A`.

Compute with sparse matrix `H`, *e. g.*, `x = H .ix. x`.

A basic feature is that there are four sparse matrix derived types, *Types (s_hbc_sparse)*, *(d_hbc_sparse)*, *(c_hbc_sparse)*, and *(z_hbc_sparse)*. These respectively handle single, double, complex and double-complex data. The defined operators work with a sparse matrix and a corresponding dense array of the same precision and data type. There is no mixing of data types such as a sparse double precision matrix multiplied by a single precision vector. To accommodate that case an intermediate double precision quantity will be created that ascends the single precision vector to a double precision vector. The table below shows the operations that are valid with sparse matrix types.

Mathematical Operation	**Operation Notation**	**Input Terms**	**Output Terms**
$y = H^{-1}x$	y = H .ix. x	$H_{n\times n}$ sparse, x(1:k), $k \geq n$	y(1:n)
$y = x^T H^{-1} \equiv H^{-T}x$	y = x .xi. H	$H_{n\times n}$ sparse, x(1:k), $k \geq n$	y(1:n)
$Y = H^{-1}X_{n\times r}$	Y= H .ix. X	$H_{n\times n}$ sparse, X(1:k,1:r), $k \geq n$	Y(1:n,1:r)
$Y = X_{r\times n}H^{-1} \equiv (H^{-T}X^T)^T$	Y = X .xi. H	$H_{n\times n}$ sparse, X(1:r,1:k), $k \geq n$	Y(1:r,1:n)
$y = Hx$	y = H .x. x	$H_{m\times n}$ sparse, x(1:k), $k \geq n$	y(1:m)
$y = x^T H \equiv H^T x$	y = x .x. H	$H_{m\times n}$ sparse, x(1:k), $k \geq m$	y(1:n)
$Y = HX_{n\times r}$	Y = H .x. X	$H_{m\times n}$ sparse, X(1:k,1:r), $k \geq n$	Y(1:m,1:r)
$Y = X_{r\times m}H$	Y = X .x. H	$H_{m\times n}$ sparse, X(1:r,1:k), $k \geq m$	Y(1:r,1:n)
$K = H^T$	K = .t. H	$H_{m\times n}$ sparse	$K_{n\times m}$ sparse
$K = H^H = \overline{H}^T$	K = .h. H	$H_{m\times n}$ sparse, complex	$K_{n\times m}$ sparse
$y = H^T x$	y = H .tx. x	$H_{m\times n}$ sparse, x(1:k), $k \geq m$	y(1:n)
$Y = H^T X_{m\times r}$	Y = H .tx. X	$H_{m\times n}$ sparse, X(1:k,1:r), $k \geq m$	Y(1:n,1:r)
$y = x^T H$	Y = x .tx. H	$H_{m\times n}$ sparse, x(1:k), $k \geq m$	y(1:n)
$Y = X^T{}_{r\times m}H$	Y = X .tx. H	$H_{m\times n}$ sparse, X(1:k,1:r), $k \geq m$	Y(1:r,1:n)
$y = Hx^T$	y = H .xt. x	$H_{m\times n}$ sparse, x(1:k), $k \geq n$	y(1:m)
$Y = HX^T{}_{n\times r}$	Y = H .xt. X	$H_{m\times n}$ sparse, x(1:k,1:r), $k \geq n$	Y(1:m,1:r)
$y = xH^T$	y = x .xt. H	$H_{m\times n}$ sparse, x(1:k), $k \geq n$	y(1:m)
$Y = X_{r\times n}H^T$	Y = X .xt. H	$H_{m\times n}$ sparse, x(1:r,1:k), $k \geq n$	Y(1:r,1:m)
$y = H^H x = \overline{H}^T x$	y = H .hx. x	$H_{m\times n}$ sparse[1], x(1:k), $k \geq m$	y(1:n)
$Y = H^H X_{m\times r} = \overline{H}^T X_{m\times r}$	Y = H .hx. X	$H_{m\times n}$ sparse, X(1:k,1:r), $k \geq m$	Y(1:n,1:r)
$y = x^H H = \overline{x}^T H$	Y = x .hx. H	$H_{m\times n}$ sparse, x(1:k), $k \geq m$	y(1:n)
$Y = X^H_{r\times m}\ H = \overline{X}^T_{r\times m}\ H$	Y = X .hx. H	$H_{m\times n}$ sparse, X(1:k,1:r), $k \geq m$	Y(1:r,1:n)
$y = Hx^H = H\overline{x}^T$	y = H .xh. x	$H_{m\times n}$ sparse, x(1:k), $k \geq n$	y(1:m)

Mathematical Operation	Operation Notation	Input Terms	Output Terms
$Y = HX^H_{n \times r} = H\overline{X}^T_{n \times r}$	Y = H .xh. X	$H_{m \times n}$ sparse, x(1:k,1:r), $k \geq n$	Y(1:m,1:r)
$y = xH^H = x\overline{H}^T$	y = x .xh H	$H_{m \times n}$ sparse, x(1:k), $k \geq n$	y(1:m)
$Y = X_{r \times n} H^H = X_{r \times n} \overline{H}^T$	Y = X .xh. H	$H_{m \times n}$ sparse, x(1:r,1:k), $k \geq n$	Y(1:r,1:m)

[1] The operators `.hx.` and `.xh.` apply to sparse complex matrices only. For real matrices use the `.tx.` and `.xt.` operators.

Derived Type Definitions

A derived type is used for the entries (triplets or coordinate format) of a sparse matrix, which consists of row and column coordinates and a corresponding value:

```
type s_entry
    integer irow
    integer jcol
    real(kind(1.e0)) value
end type
```

Additionally, type (`d_entry`), type (`c_entry`), and type (`z_entry`) are defined similarly. These support double precision, complex and complex-double precision accuracy and types.

Thus for a sparse matrix *A*, the entry at the intersection of row `irow` and column `jcol` is the scalar `value`. We define a sparse matrix representation in terms of a collection of triplets. This is a convenient way for a user to define a sparse matrix. This representation is used to define the matrix entries in a user's program using overloaded assignment. There is no implied order on the collection of triplets that define this sparse matrix. Our experience shows that for writing application code the technique of using triplets to define the matrix entries is convenient and provides a workable transition from mathematical definitions of the entries to computer code. Also note that there is generally no need for the programmer to allocate the components of a matrix of type `s_sparse` when using the overloaded assignment: `s_sparse = s_entry`. The software handles this detail by reallocating and expanding those components of the `s_sparse` matrix as required. (For this task we use the Fortran 2003 intrinsic subroutine `move_alloc()`, when it is available. This routine provides an efficient way to perform a reallocation.) The amount reallocated is controlled by an expansion factor that is a component of the derived type `SLU_options`.

```
type s_sparse
    integer :: mrows = 0
    integer :: ncols = 0
    integer :: numnz = 0
    integer, allocatable, dimension(:) :: irow
    integer, allocatable, dimension(:) :: jcol
    real(kind(1.e0)), allocatable, dimension(:) :: value
    type (SLU_options) options
```

```
      end type
```

When performing matrix computations we use the *Harwell-Boeing* column-oriented derived type. The row indices, for each column, are unique and increasing. The values in the `colptr(1:ncols)` component mark the start of the row indices and corresponding matrix entries for that column. The value `colptr(ncols+1)-1` will equal the value `numnz` after the matrix is defined with non-zero entries. The row indices for each column are in array `irow(:)`. They are unique and sorted into increasing order.

```
      type s_hbc_sparse
          integer :: mrows = 0
          integer :: ncols = 0
          integer :: numnz = 0
          integer, allocatable, dimension(:) :: irow
          integer, allocatable, dimension(:) :: colptr
          real(kind(1.e0)), allocatable, dimension(:) :: value
          type(SLU_options) options
      end type
```

Additionally we support types `(d_hbc_sparse)`, type `(c_hbc_sparse)`, and type `(z_hbc_sparse)`. These will have analogous support for the operations defined with type `(s_hbc_sparse)` and others that follow. From now on we only mention type `(s_hbc_sparse)`.

All components of the type `(s_sparse)` object are self-explanatory except for the one named `type(SLU_options)`. This component contains various parameters for managing the data structure, and for computing matrix products and linear system solutions. Normally these components do not need to be changed from their default values.

The derived type `SLU_Options` carries extra required information. That data needed for SuperLU[2] is labeled with a comment. The remaining data is needed by IMSL codes that call on SuperLU. Of particular importance is the `Sequence` attribute statement. This prevents the Fortran compiler from rearranging the order of the components. Maintaining this order is required since the derived type `SLU_Options` is passed to a IMSL C code that uses the information as a C *structure*. The `Sequence` statement orders the Fortran-defined data so that it matches the C code structure.

> SuperLU is used to support the defined operations `.ix.` and `.xi.`, and the condition number function, `cond()`. SuperLU is well-tested. Distributed and threaded versions are available but these are not used here in our software at present. SuperLU was developed by James W. Demmel, Stanley C. Eisenstat, John R. Gilbert, Xiaoye S. Li, and Joseph W. H. Liu. Note that the authors do not support the package in the context used in the IMSL Libraries.

```
  Type SLU_options
           Sequence
           Integer :: unique = 1 ! Each new entry is unique -IMSL
           Integer :: Accumulate = 0
                                 ! Accumulate or assemble duplicated entries in
                                 ! a ?_sparse matrix.  This flag is checked
                                 ! when executing an overloaded assignment
                                 ! with a Harwell-Boeing = ?_sparse matrix.
                                 ! The default is not to accumulate (0)
                                 ! Assign the value 1 to accumulate.
```

```
           Integer :: handle(2) = 0
                               ! Each HBC matrix requiring an LU
                               ! decomposition will have allocated
                               ! arrays whose start is pointed to by
                               ! this value.  In cases where the OS
                               ! uses 64 bit addressing 8 bytes are used.
           Integer :: Info = - 1
                               ! Flag returned after LU factorization (SuperLU)
           Integer :: Fact = 0 !DOFACT - SuperLU
           Integer :: Equil = 1 !YES
           Integer :: ColPerm = 3 !COLAMD
           Integer :: Trans = 0 !NOTRANS
           Integer :: IterRefine = 1 !REFINE
           Integer :: PrintStat = 0  !NO
           Integer :: SymmetricMode = 0 !NO
           Integer :: PivotGrowth = 0 !NO
           Integer :: ConditionNumber = 0 !NO
           Integer :: RowPerm = 0 !NO
           Integer :: ReplaceTinyPivot = 0 !NO
           Integer :: SolveInitialized = 0 !NO
           Integer :: RefineInitialized = 0 !NO
           Real (Kind(1.d0)) :: DiagPivotThresh = 1.d0 ! SuperLU
           Real (Kind(1.d0)) :: expansion_factor = 1.2 ! VNI -
  ! The factor to use when expanding storage.  Any value > 1.
  ! can be used such that the integer part of this factor times
  ! any integer > 9 provides at least a value of 1 increase.
           Integer :: Cond_Iteration_Max = 30
  ! Maximum number of Lanczos and inverse iterations with sparse COND().
            Integer Alignment_Dummy
       End Type
```

Overloaded Assignments

A natural way to define a sparse matrix is in terms of its triplets. The basic tool used here to define all the non-zero entries is *overloaded assignment*. Fortran 90, and further updates to the standard, supports a hidden subroutine call, packaged in a module, when an assignment is executed between differing derived types. Thus if a Fortran program has a declaration `type(s_sparse) A`, then the overloaded assignment statement

```
A = s_entry(I, J, value)
```

has the effect of calling subroutines that result in joining the matrix entry ***value*** at the intersection of row `I` and column `J`. The components of `A` are managed to hold any number of values. The number of rows, columns and non-zero values are updated as new triplets are assigned. Also the arrays that hold the triplets are re-allocated and expanded, as required, to hold newly assigned triplets.

The code snippet for this operation, and others that follow, will require use of the module `linear_operators`. If new space is required in the assignment, a reallocation of the components of the matrix `A` will occur. The user does not have to manage the details.

```
Use linear_operators
Type(s_sparse) A
…

{For all entries in A, A = s_entry(I, J, Value)}
```

Sparse = Collection of Triplets

The Harwell-Boeing sparse matrix data types are used for computations. An assignment, H = A, implies deallocating any allocated components of H, allocating new storage, and sorting the collection of triplets provided as input in the sparse matrix A. If the accumulation flag is set in H%options%accumulate, the duplicate row indices in a column are reduced to a single entry and the corresponding values are added to yield a final value. The assignment H = 0 deallocates the allocated components and returns H to its initialized state, except for any changes to the component SLU_options. A similar comment holds for the assignment, A = 0.

```
Use linear_operators
Type(s_sparse) A
Type(s_hbc_sparse) H
…
{For all nonzero matrix entries, A = s_entry(I, J, Value)}

H = A
A = 0   ! Clear and deallocate components of A
…
H = 0   ! Clear and deallocate components of H
```

Sparse = Dense

The non-zero entries of the dense array are converted to a Harwell-Boeing sparse matrix. As a first step any allocated components are cleared and then allocated as needed to hold the non-zero values of the dense array. The specific dimensions of array D are arbitrary.

```
Use linear_operators
Type(s_hbc_sparse) H
Integer, parameter :: M=1000, N=1000
Real (kind(1.e0)) D(M,N)
{Define entries of D}
H = D
```

Dense = Sparse

For some applications it is convenient to expand a sparse matrix into a dense matrix. The specific dimensions of array D are arbitrary.

```
Use linear_operators
Type(s_hbc_sparse) H
Integer, parameter :: M=1000, N=1000
Real (kind(1.e0)) D(M,N)
{Define entries of H}
D = H
```

Scalar = s_hbc_entry(Sparse, I, J)

This assignment gets the value at the intersection of row I and column J of the Harwell-Boeing sparse matrix. There must be type agreement with the function and sparse matrix type. Use a prefix of d_, c_, or z_ for double, complex, or double complex values.

```
Use inear_operators
Type(s_hbc_sparse) H
Real (kind(1.e0)) value
{Define entries of H, I and J}
value = s_hbc_entry(H, I, J)
```

.x.

Computes matrix-matrix or matrix-vector product.

Operator Return Value

Matrix containing the product of A and B. (Output)

Required Operands

A — Left operand matrix or vector. This is an array of rank 1, 2, or 3. It may be real, double, complex, double complex, or one of the computational sparse matrix derived types, `?_hbc_sparse`. (Input)
Note that A and B cannot both be `?_hbc_sparse`.

B — Right operand matrix or vector. This is an array of rank 1, 2, or 3. It may be real, double, complex, double complex, or one of the computational sparse matrix derived types, `?_hbc_sparse`. (Input)
Note that A and B cannot both be `?_hbc_sparse`.

If A has rank one, B must have rank two.
If B has rank one, A must have rank two.
If A has rank three, B must have rank three.
If B has rank three, A must have rank three.

FORTRAN 90 Interface

```
A .x. B
```

Description

Computes the product of matrix or vector A and matrix or vector B. The results are in a precision and data type that ascends to the most accurate or complex operand.

Rank three operation is defined as follows:

```
do i = 1, min(size(A,3), size(B,3))
   X(:,:,i) =  A(:,:,i) .x. B(:,:,i)
end do
```

`.x.` can be used with either dense or sparse matrices. It is MPI capable for dense matrices only.

Examples

Dense Matrix Example (operator_ex03.f90)

```
   use linear_operators
       implicit none

! This is the equivalent of Example 3 for LIN_SOL_GEN using operators.
       integer, parameter :: n=32
       real(kind(1e0)) :: one=1e0, zero=0e0, A(n,n), b(n), x(n)
       real(kind(1e0)) change_new, change_old
       real(kind(1d0)) :: d_zero=0d0, c(n), d(n,n), y(n)

! Generate a random matrix and right-hand side.
       A = rand(A); b= rand(b)

! Save double precision copies of the matrix and right-hand side.
       D = A
       c = b
! Compute single precision inverse to compute the iterative refinement.
       A = .i. A

! Start solution at zero.  Update it to an accurate solution
! with each iteration.
       y = d_zero
       change_old = huge(one)

       iterative_refinement: do
! Compute the residual with higher accuracy than the data.
          b = c - (D .x. y)

! Compute the update in single precision.
          x = A .x. b
          y = x + y
          change_new = norm(x)

! Exit when changes are no longer decreasing.
          if (change_new >= change_old) exit iterative_refinement
          change_old = change_new
       end do iterative_refinement

       write (*,*) 'Example 3 for LIN_SOL_GEN (operators) is correct.'
       end
```

Sparse Matrix Example

Consider the one-dimensional Dirichlet problem

$$\frac{d^2u}{dx^2} = f(x), \quad a < x < b, \quad u(a) = u_a = u_1, u(b) = u_b = u_N$$

Using a standard approach to solving this involves approximating the second derivative operator with central divided differences

$$\frac{d^2u}{dx^2} \approx \frac{u_{i-1} - 2u_i + u_{i+1}}{h^2}, \quad h = (b-a)/(N-1), \quad i = 2, \ldots, N-1, \quad N > 2$$

This leads to the sparse linear algebraic system *Mu* = *w*. The definitions for these terms are implied in the following Fortran program.

```
Subroutine document_ex1
! Illustrate a 1D Poisson equation with Dirichlet boundary conditions.
! This module defines the structures and overloaded assignment code.
      Use linear_operators
      Implicit None
!
      Integer :: I
      Integer, Parameter :: N = 1000
      Real (Kind(1.d0)) :: f, h, r, w (N), a = 0.d0, b = 1.d0, &
      u_a = 0.d0, u_b = 1.d0, u (N)
      Type (d_sparse) M
      Type (d_hbc_sparse) K
      External f
! Define the difference used.
      h = (b-a) / (N-1)
      r = 1.d0 / h ** 2
! Fill in the matrix entries.
! Isolated equation for the left boundary condition.
      M = d_entry (1, 1, r)
      Do I = 2, N - 1
         M = d_entry (I, I-1, r)
         M = d_entry (I, I,-2*r)
         M = d_entry (I, I+1, r)
      End Do

! Isolated equation for the right boundary condition.
      M = d_entry (N, N, r)

! Fill in the right-hand side (a dense vector).
      Do I = 2, N - 1
         w (I) = f (a+(I-1)*h)
      End Do
! Insert the known end conditions.  These should be satisfied
! almost exactly, up to rounding errors.
      w (1) = u_a * r
      w (N) = u_b * r
! Ready to solve …
! Conversion to Harwell-Boeing format using overloaded assignment

      K = M
! Solve the system using an IMSL defined operator.

      u = K .ix. w
! The parentheses are needed because of precedence rules.
! Compute residuals and overwrite w(:) with these values.

      w = w - (K .x. u)
End Subroutine
!
```

```
Function f (x)
      Real (Kind(1.d0)) :: f, x
! Define a hat function, peaked at x=0.5.
      If (x <= 0.5d0) Then
         f = x
      Else
         f = 1.d0 - x
      End If
End Function
```

Parallel Example (parallel_ex03.f90)

This example shows the box data type used while obtaining an accurate solution of several systems. Important in this example is the fact that only the root will achieve convergence, which controls program flow out of the loop. Therefore the nodes must share the root's view of convergence, and that is the reason for the broadcast of the update from root to the nodes. Note that when writing an explicit call to an MPI routine there must be the line `INCLUDE` '`mpif.h`', placed just after the `IMPLICIT NONE` statement. Any number of nodes can be used.

```
      use linear_operators
      use mpi_setup_int

      implicit none
      INCLUDE 'mpif.h'

! This is the equivalent of Parallel Example 3 for .i. and iterative
! refinement with box date types, operators and functions.
      integer, parameter :: n=32, nr=4
      integer IERROR
      real(kind(1e0)) :: one=1e0, zero=0e0
      real(kind(1e0)) :: A(n,n,nr), b(n,1,nr), x(n,1,nr)
      real(kind(1e0)) change_old(nr), change_new(nr)
      real(kind(1d0)) :: d_zero=0d0, c(n,1,nr), D(n,n,nr), y(n,1,nr)

! Setup for MPI.
      MP_NPROCS=MP_SETUP()

! Generate a random matrix and right-hand side.
      A = rand(A); b= rand(b)

! Save double precision copies of the matrix and right-hand side.
      D = A
      c = b

! Get single precision inverse to compute the iterative refinement.
      A = .i. A

! Start solution at zero.  Update it to a more accurate solution
! with each iteration.
      y = d_zero
      change_old = huge(one)

      ITERATIVE_REFINEMENT: DO

! Compute the residual with higher accuracy than the data.
         b = c - (D .x. y)

! Compute the update in single precision.
         x = A .x. b
         y = x + y
         change_new = norm(x)
```

```
! All processors must share the root's test of convergence.
         CALL MPI_BCAST(change_new, nr, MPI_REAL, 0, &
           MP_LIBRARY_WORLD, IERROR)

! Exit when changes are no longer decreasing.
         if (ALL(change_new >= change_old)) exit iterative_refinement
         change_old = change_new
      end DO ITERATIVE_REFINEMENT

        IF(MP_RANK == 0) write (*,*) 'Parallel Example 3 is correct.'

! See to any error messages and quit MPI.
      MP_NPROCS=MP_SETUP('Final')
      end
```

.tx.

more... more...

Computes transpose matrix-matrix or transpose matrix-vector product.

Operator Return Value

Matrix containing the product of A^T and B. (Output)

Required Operands

A — Left operand matrix. This is an array of rank 2 or 3. It may be real, double, complex, double complex, or one of the computational sparse matrix derived types, `?_hbc_sparse`. (Input)
Note that A and B cannot both be `?_hbc_sparse`.

B — Right operand matrix or vector. This is an array of rank 1, 2, or 3. It may be real, double, complex, double complex, or one of the computational sparse matrix derived types, `?_hbc_sparse`. (Input)
Note that A and B cannot both be `?_hbc_sparse`.

If A has rank three, B must have rank three.
If B has rank three, A must have rank three.

FORTRAN 90 Interface

```
A .tx. B
```

Description

Computes the product of the transpose of matrix A and matrix or vector B. The results are in a precision and data type that ascends to the most accurate or complex operand.

Rank three operation is defined as follows:

```
do i = 1, min(size(A,3), size(B,3))
       X(:,:,i) =  A(:,:,i) .tx. B(:,:,i)
  end do
```

`.tx.` can be used with either dense or sparse matrices. It is MPI capable for dense matrices only.

Examples

Dense Matrix Example (operator_ex05.f90)

```
use linear_operators
      implicit none

! This is the equivalent of Example 1 for LIN_SOL_SELF using operators
! and functions.
      integer, parameter :: m=64, n=32
      real(kind(1e0)) :: one=1.0e0, err
      real(kind(1e0)) A(n,n), b(n,n), C(m,n), d(m,n), x(n,n)

! Generate two rectangular random matrices.
      C = rand(C); d=rand(d)

! Form the normal equations for the rectangular system.
      A = C .tx. C; b = C .tx. d

! Compute the solution for Ax = b, A is symmetric.
      x = A .ix. b

! Check the results.
      err = norm(b - (A .x. x))/(norm(A)+norm(b))
      if (err <= sqrt(epsilon(one))) then
         write (*,*) 'Example 1 for LIN_SOL_SELF (operators) is correct.'
      end if

      end
```

Sparse Matrix Example

```
 use wrrrn_int
 use linear_operators

 type (s_sparse) S
 type (s_hbc_sparse) H
 integer, parameter :: N=3
 real (kind(1.e0)) x(N,N), y(N,N), B(N,N)
 real (kind(1.e0)) err

 S = s_entry (1, 1, 2.0)
 S = s_entry (1, 3, 1.0)
 S = s_entry (2, 2, 4.0)
 S = s_entry (3, 3, 6.0)
 H = S   ! sparse
 X = H   ! dense equivalent of H
 B = rand(B)
 Y = H .tx. B
  call wrrrn ( 'H', X)
  call wrrrn ( 'B', b)
  call wrrrn ( 'H .tx. B ', y)
```

```
! Check the results.
     err =  norm(y - (X .tx. B))
      if (err <= sqrt(epsilon(one))) then
         write (*,*) 'Sparse example for .tx. operator is correct.'
      end if

 end
```

Output

```
              H
        1       2       3
 1   2.000   0.000   1.000
 2   0.000   4.000   0.000
 3   0.000   0.000   6.000

                B
         1        2        3
 1   0.8711   0.4467   0.4743
 2   0.8315   0.7257   0.4518
 3   0.6839   0.0561   0.6972

         H .tx. B
        1       2       3
 1   1.742   0.893   0.949
 2   3.326   2.903   1.807
 3   4.975   0.784   4.657
 Sparse example for .tx. operator is correct.
```

Parallel Example (parallel_ex05.f90)

```
      use linear_operators
      use mpi_setup_int

      implicit none

! This is the equivalent of Parallel Example 5 using box data types,
! operators and functions.

      integer, parameter :: m=64, n=32, nr=4
      real(kind(1e0)) :: one=1e0, err(nr)
      real(kind(1e0)), dimension(n,n,nr) :: A, b, x
      real(kind(1e0)), dimension(m,n,nr) :: C, d

! Setup for MPI.
      mp_nprocs = mp_setup()

! Generate two rectangular random matrices, only
! at the root node.
      if (mp_rank == 0) then
      C = rand(C); d=rand(d)
      endif

! Form the normal equations for the rectangular system.
      A = C .tx. C; b = C .tx. d

! Compute the solution for Ax = b.
      x = A .ix. b

! Check the results.
      err = norm(b - (A .x. x))/(norm(A)+norm(b))
      if (ALL(err <= sqrt(epsilon(one))) .AND. MP_RANK == 0) &
         write (*,*) 'Parallel Example 5 is correct.'
```

```
! See to any error messages and quit MPI.
      mp_nprocs = mp_setup('Final')

      end
```

.xt.

more... more...

Computes matrix-transpose matrix product.

Operator Return Value

Matrix containing the product of A and B^T. (Output)

Required Operands

A — Left operand matrix or vector. This is an array of rank 1, 2, or 3. It may be real, double, complex, double complex, or one of the computational sparse matrix derived types, `?_hbc_sparse`. (Input)
Note that A and B cannot both be `?_hbc_sparse`.

B — Right operand matrix. This is an array of rank 2 or 3. It may be real, double, complex, double complex, or one of the computational sparse matrix derived types, `?_hbc_sparse`. (Input)
Note that A and B cannot both be `?_hbc_sparse`.

If A has rank three, B must have rank three.
If B has rank three, A must have rank three.

FORTRAN 90 Interface

```
A .xt. B
```

Description

Computes the product of matrix or vector A and the transpose of matrix B. The results are in a precision and data type that ascends to the most accurate or complex operand.

Rank three operation is defined as follows:

```
do i = 1, min(size(A,3), size(B,3))
  X(:,:,i) =  A(:,:,i) .xt. B(:,:,i)
end do
```

`.xt.` can be used with either dense or sparse matrices. It is MPI capable for dense matrices only.

Examples

Dense Matrix Example (operator_ex14.f90)

```
      use linear_operators
      implicit none

!
      integer, parameter :: n=32
      real(kind(1d0)) :: one=1d0, zero=0d0
      real(kind(1d0)) A(n,n), P(n,n), Q(n,n), &
             S_D(n), U_D(n,n), V_D(n,n)

! Generate a random matrix.
      A = rand(A)

! Compute the singular value decomposition.
      S_D = SVD(A, U=U_D, V=V_D)

! Compute the (left) orthogonal factor.
      P = U_D .xt. V_D

! Compute the (right) self-adjoint factor.
      Q = V_D .x. diag(S_D) .xt. V_D

! Check the results.
      if (norm( EYE(n) - (P .xt. P)) &
               <= sqrt(epsilon(one))) then
         if (norm(A - (P .x. Q))/norm(A) &
               <= sqrt(epsilon(one))) then
            write (*,*) 'Example 2 for LIN_SOL_SVD (operators) is correct.'
         end if
      end if
      end
```

Sparse Matrix Example

```
   use wrrrn_int
   use linear_operators

   type (s_sparse) S
   type (s_hbc_sparse) H
   integer, parameter :: N=3
   real (kind(1.e0)) x(N,N), y(N,N), a(N,N)
   real (kind(1.e0)) err
   S = s_entry (1, 1, 2.0)
   S = s_entry (1, 3, 1.0)
   S = s_entry (2, 2, 4.0)
   S = s_entry (3, 3, 6.0)
   H = S   ! sparse
   X = H   ! dense equivalent of H
   A = rand(A)
```

```
   Y = A .xt. H
    call wrrrn ( 'A', A)
    call wrrrn ( 'H', X)
    call wrrrn ( 'A .xt. H', y)

  ! Check the results.
       err =  norm(y - (A .xt. X))
        if (err <= sqrt(epsilon(one))) then
           write (*,*) 'Sparse example for .xt. operator is correct.'
        end if

   end
```

Output

```
                 A
            1        2        3
   1   0.5423   0.2380   0.9250
   2   0.0844   0.1323   0.1937
   3   0.4146   0.3135   0.7757

               H
           1       2       3
   1   2.000   0.000   1.000
   2   0.000   4.000   0.000
   3   0.000   0.000   6.000

           A .xt. H
           1       2       3
   1   2.010   0.952   5.550
   2   0.363   0.529   1.162
   3   1.605   1.254   4.654
   Sparse example for .xt. operator is correct.
```

Parallel Example (parallel_ex15.f90)

A “Polar Decomposition” of several matrices are computed. The box data type and the `SVD()` function are used. Orthogonality and small residuals are checked to verify that the results are correct.

```
        use linear_operators
        use mpi_setup_int
        implicit none

  ! This is the equivalent of Parallel Example 15 using operators and,
  ! functions for a polar decomposition.
        integer, parameter :: n=33, nr=3
        real(kind(1d0)) :: one=1d0, zero=0d0
        real(kind(1d0)),dimension(n,n,nr) :: A, P, Q, &
               S_D(n,nr), U_D, V_D
        real(kind(1d0)) TEMP1(nr), TEMP2(nr)

  ! Setup for MPI:
        mp_nprocs = mp_setup()

  ! Generate a random matrix.
        if(mp_rank == 0) A = rand(A)

  ! Compute the singular value decomposition.
        S_D = SVD(A, U=U_D, V=V_D)

  ! Compute the (left) orthogonal factor.
        P = U_D .xt. V_D
```

```
! Compute the (right) self-adjoint factor.
      Q = V_D .x. diag(S_D) .xt. V_D
! Check the results for orthogonality and
! small residuals.
      TEMP1 = NORM(spread(EYE(n),3,nr) - (p .xt. p))
      TEMP2 = NORM(A -(P .X. Q)) / NORM(A)
      if (ALL(TEMP1 <= sqrt(epsilon(one))) .and. &
          ALL(TEMP2 <= sqrt(epsilon(one)))) then
            if(mp_rank == 0)&
            write (*,*) 'Parallel Example 15 is correct.'
      end if

! See to any error messages and exit MPI.
      mp_nprocs = mp_setup('Final')

      end
```

.hx.

more... more...

Computes conjugate transpose matrix-matrix product.

Operator Return Value

Matrix containing the product of A^H and B. (Output)

Required Operands

A — Left operand matrix. This is an array of rank 2 or 3. It may be real, double, complex, double complex, or one of the computational sparse matrix derived types, `c_hbc_sparse` or `z_hbc_sparse`. (Input)
Note that A and B cannot both be `?_hbc_sparse`.

B — Right operand matrix or vector. This is an array of rank 1, 2, or 3. It may be real, double, complex, double complex, or one of the computational sparse matrix derived types, `c_hbc_sparse` or `z_hbc_sparse`. (Input)

Note that A and B cannot both be `?_hbc_sparse`.

If A has rank three, B must have rank three.

If B has rank three, A must have rank three.

FORTRAN 90 Interface

```
A .hx. B
```

Description

Computes the product of the conjugate transpose of matrix A and matrix or vector B. The results are in a precision and data type that ascends to the most accurate or complex operand.

Rank three operation is defined as follows:

```
do i = 1, min(size(A,3), size(B,3))
  X(:,:,i) =  A(:,:,i) .hx. B(:,:,i)
end do
```

`.hx.` can be used with either dense or sparse matrices. It is MPI capable for dense matrices only.

Examples

Dense Matrix Example (operator_ex32.f90)

```
      use linear_operators
      implicit none
! This is the equivalent of Example 4 (using operators) for LIN_EIG_GEN.

      integer, parameter :: n=17
      real(kind(1d0)), parameter :: one=1d0
      real(kind(1d0)), dimension(n,n) :: A, C
      real(kind(1d0)) variation(n), eta
      complex(kind(1d0)), dimension(n,n) :: U, V, e(n), d(n)

! Generate a random matrix.
      A = rand(A)

! Compute the eigenvalues, left- and right- eigenvectors.
      D = EIG(A, W=V); E = EIG(.t.A, W=U)

! Compute condition numbers and variations of eigenvalues.
      variation = norm(A)/abs(diagonals( U .hx. V))

! Now perturb the data in the matrix by the relative factors
! eta=sqrt(epsilon) and solve for values again.  Check the
! differences compared to the estimates.  They should not exceed
! the bounds.
      eta = sqrt(epsilon(one))
      C = A + eta*(2*rand(A)-1)*A
      D = EIG(C)

! Looking at the differences of absolute values accounts for
! switching signs on the imaginary parts.
      if (count(abs(d)-abs(e) > eta*variation) == 0) then
         write (*,*) 'Example 4 for LIN_EIG_GEN (operators) is correct.'
      end if
      end
```

Sparse Matrix Example

```
   use wrcrn_int
   use linear_operators

   type (c_sparse) S
```

```
   type (c_hbc_sparse) H
   integer, parameter :: N=3
   complex (kind(1.e0)) x(N,N), y(N,N), A(N,N)
   real (kind(1.e0)) err
   S = c_entry (1, 1, (2.0, 1.0) )
   S = c_entry (1, 3, (1.0, 3.0))
   S = c_entry (2, 2, (4.0, -1.0))
   S = c_entry (3, 3, (6.0, 2.0))
   H = S   ! sparse
   X = H   ! dense equivalent of H
   A= rand(A)
   Y = H .hx. A
    call wrcrn ( 'H', X)
    call wrcrn ( 'A', a)
    call wrcrn ( 'H .hx. A ', y)

  ! Check the results.
      err =  norm(y - (X .hx. A))
       if (err <= sqrt(epsilon(one))) then
          write (*,*) 'Sparse example for .hx. operator is correct.'
       end if

   end
```

Output

```
                                 H
                    1                  2                  3
   1  ( 2.000, 1.000)  ( 0.000, 0.000)  ( 1.000, 3.000)
   2  ( 0.000, 0.000)  ( 4.000,-1.000)  ( 0.000, 0.000)
   3  ( 0.000, 0.000)  ( 0.000, 0.000)  ( 6.000, 2.000)

                                    A
                      1                    2                    3
   1  ( 0.6278, 0.8475)  ( 0.8007, 0.4179)  ( 0.4512, 0.2601)
   2  ( 0.1249, 0.4675)  ( 0.7957, 0.1609)  ( 0.4228, 0.0507)
   3  ( 0.4608, 0.0891)  ( 0.3181, 0.9180)  ( 0.9961, 0.1939)

                             H .hx. A
                    1                  2                  3
   1  ( 2.103, 1.067)  ( 2.019, 0.035)  ( 1.163, 0.069)
   2  ( 0.032, 1.995)  ( 3.022, 1.439)  ( 1.640, 0.626)
   3  ( 6.113,-1.423)  ( 5.799, 2.888)  ( 7.596,-1.922)
   Sparse example for .hx. operator is correct.
```

Parallel Example

```
   use linear_operators
   use mpi_setup_int

   integer, parameter :: N=32, nr=4
   complex (kind(1.e0)) A(N,N,nr), B(N,N,nr), Y(N,N,nr)
  ! Setup for MPI
    mp_nprocs = mp_setup()

   if (mp_rank == 0) then
     A = rand(A)
     B = rand(B)
   end if

   Y = A .hx. B

   mp_nprocs = mp_setup ('Final')
```

```
    end
```

.xh.

more... more...

Computes a matrix-conjugate transpose matrix product.

Operator Return Value

Matrix containing the product of A and B^{H}. (Output)

Required Operands

A — Left operand matrix or vector. This is an array of rank 1, 2, or 3. It may be real, double, complex, double complex, or one of the computational sparse matrix derived types, `c_hbc_sparse` or `z_hbc_sparse`. (Input)
Note that A and B cannot both be `?_hbc_sparse`.

B — Right operand matrix. This is an array of rank 2, or 3. It may be real, double, complex, double complex, or one of the computational sparse matrix derived types, `c_hbc_sparse` or `z_hbc_sparse`. (Input)
Note that A and B cannot both be `?_hbc_sparse`.

If A has rank three, B must have rank three.

If B has rank three,

A must have rank three.

FORTRAN 90 Interface

```
A .xh. B
```

Description

Computes the product of matrix or vector A and the conjugate transpose of matrix B. The results are in a precision and data type that ascends to the most accurate or complex operand.

Rank three operation is defined as follows:

```
do i = 1, min(size(A,3), size(B,3))
  X(:,:,i) =  A(:,:,i) .xh. B(:,:,i)
end do
```

`.xh.` can be used with either dense or sparse matrices. It is MPI capable for dense matrices only.

Examples

Dense Matrix Example

```
use wrcrn_int
use linear_operators
integer, parameter :: N=3
complex (kind(1.e0)) A(N,N), B(N,N), Y(N,N)

A = rand(A)
B = rand(B)
Y = A .xh. B
 call wrcrn ( 'A', a)
 call wrcrn ( 'B', b)
 call wrcrn ( 'A .xh. B ', y)
end
```

Output

```
                            A
                   1                   2                   3
1  ( 0.8071, 0.0054)  ( 0.5617, 0.2508)  ( 0.0223, 0.5555)
2  ( 0.9380, 0.5181)  ( 0.8895, 0.9512)  ( 0.7951, 0.6010)
3  ( 0.8349, 0.7291)  ( 0.4162, 0.5255)  ( 0.7388, 0.0309)

                            B
                   1                   2                   3
1  ( 0.5342, 0.2246)  ( 0.9045, 0.0550)  ( 0.4576, 0.3173)
2  ( 0.5531, 0.3362)  ( 0.0757, 0.3970)  ( 0.6807, 0.8625)
3  ( 0.3553, 0.9157)  ( 0.0951, 0.7807)  ( 0.4853, 0.0617)

                     A .xh. B
                 1                 2                 3
1  ( 1.141, 0.265)  ( 1.085,-0.113)  ( 0.586,-0.884)
2  ( 2.029, 0.900)  ( 2.198,-0.587)  ( 2.058,-1.036)
3  ( 1.363, 0.434)  ( 1.477,-0.619)  ( 1.775,-0.811)
```

Sparse Matrix Example

```
use wrcrn_int
use linear_operators

type (c_sparse) S
```

```
   type (c_hbc_sparse) H
   integer, parameter :: N=3
   complex (kind(1.e0)) x(N,N), y(N,N), A(N,N)
   real (kind(1.e0)) err
   S = c_entry (1, 1, (2.0, 1.0) )
   S = c_entry (1, 3, (1.0, 3.0))
   S = c_entry (2, 2, (4.0, -1.0))
   S = c_entry (3, 3, (6.0, 2.0))
   H = S   ! sparse
   X = H   ! dense equivalent of H
   A= rand(A)
   Y = A .xh. H
    call wrcrn ( 'A', a)
    call wrcrn ( 'H', X)
    call wrcrn ( 'A .xh. H ', y)

  ! Check the results.
      err =  norm(y - (A .xh. X))
       if (err <= sqrt(epsilon(one))) then
          write (*,*) 'Sparse example for .xh. operator is correct.'
       end if

   end
```

Output

```
                              A
                      1                  2                  3
   1  ( 0.8526, 0.3532)  ( 0.1822, 0.3938)  ( 0.8008, 0.1308)
   2  ( 0.5599, 0.8914)  ( 0.7541, 0.5163)  ( 0.8713, 0.9580)
   3  ( 0.9947, 0.2735)  ( 0.6237, 0.2137)  ( 0.3802, 0.8903)

                           H
                    1                 2                 3
   1  ( 2.000, 1.000)  ( 0.000, 0.000)  ( 1.000, 3.000)
   2  ( 0.000, 0.000)  ( 4.000,-1.000)  ( 0.000, 0.000)
   3  ( 0.000, 0.000)  ( 0.000, 0.000)  ( 6.000, 2.000)

                        A .xh. H
                    1                 2                 3
   1  ( 3.252,-2.418)  ( 0.335, 1.757)  ( 5.066,-0.817)
   2  ( 5.757,-0.433)  ( 2.500, 2.819)  ( 7.144, 4.005)
   3  ( 5.314,-0.698)  ( 2.281, 1.478)  ( 4.062, 4.581)
   Sparse example for .xh. operator is correct.
```

Parallel Example

```
   use linear_operators
   use mpi_setup_int

   integer, parameter :: N=32, nr=4
   complex (kind(1.e0)) A(N,N,nr), B(N,N,nr), Y(N,N,nr)
  ! Setup for MPI
    mp_nprocs = mp_setup()

   if (mp_rank == 0) then
     A = rand(A)
     B = rand(B)
   end if

   Y = A .xh. B

   mp_nprocs = mp_setup ('Final')
```

```
  end
```

.t.

Computes the transpose of a matrix.

Operator Return Value

Matrix containing the transpose of `A`. (Output)

Required Operand

A — Matrix for which the transpose is to be computed. This is a real, double, complex, double complex, or one of the computational sparse matrix derived types, `c_hbc_sparse` or `z_hbc_sparse`. (Input).

FORTRAN 90 Interface

```
.t. A
```

Description

Computes the transpose of matrix A. The operation may be read *transpose*, and the results are the mathematical objects in a precision and data type that matches the operand. Since this is a unary operation, it has *higher* Fortran 90 precedence than any other intrinsic unary array operation.

`.t.` can be used with either dense or sparse matrices.

Examples

Dense Matrix Example (operator_ex07.f90)

```
use linear_operators

      implicit none

! This is the equivalent of Example 3 (using operators) for LIN_SOL_SELF.

      integer tries
      integer, parameter :: m=8, n=4, k=2
      integer ipivots(n+1)
      real(kind(1d0)) :: one=1.0d0, err
```

```
      real(kind(1d0)) a(n,n), b(n,1), c(m,n), x(n,1), &
             e(n), ATEMP(n,n)
      type(d_options) :: iopti(4)

! Generate a random rectangular matrix.
      C = rand(C)

! Generate a random right hand side for use in the inverse
! iteration.
      b = rand(b)

! Compute the positive definite matrix.
      A = C .tx. C; A = (A+.t.A)/2

! Obtain just the eigenvalues.
      E = EIG(A)

! Use packaged option to reset the value of a small diagonal.
      iopti(4) = 0
      iopti(1) = d_options(d_lin_sol_self_set_small,&
                 epsilon(one)*abs(E(1)))

! Use packaged option to save the factorization.
      iopti(2) = d_lin_sol_self_save_factors

! Suppress error messages and stopping due to singularity
! of the matrix, which is expected.
      iopti(3) = d_lin_sol_self_no_sing_mess

      ATEMP = A

! Compute A-eigenvalue*I as the coefficient matrix.
! Use eigenvalue number k.
      A = A - e(k)*EYE(n)

      do tries=1,2
         call lin_sol_self(A, b, x, &
                   pivots=ipivots, iopt=iopti)
! When code is re-entered, the already computed factorization
! is used.
         iopti(4) = d_lin_sol_self_solve_A

! Reset right-hand side in the direction of the eigenvector.
         B = UNIT(x)
      end do

! Normalize the eigenvector.
      x = UNIT(x)

! Check the results.
      b=ATEMP .x. x
      err =  dot_product(x(1:n,1), b(1:n,1)) - e(k)

! If any result is not accurate, quit with no printing.
      if (abs(err) <= sqrt(epsilon(one))*E(1)) then
        write (*,*) 'Example 3 for LIN_SOL_SELF (operators) is correct.'
      end if

      end
```

Sparse Matrix Example

```
   use wrrrn_int
   use linear_operators
```

```
   type (s_sparse) S
   type (s_hbc_sparse) H, HT
   integer, parameter :: N=3
   real (kind(1.e0)) X(3,3), XT(3,3)
   real (kind(1.e0)) err
   S = s_entry (1, 1, 2.0)
   S = s_entry (1, 3, 1.0)
   S = s_entry (2, 2, 4.0)
   S = s_entry (3, 3, 6.0)
   H = S   ! sparse
   X = H   ! dense equivalent of H
   HT = .t. H
   XT = HT ! dense equivalent of HT
    call wrrrn ( 'H', X)
    call wrrrn ( 'H Transpose', XT)

  ! Check the results.
       err =  norm(XT - (.t. X))
        if (err <= sqrt(epsilon(one))) then
           write (*,*) 'Sparse example for .t. operator is correct.'
        end if

   end
```

Output

```
                H
           1       2       3
   1   2.000   0.000   1.000
   2   0.000   4.000   0.000
   3   0.000   0.000   6.000

          H Transpose
           1       2       3
   1   2.000   0.000   0.000
   2   0.000   4.000   0.000
   3   1.000   0.000   6.000
   Sparse example for .t. operator is correct.
```

.h.

Computes the conjugate transpose of a matrix.

Operator Return Value

Matrix containing the conjugate transpose of A. (Output)

Required Operand

A — Matrix for which the conjugate transpose is to be computed. This is an array of rank 2 or 3. It may be real, double, complex, double complex, or one of the computational sparse matrix derived types, `c_hbc_sparse` or `z_hbc_sparse`. (Input)

FORTRAN 90 Interface

```
.h. A
```

Description

Computes the conjugate transpose of matrix A. The operation may be read *adjoint*, and the results are the mathematical objects in a precision and data type that matches the operand. Since this is a unary operation, it has *higher* Fortran 90 precedence than any other intrinsic unary array operation.

`.h.` can be used with either dense or sparse matrices.

Examples

Dense Matrix Example (operator_ex34.f90)

```
      use linear_operators

      implicit none

! This is the equivalent of Example 2 (using operators) for LIN_GEIG_GEN.

      integer, parameter :: n=32
      real(kind(1d0)), parameter :: one=1d0, zero=0d0
      real(kind(1d0)) err, alpha(n)
      complex(kind(1d0)), dimension(n,n) :: A, B, C, D, V
```

```
! Generate random matrices for both A and B.
      C = rand(C); D = rand(D)
      A = C + .h.C; B = D .hx. D; B = (B + .h.B)/2

      ALPHA = EIG(A, B=B, W=V)

! Check that residuals are small.  Use a real array for  alpha
! since the eigenvalues are known to be real.
      err= norm((A .x. V) - (B .x. V .x. diag(alpha)),1)/&
           (norm(A,1)+norm(B,1)*norm(alpha,1))
      if (err <= sqrt(epsilon(one))) then
         write (*,*) 'Example 2 for LIN_GEIG_GEN (operators) is correct.'
      end if

      end
```

Sparse Matrix Example

```
  use wrcrn_int
  use linear_operators

  type (c_sparse) S
  type (c_hbc_sparse) H, HT
  integer, parameter :: N=3
  complex (kind(1.e0)) X(3,3), XT(3,3)
  real (kind(1.e0)) err
  S = c_entry (1, 1, (2.0, 1.0) )
  S = c_entry (1, 3, (1.0, 3.0))
  S = c_entry (2, 2, (4.0, -1.0))
  S = c_entry (3, 3, (6.0, 2.0))
  H = S    ! sparse
  X = H    ! dense equivalent of H
  HT = .h. H
  XT = HT ! dense equivalent of HT
   call wrcrn ( 'H', X)
   call wrcrn ( 'H Conjugate Transpose', XT)

! Check the results.
     err =  norm(XT - (.h. X))
      if (err <= sqrt(epsilon(one))) then
         write (*,*) 'Sparse example for .h. operator is correct.'
      end if

  end
```

Output

```
                            H
                 1                 2                 3
  1  ( 2.000, 1.000)  ( 0.000, 0.000)  ( 1.000, 3.000)
  2  ( 0.000, 0.000)  ( 4.000,-1.000)  ( 0.000, 0.000)
  3  ( 0.000, 0.000)  ( 0.000, 0.000)  ( 6.000, 2.000)

                H Conjugate Transpose
                 1                 2                 3
  1  ( 2.000,-1.000)  ( 0.000, 0.000)  ( 0.000, 0.000)
  2  ( 0.000, 0.000)  ( 4.000, 1.000)  ( 0.000, 0.000)
  3  ( 1.000,-3.000)  ( 0.000, 0.000)  ( 6.000,-2.000)
  Sparse example for .h. operator is correct.
```

.i.

more... more...

Computes the inverse matrix.

Operator Return Value

Matrix containing the inverse of A. (Output)

Required Operand

A — Matrix for which the inverse is to be computed. This is an array of rank 2 or 3. It may be real, double, complex, double complex. (Input)

Optional Variables, Reserved Names

This operator uses the routines `LIN_SOL_GEN` or `LIN_SOL_LSQ` (See *Chapter 1, "Linear Systems"*).

The option and derived type names are given in the following tables:

Option Names for .i.	Option Value
Use_lin_sol_gen_only	1
Use_lin_sol_lsq_only	2
I_options_for_lin_sol_gen	3
I_options_for_lin_sol_lsq	4
Skip_error_processing	5

Name of Unallocated Option Array to Use for Setting Options	Use	Derived Type
?_inv_options(:)	Use when setting options for calls hereafter.	?_options
?_inv_options_once(:)	Use when setting options for next call only.	?_options

For a description on how to use these options, see *Matrix Optional Data Changes*. See `LIN_SOL_GEN` and `LIN_SOL_LSQ` in *Chapter 1, "Linear Systems"* for the specific options for these routines.

FORTRAN 90 Interface

```
.i. A
```

Description

Computes the inverse matrix for square non-singular matrices using `LIN_SOL_GEN`, or the Moore-Penrose generalized inverse matrix for singular square matrices or rectangular matrices using `LIN_SOL_LSQ`. The operation may be read *inverse or generalized inverse*, and the results are in a precision and data type that matches the operand.

This operator requires a single operand. Since this is a unary operation, it has *higher* Fortran 90 precedence than any other intrinsic array operation.

Examples

Dense Matrix Example (operator_ex02.f90)

```
      use linear_operators
      implicit none

! This is the equivalent of Example 2 for LIN_SOL_GEN using operators
! and functions.

      integer, parameter :: n=32
      real(kind(1e0)) :: one=1e0, err, det_A, det_i
      real(kind(1e0)), dimension(n,n) :: A, inv

! Generate a random matrix.
      A = rand(A)
! Compute the matrix inverse and its determinant.
      inv = .i.A; det_A = det(A)
! Compute the determinant for the inverse matrix.
      det_i = det(inv)
```

```
! Check the quality of both left and right inverses.
      err = (norm(EYE(n)-(A .x. inv))+norm(EYE(n)-(inv.x.A)))/cond(A)
      if (err <= sqrt(epsilon(one)) .and. abs(det_A*det_i - one) <= &
                   sqrt(epsilon(one))) &
      write (*,*) 'Example 2 for LIN_SOL_GEN (operators) is correct.'
      end
```

Parallel Example (parallel_ex02.f90)

```
      use linear_operators
      use mpi_setup_int

      implicit none

! This is the equivalent of Parallel Example 2 for .i. and det() with box
! data types, operators and functions.

      integer, parameter :: n=32, nr=4
      integer J
      real(kind(1e0)) :: one=1e0
      real(kind(1e0)), dimension(nr) :: err, det_A, det_i
      real(kind(1e0)), dimension(n,n,nr) :: A, inv, R, S

! Setup for MPI.
      MP_NPROCS=MP_SETUP()
! Generate a random matrix.
      A = rand(A)
! Compute the matrix inverse and its determinant.
      inv = .i.A; det_A = det(A)
! Compute the determinant for the inverse matrix.
      det_i = det(inv)
! Check the quality of both left and right inverses.
      DO J=1,nr; R(:,:,J)=EYE(N); END DO

      S=R; R=R-(A .x. inv); S=S-(inv .x. A)
      err = (norm(R)+norm(S))/cond(A)
      if (ALL(err <= sqrt(epsilon(one)) .and. &
        abs(det_A*det_i - one) <= sqrt(epsilon(one)))&
       .and. MP_RANK == 0) &
        write (*,*) 'Parallel Example 2 is correct.'

! See to any error messages and quit MPI.
      MP_NPROCS=MP_SETUP('Final')

      end
```

.ix.

more... more...

Computes the product of the inverse of a matrix and a vector or matrix.

Operator Return Value

Matrix containing the product of A^{-1} and B. (Output)

Required Operands

A — Left operand matrix. This is an array of rank 2 or 3. It may be real, double, complex, double complex, or one of the computational sparse matrix derived types, `?_hbc_sparse`. (Input)

B — Right operand matrix or vector. This is an array of rank 1, 2, or 3. It may be real, double, complex, or double complex. (Input)

Optional Variables, Reserved Names

This operator uses the routines `LIN_SOL_GEN` or `LIN_SOL_LSQ` (See *Chapter 1, "Linear Systems"*).

The option and derived type names are given in the following tables:

Option Names for .ix.	**Option Value**
Use_lin_sol_gen_only	1
Use_lin_sol_lsq_only	2
ix_options_for_lin_sol_gen	3
ix_options_for_lin_sol_lsq	4
Skip_error_processing	5

Name of Unallocated Option Array to Use for Setting Options	Use	Derived Type
?_invx_options(:)	Use when setting options for calls hereafter.	?_options
?_invx_options_once(:)	Use when setting options for next call only.	?_options

For a description on how to use these options, see *Matrix Optional Data Changes*. See `LIN_SOL_GEN` and `LIN_SOL_LSQ` in *Chapter 1, "Linear Systems"* for the specific options for these routines.

FORTRAN 90 Interface

```
A .ix. B
```

Description

Computes the product of the inverse of matrix A and vector or matrix B, for square non-singular matrices or the corresponding Moore-Penrose generalized inverse matrix for singular square matrices or rectangular matrices. The operation may be read *generalized inverse times*. The results are in a precision and data type that matches the most accurate or complex operand.

`.ix.` can be used with either dense or sparse matrices. It is MPI capable for dense matrices only.

Examples

Dense Matrix Example (operator_ex01.f90)

```
  use linear_operators
      implicit none

! This is the equivalent of Example 1 for LIN_SOL_GEN, with operators
! and functions.

      integer, parameter :: n=32
      real(kind(1e0)) :: one=1.0e0, err
      real(kind(1e0)), dimension(n,n) :: A, b, x

! Generate random matrices for A and b:
      A = rand(A); b=rand(b)

! Compute the solution matrix of Ax = b.
      x = A .ix. b

! Check the results.
      err = norm(b - (A .x. x))/(norm(A)*norm(x)+norm(b))
```

```
      if (err <= sqrt(epsilon(one))) &
         write (*,*) 'Example 1 for LIN_SOL_GEN (operators) is correct.'
      end
```

Sparse Matrix Example 1

```
  use wrrrn_int
  use linear_operators

  type (s_sparse) S
  type (s_hbc_sparse) H
  integer, parameter :: N=3
  real (kind(1.e0)) x(N,N), y(N,N), B(N,N)
  real (kind(1.e0)) err
  S = s_entry (1, 1, 2.0)
  S = s_entry (1, 3, 1.0)
  S = s_entry (2, 2, 4.0)
  S = s_entry (3, 3, 6.0)
  H = S   ! sparse
  X = H   ! dense equivalent of H
  B= rand(B)
  Y = H .ix. B
   call wrrrn ( 'H', X)
   call wrrrn ( 'B', b)
   call wrrrn ( 'H .ix. B ', y)

 ! Check the results.
     err =  norm(y - (X .ix. B))
      if (err <= sqrt(epsilon(one))) then
         write (*,*) 'Sparse example for .ix. operator is correct.'
      end if

  end
```

Output

```
              H
          1        2        3
  1   2.000    0.000    1.000
  2   0.000    4.000    0.000
  3   0.000    0.000    6.000

                  B
           1         2         3
  1   0.8292    0.5697    0.1687
  2   0.9670    0.7296    0.0603
  3   0.1458    0.2726    0.8809

             H .ix. B
           1         2         3
  1   0.4025    0.2621    0.0109
  2   0.2417    0.1824    0.0151
  3   0.0243    0.0454    0.1468
```

Sparse Matrix Example 2: Plane Poisson Problem with Dirichlet Boundary Conditions

We want to calculate a numerical solution, which approximates the true solution of the Poisson (boundary value) problem in the solution domain Ω, a rectangle in $\mathbb{R}^2$. The equation is

$$\Delta u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f \quad \text{in } \Omega$$

There are Dirichlet boundary conditions $u = g$ on $\partial_1\Omega$

There are further Neumann boundary conditions $\frac{\partial u}{\partial n} = h$ on $\partial_2\Omega$.

The boundary arcs comprising $\partial_1\Omega \cup \partial_2\Omega = \partial\Omega$ are mutually exclusive of each other. The functions *f*, *g*, *h* are defined on their respective domains.

We will solve an instance of this problem by using finite differences to approximate the derivatives. This will lead to a sparse system of linear algebraic equations. Note that particular cases of this problem can be solved with methods that are likely to be more efficient or more appropriate than the one illustrated here. We use this method to illustrate our matrix data handling routines and defined operators.

The area of the rectangle Ω is $a \times b$ with the origin fixed at the lower left or SW corner. The dimension along the *x* axis is *a* and along the *y* axis is *b*. A rectangular $n \times m$ uniform grid is defined on Ω where each sub-rectangle in the grid has sides $\Delta x = a/(n-1)$ and $\Delta y = a/(m-1)$. What is perhaps novel in our development is that the boundary values are written into the $(m \times n)^2$ linear system as trivial equations. This leads to more unknowns than standard approaches to this problem but the complexity of describing the equations into computer code is reduced. The boundary conditions are naturally in place when the solution is obtained. No reshaping is required.

We number the approximate values of *u* at the grid points and collapse them into a single vector. Given a coordinate of the grid (i, j), $((i = 1, \ldots, \text{n}), j = 1, \ldots, m)$, we use the mapping $J = i + (j - 1)n$ to define coordinate J of this vector. This mapping enables us to define the matrix that is used to solve for the values of *u* at the grid points.

For the Neumann boundary conditions we take $\partial_2\Omega$ to be the East face of the rectangle. Along that edge we have $\frac{\partial u}{\partial n} = \frac{\partial u}{\partial x}$, and we impose the smooth interface $h = 0$.

Our use of finite differences is standard. For the differential equation we approximate

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \doteq \left(\frac{u_{i-1,j} - 2u_{i,j} + u_{i+1,j}}{\Delta x^2}\right)\left(\frac{u_{i,j-1} - 2u_{i,j} + u_{i,j+1}}{\Delta y^2}\right) = f(x_i, y_j)$$

at the inner grid points (i, j), $((i = 2, \ldots, \text{n}-1), j = 2, \ldots, m-1)$. For the Neumann condition we approximate

$$\frac{\partial u}{\partial x} \doteq \left(\frac{u_{n,j} - u_{n-1,j}}{\Delta x}\right) = 0, \quad j = 1, \ \ldots, m$$

The remaining equations come from the Dirichlet conditions given on $\partial_1\Omega$.

To illustrate three examples of solutions to this problem we consider

1. A Laplace Equation with the boundary conditions
   u = 0, on the South Edge
   u = 0.7, on the East Edge
   u = 1, on the North Edge
   u = 0.3, on the West Edge
   The function *f* = 0 for all (*x*, *y*). Graphical results are shown below with the title *Problem Case 1*.

2. A Poisson equation with the boundary conditions *u* = 0 on all of the edges and f(x, y) = −sin(π *x*) sin(π *y*). This problem has the solution *u*(x, y) = −f(x, y)/(2π^2), and this identity provides a way of verifying that the accuracy is within the truncation error implied by the difference equations. Graphical results are shown with the title *Problem Case 2* The residual function verifies the expected accuracy.

3. The Laplace Equation with the boundary conditions of Problem Case 1 except that the boundary condition on the East Edge is replaced by the Neumann condition $\frac{\partial u}{\partial x} = 0$. Graphical results are shown as *Problem Case 3*.

```
Subroutine document_ex2
! Illustrate a 2D Poisson equation with Dirichlet and
! Neumann boundary conditions.
! These modules defines the structures and overloaded assignment code.
      Use linear_operators
      Implicit None
      Integer :: I, J, JJ, MY_CASE, IFILE
      Integer, Parameter :: N = 300, M = 300
      Real (Kind(1.d0)) :: a = 1.d0, b = 1.d0
      Real (Kind(1.d0)) :: delx, dely, r, s, pi, scale
      Real (Kind(1.d0)) ::  u(N*M), w(N*M), P(N, M)
      Real (Kind(1.e0)) :: TS, TE
      CHARACTER(LEN=12) :: PR_LABEL(3)=&
                          (/'Laplace','Poisson','Neumann'/)
! Mapping function (in-line) for grid coordinate to
! matrix-vector indexing.
      JJ (I, J) = I + (J-1) * N

! Define sparse matrices to hold problem data.
      Type (d_sparse) C
      Type (d_hbc_sparse) D
! Define differences and related parameters.
      delx = a / (N-1)
      dely = b / (M-1)
      r = 1.d0 / delx ** 2
      s = 1.d0 / dely ** 2
      Do MY_CASE = 1, 3
! For MY_CASE =
! 1. Solve boundary value problem with f=0 and Dirichlet
!    boundary conditions.
! 2. Solve Poisson equation with f such that a solution is known.
!    Use zero boundary condtions.
! 3. Solve boundary value problem with Dirichlet condtions as in 1.
!    except on the East edge.  There the partial WRT x is zero.
! Set timer for building the matrix.
         Call cpu_time (TS)
         Do I = 2, N - 1
            Do J = 2, M - 1
! Write entries for second partials WRT x and y.
               C = d_entry (JJ(I, J), JJ(I-1, J), r)
```

```
                 C = d_entry (JJ(I, J), JJ(I+1, J), r)
                 C = d_entry (JJ(I, J), JJ(I, J),-2*(r+s))
                 C = d_entry (JJ(I, J), JJ(I, J-1), s)
                 C = d_entry (JJ(I, J), JJ(I, J+1), s)
!
! Define components of the right-hand side.
                 w (JJ(I, J)) = f((I-1)*delx, (J-1)*dely, MY_CASE)
              End Do
           End Do
! Write entries for Dirichlet boundary conditions.
! First do the South edge, then the West, then the North.
           Select Case (MY_CASE)
           Case (1:2)
              Do I = 1, N
                 C = d_entry (JJ(I, 1), JJ(I, 1), r+s)
                 w (JJ(I, 1)) = g ((I-1)*delx, 0.d0, MY_CASE) * (r+s)
              End Do
              Do J = 2, M - 1
                 C = d_entry (JJ(1, J), JJ(1, J), r+s)
                 w (JJ(1, J)) = g (0.d0, (J-1)*dely, MY_CASE) * (r+s)
              End Do
              Do I = 1, N
                 C = d_entry (JJ(I, M), JJ(I, M), r+s)
                 w (JJ(I, M)) = g ((I-1)*delx, b, MY_CASE) * (r+s)
              End Do
              Do J = 2, M - 1
                 C = d_entry (JJ(N, J), JJ(N, J), (r+s))
                 w (JJ(N, J)) = g (a, (J-1)*dely, MY_CASE) * (r+s)
              End Do
           Case (3)
! Write entries for the boundary values but avoid the East edge.
              Do I = 1, N - 1
                 C = d_entry (JJ(I, 1), JJ(I, 1), r+s)
                 w (JJ(I, 1)) = g ((I-1)*delx, 0.d0, MY_CASE) * (r+s)
              End Do
              Do J = 2, M - 1
                 C = d_entry (JJ(1, J), JJ(1, J), r+s)
                 w (JJ(1, J)) = g (0.d0, (J-1)*dely, MY_CASE) * (r+s)
              End Do
              Do I = 1, N - 1
                 C = d_entry (JJ(I, M), JJ(I, M), r+s)
                 w (JJ(I, M)) = g ((I-1)*delx, b, MY_CASE) * (r+s)
              End Do
! Write entries for the Neumann condition on the East edge.
              Do J = 1, M
                 C = d_entry (JJ(N, J), JJ(N, J), 1.d0/delx)
                 C = d_entry (JJ(N, J), JJ(N-2, J),-1.d0/delx)
                 w (JJ(N, J)) = 0.d0
              End Do
           End Select
!
! Convert to Harwell-Boeing format for solving.
           D = C
!
           Call cpu_time (TE)
           Write (*,'(A,F6.2," S. - ",A)') "Time to build  matrix = ", &
                                           TE - TS, PR_LABEL(MY_CASE)
! Clear sparse triplets.
           C = 0
!
! Turn off iterative refinement for maximal performance.
! This is generally not recommended unless
! the problem is known not to require it.
           If (MY_CASE == 2) D%options%iterRefine = 0
! This is the solve step.
           Call cpu_time (TS)
```

```
          u  = D .ix. w
          Call cpu_time (TE)
          Write (*,'(A,I6," is",F6.2," S")') &
            "Time to solve system of size = ", N * M, TE - TS
! This is a second solve step using the factorization
! from the first step.
          Call cpu_time (TS)
          u  = D .ix. w
          Call cpu_time (TE)
!
          If(MY_CASE == 1) then
          Write (*,'(A,I6," is",F6.2," S")') &
            "Time for a 2nd system of size (iterative refinement) =", &
             N * M, TE - TS
          Else
          Write (*,'(A,I6," is",F6.2," S")') &
            "Time for a 2nd system of size (without refinement) =", &
             N * M, TE - TS
          End if
! Convert solution vector to a 2D array of values.
          P = reshape (u , (/ N, M /))
          If (MY_CASE == 2) Then
             pi = dconst ('pi')
!
             scale = - 0.5 / pi ** 2
             Do I = 1, N
                Do J = 1, M
! This uses the known form of the solution to compute residuals.
                   P (I, J) = P (I, J) - scale * f ((I-1)*delx, &
                  (J-1)*dely, MY_CASE)
                End Do
             End Do
!
             write (*,*) minval (P), " = min solution error "
             write (*,*) maxval (P), " = max solution error "
          End If
          Write (*,'(A,1pE12.4/)') "Condition number of matrix", cond (D)
! Clear all matrix data for next problem case.
          D = 0
!
      End Do ! MY_CASE
Contains
      Function f (x, y, MY_CASE)
      implicit none
! Define the right-hand side function associated with the
! "del" operator.
          Real (Kind(1.d0)) x, y, f, pi
          Integer MY_CASE
          if(MY_CASE == 2) THEN
             pi = dconst ('pi')
             f = - Sin (pi*x) * Sin (pi*y)
          Else
             f = 0.d0
          End If
      End Function
!
      Function g (x, y, MY_CASE)
      implicit none
! Define the edge values, except along East edge, x = a.
          Real (Kind(1.d0)) x, y, g
          Integer MY_CASE
! Fill in a constant value along each edge.
          If (MY_CASE == 1 .Or. MY_CASE == 3) Then
             If (y == 0.d0) Then
                g = 0.d0
                Return
```

```
               End If
               If (y == b) Then
                  g = 1.d0
                  Return
               End If
               If (x == 0.d0) Then
                  g = 0.3d0
                  Return
               End If
               If (x == a) Then
                  g = 0.7d0
               End If
            Else
               g = 0.d0
!
            End If
!
         End Function
   End Subroutine
```

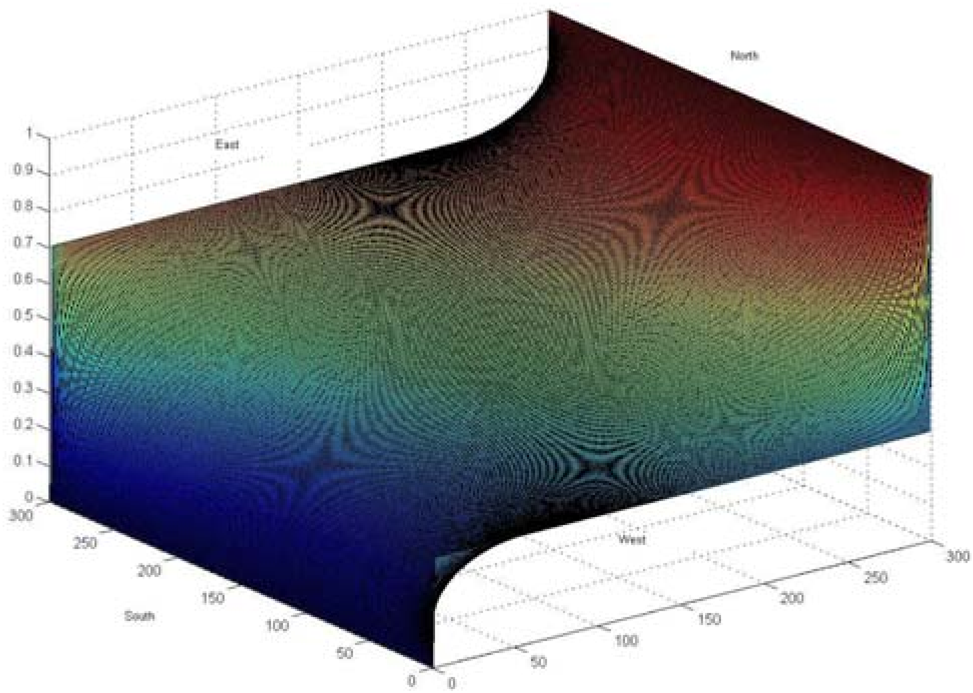


Figure 12, Problem Case 1

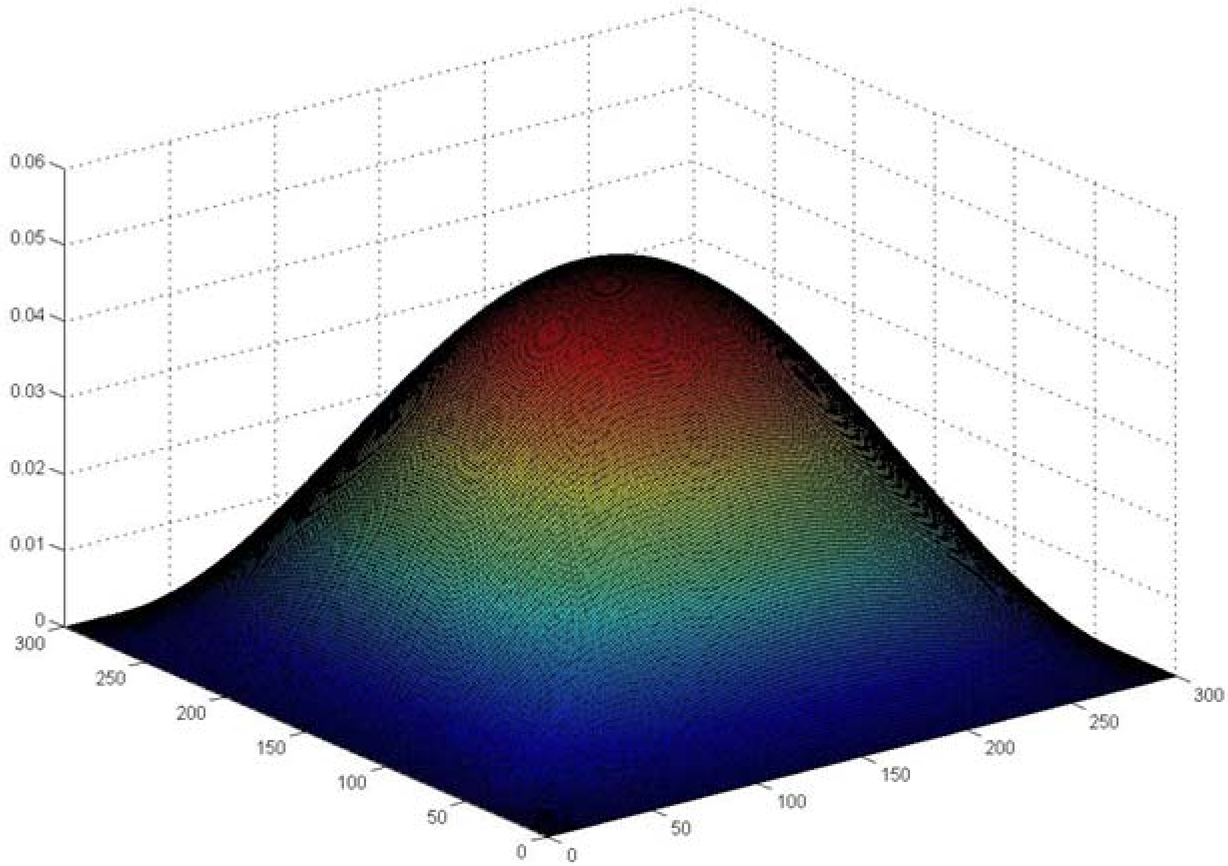


Figure 13, Problem Case 2

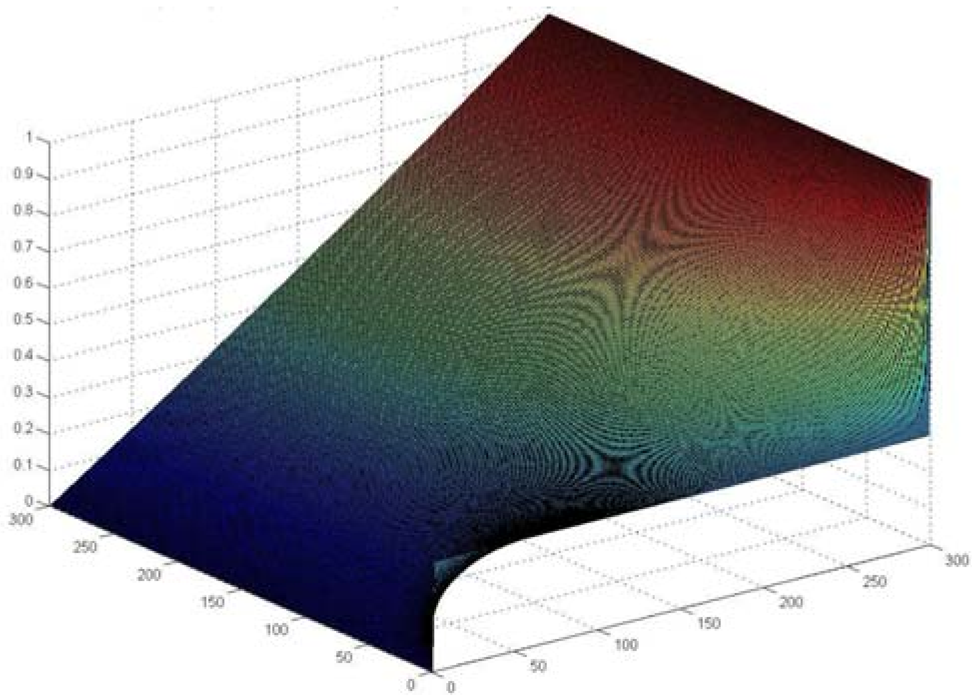


Figure 14, Problem Case 3

Parallel Example (parallel_ex01.f90)

```
      use linear_operators
      use mpi_setup_int

      implicit none

! This is the equivalent of Parallel Example 1 for .ix., with box data types
! and functions.

      integer, parameter :: n=32, nr=4
      real(kind(1e0)) :: one=1e0
      real(kind(1e0)), dimension(n,n,nr) :: A, b, x, err(nr)

! Setup for MPI.
      MP_NPROCS=MP_SETUP()

! Generate random matrices for A and b:
      A = rand(A); b=rand(b)
! Compute the box solution matrix of Ax = b.
      x = A .ix. b

! Check the results.
      err = norm(b - (A .x. x))/(norm(A)*norm(x)+norm(b))
      if (ALL(err <= sqrt(epsilon(one))) .and. MP_RANK == 0) &
        write (*,*) 'Parallel Example 1 is correct.'
! See to any error messages and quit MPI.
      MP_NPROCS=MP_SETUP('Final')
```

```
        end
```

.xi.

more... more...

Computes the product of a matrix or vector and the inverse of a matrix.

Operator Return Value

Matrix containing the product of A and B^{-1}. (Output)

Required Operands

A — Right operand matrix or vector. This is an array of rank 1, 2, or 3. It may be real, double, complex, or double complex. (Input)

B — Left operand matrix. This is an array of rank 2 or 3. It may be real, double, complex, double complex, or one of the computational sparse matrix derived types, `?_hbc_sparse`. (Input)

Optional Variables, Reserved Names

This operator uses the routines `LIN_SOL_GEN` or `LIN_SOL_LSQ` (See *Chapter 1, "Linear Systems"*).

The option and derived type names are given in the following tables:

Option Names for `.xi.`	**Option Value**
Use_lin_sol_gen_only	1
Use_lin_sol_lsq_only	2
xi_options_for_lin_sol_gen	3
xi_options_for_lin_sol_lsq	4
Skip_error_processing	5

Name of Unallocated Option Array to Use for Setting Options	Use	Derived Type
?_xinv_options(:)	Use when setting options for calls hereafter.	?_options
?_xinv_options_once(:)	Use when setting options for next call only.	?_options

For a description on how to use these options, see *Matrix Optional Data Changes*. See `LIN_SOL_GEN` and `LIN_SOL_LSQ` in *Chapter 1, "Linear Systems"* for the specific options for these routines.

FORTRAN 90 Interface

```
A .xi. B
```

Description

Computes the product of matrix A and the inverse of matrix B, for square non-singular matrices or the corresponding Moore-Penrose generalized inverse matrix for singular square matrices or rectangular matrices. The operation may be read *times generalized inverse*. The results are in a precision and data type that matches the most accurate or complex operand.

`.xi.` can be used with either dense or sparse matrices. It is MPI capable for dense matrices only.

Examples

Dense Matrix Example

```
      use linear_operators
      implicit none

      integer, parameter :: n=32
      real(kind(1e0)) :: one=1.0e0, err
      real(kind(1e0)), dimension(n,n) :: A, b, x

! Generate random matrices for A and b:
      A = rand(A); b=rand(b)

! Compute the solution matrix of xA = b.
      x = b .xi. A

! Check the results.
      err = norm(b - (x .x. A))/(norm(A)*norm(x)+norm(b))
      if (err <= sqrt(epsilon(one))) &
         write (*,*) 'Example  for .xi. operator is correct.'
      end
```

Sparse Matrix Example

```
use wrrrn_int
use linear_operators

type (s_sparse) S
type (s_hbc_sparse) H
integer, parameter :: N=3
real (kind(1.e0)) x(N,N), y(N,N), a(N,N)
real (kind(1.e0)) err
S = s_entry (1, 1, 2.0)
S = s_entry (1, 3, 1.0)
S = s_entry (2, 2, 4.0)
S = s_entry (3, 3, 6.0)
H = S   ! sparse
X = H   ! dense equivalent of H
A = rand(A)
Y = A .xi. H
 call wrrrn ( 'A', A)
 call wrrrn ( 'H', X)
 call wrrrn ( 'A .xi. H', y)

! Check the results.
    err =  norm(y - (A .xi. X))
     if (err <= sqrt(epsilon(one))) then
        write (*,*) 'Sparse example for .xi. operator is correct.'
     end if

end
```

Output

```
                 A
         1         2         3
1   0.5926   0.5015   0.5368
2   0.4001   0.9529   0.6988
3   0.0412   0.0633   0.3821

               H
        1        2        3
1   2.000    0.000    1.000
2   0.000    4.000    0.000
3   0.000    0.000    6.000

          A .xi. H
         1         2         3
1   0.2963   0.1254   0.0401
2   0.2001   0.2382   0.0831
3   0.0206   0.0158   0.0602
Sparse example for .xi. operator is correct.
```

Parallel Example

```
      use linear_operators
      use mpi_setup_int

      implicit none

! This is the equivalent of Parallel Example 1 for .xi., with box data types
! and functions.

      integer, parameter :: n=32, nr=4
      real(kind(1e0)) :: one=1e0
```

```
      real(kind(1e0)), dimension(n,n,nr) :: A, b, x, err(nr)

! Setup for MPI.
      MP_NPROCS=MP_SETUP()

! Generate random matrices for A and b:
      A = rand(A); b=rand(b)

! Compute the box solution matrix of xA = b.
      x = b .xi. A

! Check the results.
      err = norm(b - (x .x. A))/(norm(A)*norm(x)+norm(b))
      if (ALL(err <= sqrt(epsilon(one))) .and. MP_RANK == 0) &
        write (*,*) 'Parallel Example 1 is correct.'

! See to any error messages and quit MPI.
      MP_NPROCS=MP_SETUP('Final')

      end
```

CHOL

more...

Computes the Cholesky factorization of a positive-definite, symmetric or self-adjoint matrix.

Function Return Value

Matrix containing the Cholesky factorization of A. The factor is upper triangular, $R^T R = A$. (Output)

Required Argument

A — Matrix to be factored. This argument must be a rank-2 or rank-3 array that contains a positive-definite, symmetric or self-adjoint matrix. It may be real, double, complex, double complex. (Input)
For rank-3 arrays each rank-2 array (for fixed third subscript) is a positive-definite, symmetric or self-adjoint matrix. In this case, the output is a rank-3 array of Cholesky factors for the individual problems.

Optional Arguments, Packaged Options

This function uses `LIN_SOL_SELF` (See *Chapter 1, "Linear Systems"*), using the appropriate options to obtain the Cholesky factorization.

The option and derived type names are given in the following tables:

Option Names for `CHOL`	**Option Value**
Use_lin_sol_gen_only	4
Use_lin_sol_lsq_only	5

Name of Unallocated Option Array to Use for Setting Options	Use	Derived Type
?_chol_options(:)	Use when setting options for calls hereafter.	?_options
?_chol_options_once(:)	Use when setting options for next call only.	?_options

For a description on how to use these options, see *Matrix Optional Data Changes*. See `LIN_SOL_SELF` in *Chapter 1, "Linear Systems"* for the specific options for these routines.

FORTRAN 90 Interface

```
CHOL(A)
```

Description

Computes the Cholesky factorization of a positive-definite, symmetric or self-adjoint matrix, A. The factor is upper triangular, $R^T R = A$.

Examples

Dense Matrix Example (operator_ex06.f90)

```
      use linear_operators

      implicit none

! This is the equivalent of Example 2 for LIN_SOL_SELF using operators
! and functions.

      integer, parameter :: m=64, n=32
      real(kind(1e0)) :: one=1e0, zero=0e0, err
      real(kind(1e0)) A(n,n), b(n), C(m,n), d(m), cov(n,n), x(n)

! Generate a random rectangular matrix and right-hand side.
      C = rand(C); d=rand(d)

! Form the normal equations for the rectangular system.
      A = C .tx. C; b = C .tx. d
      COV = .i. CHOL(A); COV = COV .xt. COV

! Compute the least-squares solution.
       x = C .ix. d

! Compare with solution obtained using the inverse matrix.
      err = norm(x - (COV .x. b))/norm(cov)
```

```
! Scale the inverse to obtain the sample covariance matrix.
      COV = sum((d - (C .x. x))**2)/(m-n) * COV
! Check the results.
      if (err <= sqrt(epsilon(one))) then
         write (*,*) 'Example 2 for LIN_SOL_SELF (operators) is correct.'
      end if

      end
```

Parallel Example (parallel_ex06.f90)

```
      use linear_operators
      use mpi_setup_int

      implicit none

! This is the equivalent of Parallel Example 6 for box data types, operators ! and
functions.

      integer, parameter :: m=64, n=32, nr=4
      real(kind(1e0)) :: one=1e0, zero=0e0, err(nr)
      real(kind(1e0)), dimension(m,n,nr) :: C, d(m,1,nr)
      real(kind(1e0)), dimension(n,n,nr) :: A, cov
      real(kind(1e0)), dimension(n,1,nr) :: b, x

! Setup for MPI:
      mp_nprocs=mp_setup()

! Generate a random rectangular matrix and right-hand side.
      if(mp_rank == 0) then
         C = rand(C); d=rand(d)
      endif

! Form the normal equations for the rectangular system.
      A = C .tx. C; b = C .tx. d
      COV = .i. CHOL(A); COV = COV .xt. COV

! Compute the least-squares solution.
       x = C .ix. d

! Compare with solution obtained using the inverse matrix.
      err = norm(x - (COV .x. b))/norm(cov)

! Check the results.
      if (ALL(err <= sqrt(epsilon(one))) .and. mp_rank == 0) &
         write (*,*) 'Parallel Example 6 is correct.'

! See to any eror messages and quit MPI
      mp_nprocs=mp_setup('Final')

      end
```

COND

more...

Computes the condition number of a matrix.

Function Return Value

Computes condition number of matrix `A`. This is a scalar for the case where `A` is rank-2 or a sparse matrix. It is a rank-1 array when `A` is a dense rank-3 array. (Output)

Required Argument

A — Matrix for which the condition number is to be computed. The matrix may be real, double, complex, double-complex, or one of the computational sparse matrix derived types, `?_hbc_sparse`. For an array of type real, double, complex, or double-complex the array may be of rank-2 or rank-3.

For a dense rank-3 array, each rank-2 array section (for fixed third subscript) is a separate problem. In this case, the output is a rank-1 array of condition numbers for each problem. (Input)

Optional Arguments, Packaged Options

NORM_CHOICE — Integer indicating the type of norm to be used in computing the condition number.

NORM_CHOICE	CONDITION Number	Square Matrix		Rectangular Matrix	
		Dense	**Sparse**	**Dense**	**Sparse**
1	L_1	Yes	Yes	No	No
2 (Default)	L_2	Yes	Yes	Yes	No
huge(1)	L_∞	Yes	Yes	No	No

This function uses `LIN_SOL_SVD` (see *Chapter 1, "Linear Systems"*).

The option and derived type names are given in the following tables:

Option Names for COND	Option Value
?_cond_set_small	1
?_cond_for_lin_sol_svd	2

Name of Unallocated Option Array to Use for Setting Options	Use	Derived Type
?_cond_options(:)	Use when setting options for calls hereafter.	?_options
?_cond_options_once(:)	Use when setting options for next call only.	?_options

For a description on how to use these options, see *Matrix Optional Data Changes*. See LIN_SOL_SVD in *Chapter 1, "Linear Systems"* for the specific options for these routines.

FORTRAN 90 Interface

```
COND (A [,...])
```

Description

The mathematical definitions of the condition numbers which this routine estimates are:

$$l_1 \text{ condition number } \kappa_1(A) = \|A\|_1 \bullet \|A^{-1}\|_1$$
$$l_2 \text{ condition number } \kappa_2(A) = \|A\|_2 \bullet \|A^{-1}\|_2$$
$$l_\infty \text{ condition number } \kappa_\infty(A) = \|A\|_\infty \bullet \|A^{-1}\|_\infty$$

COND can be used with either dense or sparse matrices as follows:

	Square Matrix		Rectangular Matrix	
	Dense	Sparse	Dense	Sparse
L_1	Yes	Yes	No	No
L_2	Yes	Yes	Yes	No
L_∞	Yes	Yes	No	No

The generic function `COND` can be used with either dense or sparse square matrices. This function uses `LIN_SOL_SVD` for dense square and rectangular matrices in computing $\kappa_2(A) = s_1/s_n$. The function uses `LIN_SOL_GEN` for dense square matrices in computing $\kappa_1(A)$ and $\kappa_\infty(A)$. For sparse square matrices, the values returned for $\kappa_1(A)$ and $\kappa_\infty(A)$ are provided by the `SuperLU` linear equation solver. The condition number $\kappa_2(A) = s_1/s_n$ is computed by an algorithm that first approximates s_1 by computing the singular values of the $\kappa \times \kappa$ bidiagonal matrix obtained using the Lanczos method found in Golub and Van Loan, Ed. 3, p. 495. Here κ is set using the value `A%Options%Cond_Iteration_Max`, which has the default value of 30. The value s_n^{-2} is obtained using the power method, Golub and Van Loan, p. 330, iterating with the inverse matrix $\left(A^T A\right)^{-1} = A^{-1} A^{-T}$. For complex matrices A^T is replaced by $A^H = \overline{A}^T$. The dominant eigenvalue of this inverse matrix is s_n^{-2}. The number of iterations is limited by the parameter value κ or relative accuracy equal to the cube root of machine epsilon. Some timing tests indicate that computing $\kappa_2(A)$ for sparse matrices by this algorithm typically requires about twice the time as for a single linear solve using the defined operator `A .ix. b`.

For computation of $\kappa_2(A)$ with rectangular sparse matrices one can use a dense matrix representation for the matrix. This is not recommended except for small problem sizes. For overdetermined systems of sparse least-squares equations $Ax \cong b$ a related square system is given by

$$C\begin{bmatrix} x \\ r \end{bmatrix} \equiv \begin{bmatrix} A & I_{m\times m} \\ 0_{n\times n} & A^T \end{bmatrix} \begin{bmatrix} x \\ r \end{bmatrix} = \begin{bmatrix} b \\ 0 \end{bmatrix}$$

One can form C, which has more than twice the number of non-zeros as A. But C is still sparse. One can use the condition number of C as an estimate of the accuracy for the solution vector x and the residual vector r. Note that this version of the condition number is not the same as the l_2 condition number of A but is relevant to determining the accuracy of the least-squares system.

Examples

Dense Matrix Example (operator_ex02.f90)

```
use wrrrn_int
use linear_operators

integer, parameter :: N=3
real (kind(1.e0)) A(N,N)
real (kind(1.e0))  C1, C2, CINF
DATA A/2.0, 2.0, -4.0, 0.0, -1.0, 2.0, 0.0, 0.0, 5.0/
CINF = COND (A, norm_choice=huge(1))
C1   = COND (A, norm_choice=1)
C2   = COND (A)
call wrrrn ( 'A', A)
write (*,*)  'L1 condition number= ', C1
```

```
write (*,*)  'L2 condition number= ', C2
write (*,*)  'L infinity condition number= ', CINF

end
```

Output

```
            A
        1       2       3
1   2.000   0.000   0.000
2   2.000  -1.000   0.000
3  -4.000   2.000   5.000

L1 condition number=  12.0
L2 condition number=  10.405088
L infinity condition number=  22.0
```

Sparse Matrix Example

```
use wrrrn_int
use linear_operators

type (s_sparse) S
type (s_hbc_sparse) H
integer, parameter :: N=3
real (kind(1.e0)) X(N,N)
real (kind(1.e0))  C1, C2, CINF
S = s_entry (1, 1, 2.0)
S = s_entry (2, 1, 2.0)
S = s_entry (3, 1, -4.0)
S = s_entry (3, 2, 2.0)
S = s_entry (2, 2, -1.0)
S = s_entry (3, 3, 5.0)
H = S   ! sparse
X = H   ! dense equivalent of H

CINF = COND (H, norm_choice=huge(1))
C1   = COND (H, norm_choice=1)
C2   = COND (H)
call wrrrn ( 'H', X)
write (*,*)  'L1 condition number= ', C1
write (*,*)  'L2 condition number= ', C2
write (*,*)  'L infinity condition number= ', CINF

end
```

Output

```
            H
        1       2       3
1   2.000   0.000   0.000
2   2.000  -1.000   0.000
3  -4.000   2.000   5.000

L1 condition number=  12.0
L2 condition number=  10.405088
L infinity condition number=  22.0
```

Parallel Example (parallel_ex02.f90)

```
     use linear_operators
```

```
      use mpi_setup_int

      implicit none

! This is the equivalent of Parallel Example 2 for .i. and det() with box
! data types, operators and functions.

      integer, parameter :: n=32, nr=4
      integer J
      real(kind(1e0)) :: one=1e0
      real(kind(1e0)), dimension(nr) :: err, det_A, det_i
      real(kind(1e0)), dimension(n,n,nr) :: A, inv, R, S

! Setup for MPI.
      MP_NPROCS=MP_SETUP()
! Generate a random matrix.
      A = rand(A)
! Compute the matrix inverse and its determinant.
      inv = .i.A; det_A = det(A)
! Compute the determinant for the inverse matrix.
      det_i = det(inv)
! Check the quality of both left and right inverses.
      DO J=1,nr; R(:,:,J)=EYE(N); END DO

      S=R; R=R-(A .x. inv); S=S-(inv .x. A)
      err = (norm(R)+norm(S))/cond(A)
      if (ALL(err <= sqrt(epsilon(one)) .and. &
        abs(det_A*det_i - one) <= sqrt(epsilon(one)))&
       .and. MP_RANK == 0) &
        write (*,*) 'Parallel Example 2 is correct.'

! See to any error messages and quit MPI.
      MP_NPROCS=MP_SETUP('Final')

      end
```

DET

more...

Computes the determinant of a rectangular matrix.

Function Return Value

Determinant of matrix A. This is a scalar for the case where A is rank 2. It is a rank-1 array of determinant values for the case where A is rank 3. (Output)

Required Argument

A — Matrix for which the determinant is to be computed. This argument must be a rank-2 or rank-3 array that contains a rectangular matrix. It may be real, double, complex, double complex. (Input)

For rank-3 arrays, each rank-2 array (for fixed third subscript) is a separate matrix. In this case, the output is a rank-1 array of determinant values for each problem.

Optional Arguments, Packaged Options

This function uses LIN_SOL_LSQ (see *Chapter 1, "Linear Systems"*) to compute the *QR* decomposition of *A*, and the logarithmic value of det(*A*), which is exponentiated for the result.

The option and derived type names are given in the following tables:

Option Names for DET	**Option Value**
?_det_for_lin_sol_lsq	1

Name of Unallocated Option Array to Use for Setting Options	Use	Derived Type
?_det_options(:)	Use when setting options for calls hereafter.	?_options
?_det_options_once(:)	Use when setting options for next call only.	?_options

For a description on how to use these options, see *Matrix Optional Data Changes*. See LIN_SOL_LSQ in *Chapter 1, "Linear Systems"* for the specific options for these routines.

FORTRAN 90 Interface

DET (A)

Description

Computes the determinant of a rectangular matrix, *A*. The evaluation is based on the *QR* decomposition,

$$QAP = \begin{bmatrix} R_{k \times k} & 0 \\ 0 & 0 \end{bmatrix}$$

and $k = rank(A)$. Thus $det(A) = s \times det(R)$ where $s = det(Q) \times det(P) = \pm 1$.

Even well-conditioned matrices can have determinants with values that have very large or very tiny magnitudes. The values may overflow or underflow. For this class of problems, the use of the logarithmic representation of the determinant found in LIN_SOL_GEN or LIN_SOL_LSQ is required.

Examples

Dense Matrix Example (operator_ex02.f90)

```
      use linear_operators
      implicit none

! This is Example 2 for LIN_SOL_GEN using operators and functions.

      integer, parameter :: n=32
      real(kind(1e0)) :: one=1e0, err, det_A, det_i
      real(kind(1e0)), dimension(n,n) :: A, inv

! Generate a random matrix.
      A = rand(A)
! Compute the matrix inverse and its determinant.
      inv = .i.A; det_A = det(A)
```

```
! Compute the determinant for the inverse matrix.
      det_i = det(inv)
! Check the quality of both left and right inverses.
      err = (norm(EYE(n)-(A .x. inv))+norm(EYE(n)-(inv.x.A)))/cond(A)
      if (err <= sqrt(epsilon(one)) .and. abs(det_A*det_i - one) <= &
                 sqrt(epsilon(one))) &
      write (*,*) 'Example 2 for LIN_SOL_GEN (operators) is correct.'
      end
```

Parallel Example (parallel_ex02.f90)

```
      use linear_operators
      use mpi_setup_int

      implicit none

! This is the equivalent of Parallel Example 2 for .i. and det() with box
! data types, operators and functions.

      integer, parameter :: n=32, nr=4
      integer J
      real(kind(1e0)) :: one=1e0
      real(kind(1e0)), dimension(nr) :: err, det_A, det_i
      real(kind(1e0)), dimension(n,n,nr) :: A, inv, R, S

! Setup for MPI.
      MP_NPROCS=MP_SETUP()
! Generate a random matrix.
      A = rand(A)
! Compute the matrix inverse and its determinant.
      inv = .i.A; det_A = det(A)
! Compute the determinant for the inverse matrix.
      det_i = det(inv)
! Check the quality of both left and right inverses.
      DO J=1,nr; R(:,:,J)=EYE(N); END DO

      S=R; R=R-(A .x. inv); S=S-(inv .x. A)
      err = (norm(R)+norm(S))/cond(A)
      if (ALL(err <= sqrt(epsilon(one)) .and. &
        abs(det_A*det_i - one) <= sqrt(epsilon(one)))&
       .and. MP_RANK == 0) &
        write (*,*) 'Parallel Example 2 is correct.'

! See to any error messages and quit MPI.
      MP_NPROCS=MP_SETUP('Final')

      end
```

DIAG

Constructs a square diagonal matrix.

Function Return Value

Square diagonal matrix of rank-2 if `A` is rank-1 or rank-3 array if `A` is rank-2. (Output)

Required Argument

A — This is a rank-1 or rank-2 array of type real, double, complex, or double complex, containing the diagonal elements. The output is a rank-2 or rank-3 array, respectively. (Input)

FORTRAN 90 Interface

`DIAG (A)`

Description

Constructs a square diagonal matrix from a rank-1 array or several diagonal matrices from a rank-2 array. The dimension of the matrix is the value of the size of the rank-1 array.

The use of `DIAG` may be obviated by observing that the defined operations `C = diag(x) .x. A` or `D = B .x. diag(x)` are respectively the array operations `C = spread(x, DIM=1, NCOPIES=size(A,1))*A`, and `D = B*spread(x,DIM=2,NCOPIES=size(B,2))`. These array products are not as easy to read as the defined operations using `DIAG` and matrix multiply, but their use results in a more efficient code.

Examples

Dense Matrix Example (operator_ex13.f90)

```
      use linear_operators
      implicit none

! This is the equivalent of Example 1 for LIN_SOL_SVD using operators
! and functions.
      integer, parameter :: m=128, n=32
```

```
      real(kind(1d0)) :: one=1d0, err
      real(kind(1d0)) A(m,n), b(m), x(n), U(m,m), V(n,n), S(n), g(m)

! Generate a random matrix and right-hand side.
      A = rand(A); b = rand(b)

! Compute the least-squares solution matrix of Ax=b.
      S = SVD(A, U = U, V = V)
      g = U .tx. b; x = V .x. diag(one/S) .x. g(1:n)

! Check the results.
      err = norm(A .tx. (b - (A .x. x)))/(norm(A)+norm(x))
      if (err <= sqrt(epsilon(one))) then
         write (*,*) 'Example 1 for LIN_SOL_SVD (operators) is correct.'
      end if

      end
```

DIAGONALS

Extracts the diagonal terms of a matrix.

Function Return Value

Array containing the diagonal terms of matrix A. It is rank-1 or rank-2 depending on the rank of A. When A is a rank-3 array, the result is a rank-2 array consisting of each separate set of diagonals. (Output)

Required Argument

A — Matrix from which to extract the diagonal. This is a rank-2 or rank-3 array of type real, double, complex, or double complex. The output is a rank-1 or rank-2 array, respectively. (Input)

FORTRAN 90 Interface

DIAGONALS (A)

Description

Extracts a rank-1 array whose values are the diagonal terms of the rank-2 array A. The size of the array is the smaller of the two dimensions of the rank-2 array.

Examples

Dense Matrix Example (operator_ex32.f90)

```
      use linear_operators
      implicit none
! This is the equivalent of Example 4 (using operators) for LIN_EIG_GEN.

      integer, parameter :: n=17
      real(kind(1d0)), parameter :: one=1d0
      real(kind(1d0)), dimension(n,n) :: A, C
      real(kind(1d0)) variation(n), eta
      complex(kind(1d0)), dimension(n,n) :: U, V, e(n), d(n)

! Generate a random matrix.
      A = rand(A)

! Compute the eigenvalues, left- and right- eigenvectors.
```

```
      D = EIG(A, W=V); E = EIG(.t.A, W=U)

! Compute condition numbers and variations of eigenvalues.
      variation = norm(A)/abs(diagonals( U .hx. V))

! Now perturb the data in the matrix by the relative factors
! eta=sqrt(epsilon) and solve for values again.  Check the
! differences compared to the estimates.  They should not exceed
! the bounds.
      eta = sqrt(epsilon(one))
      C = A + eta*(2*rand(A)-1)*A
      D = EIG(C)

! Looking at the differences of absolute values accounts for
! switching signs on the imaginary parts.
      if (count(abs(d)-abs(e) > eta*variation) == 0) then
         write (*,*) 'Example 4 for LIN_EIG_GEN (operators) is correct.'
      end if
      end
```

EIG

more...

Computes the eigenvalue-eigenvector decomposition of an ordinary or generalized eigenvalue problem.

Function Return Value

Rank-1 or rank-2 real or complex array of eigenvalues. (Output)

Required Argument

A — Matrix for which the eigenexpansion is to be computed. This is a square rank-2 array or a rank-3 array with square first rank-2 sections of type single, double, complex, or double complex. (Input)

Optional Arguments, Packaged Options

B — Matrix `B` for the generalized problem, $Ax = eBx$. `B` must be the same type as `A`. (Input)

D — Array containing the real diagonal matrix factors of the generalized eigenvalues. (Output)

V — Array of real eigenvectors for both the ordinary and generalized problem. Used only for the generalized problem when matrix B is singular. (Output)

W — Array of complex eigenvectors for both the ordinary and generalized problem. Do not use optional argument `V` when `W` is present. (Output)

This function uses `LIN_EIG_SELF`, `LIN_EIG_GEN`, and `LIN_GEIG_GEN` to compute the decompositions. See *Chapter 2, "Eigensystem Analysis"*.

The option and derived type names are given in the following tables:

Option Names for `EIG`	**Option Value**
Options_for_lin_eig_self	1
Options_for_lin_eig_gen	2

Option Names for `EIG`	Option Value
Options_for_lin_geig_gen	3
Skip_error_processing	5

Name of Unallocated Option Array to Use for Setting Options	Use	Derived Type
?_eig_options(:)	Use when setting options for calls hereafter.	?_options
?_eig_options_once(:)	Use when setting options for next call only.	?_options

For a description on how to use these options, see "Matrix Optional Data Changes". See `LIN_EIG_SELF`, `LIN_EIG_GEN`, and `LIN_GEIG_GEN` located in *Chapter 2, "Eigensystem Analysis"* for the specific options for these routines.

FORTRAN 90 Interface

```
EIG (A [,…])
```

Description

Computes the eigenvalue-eigenvector decomposition of an ordinary or generalized eigenvalue problem.

For the ordinary eigenvalue problem $Ax = ex$, optional argument B is not used. With the generalized problem $Ax = eBx$, the optional argument `B` is used to input the matrix B. Optional output argument `D` is an array required only for the generalized problem and then only when the matrix B is singular.

The array of real eigenvectors is an optional output (`V`) for both the ordinary and the generalized problem. If any eigenvectors are complex, optional output `W` must be present. In that case `V` is not used.

Examples

Dense Matrix Example 1 (operator_ex26.f90)

```
      use linear_operators
      implicit none
! This is the equivalent of Example 2 (using operators) for LIN_EIG_SELF.
```

```
      integer, parameter :: n=8
      real(kind(1e0)), parameter :: one=1e0
      real(kind(1e0)), dimension(n,n) :: A, d(n), v_s

! Generate a random self-adjoint matrix.
      A = rand(A); A = A + .t.A

! Compute the eigenvalues and eigenvectors.
      D = EIG(A,V=v_s)

! Check the results for small residuals.
      if (norm((A .x. v_s) - (v_s .x. diag(D)))/abs(d(1)) <= &
              sqrt(epsilon(one))) then
         write (*,*) 'Example 2 for LIN_EIG_SELF (operators) is correct.'
      end if

      end
```

Dense Matrix Example 2 (operator_ex33.f90)

```
      use linear_operators

      implicit none

! This is the equivalent of Example 1 (using operators) for LIN_GEIG_GEN.

      integer, parameter :: n=32
      real(kind(1d0)), parameter :: one=1d0
      real(kind(1d0)) A(n,n), B(n,n), bta(n), beta_t(n), err
      complex(kind(1d0)) alpha(n), alpha_t(n), V(n,n)

! Generate random matrices for both A and B.
      A = rand(A); B = rand(B)

! Compute the generalized eigenvalues.
      alpha = EIG(A, B=B, D=bta)

! Compute the full decomposition once again, A*V = B*V*values,
! and check for any error messages.
      alpha_t = EIG(A, B=B, D=beta_t, W = V)

! Use values from the first decomposition, vectors from the
! second decomposition, and check for small residuals.
      err = norm((A .x. V .x. diag(bta)) - (B .x. V .x. diag(alpha)),1)/&
             (norm(A,1)*norm(bta,1) + norm(B,1)*norm(alpha,1))
      if (err  <= sqrt(epsilon(one))) then
         write (*,*) 'Example 1 for LIN_GEIG_GEN (operators) is correct.'
      end if

      end
```

Parallel Example (parallel_ex04.f90)

Here an alternate node is used to compute the majority of a single application, and the user does not need to make any explicit calls to MPI routines. The time-consuming parts are the evaluation of the eigenvalue-eigenvector expansion, the solving step, and the residuals. To do this, the rank-2 arrays are changed to a box data type with a unit third dimension. This uses parallel computing. The node priority order is established by the initial function call, `MP_SETUP(n)`. The root is restricted from working on the box data type by assigning `MPI_ROOT_WORKS=.false.`. This example anticipates that the most efficient node, other than the root, will perform the heavy computing. Two nodes are required to execute.

```
      use linear_operators
      use mpi_setup_int

      implicit none

! This is the equivalent of Parallel Example 4 for matrix exponential.
! The box dimension has a single rack.
      integer, parameter :: n=32, k=128, nr=1
      integer i
      real(kind(1e0)), parameter :: one=1e0, t_max=one, delta_t=t_max/(k-1)
      real(kind(1e0)) err(nr), sizes(nr), A(n,n,nr)
      real(kind(1e0)) t(k), y(n,k,nr), y_prime(n,k,nr)
      complex(kind(1e0)), dimension(n,nr) :: x(n,n,nr), z_0, &
        Z_1(n,nr,nr), y_0, d

! Setup for MPI.  Establish a node priority order.
! Restrict the root from significant computing.
! Illustrates using the 'best' performing node that
! is not the root for a single task.
      MP_NPROCS=MP_SETUP(n)

      MPI_ROOT_WORKS=.false.

! Generate a random coefficient matrix.
      A = rand(A)

! Compute the eigenvalue-eigenvector decomposition
! of the system coefficient matrix on an alternate node.
      D = EIG(A, W=X)

! Generate a random initial value for the ODE system.
      y_0 = rand(y_0)

! Solve complex data system that transforms the initial
! values, X z_0=y_0.

      z_1= X .ix. y_0 ; z_0(:,nr) = z_1(:,nr,nr)

! The grid of points where a solution is computed:
      t = (/(i*delta_t,i=0,k-1)/)


! Compute y and y' at the values t(1:k).
! With the eigenvalue-eigenvector decomposition AX = XD, this
! is an evaluation of EXP(A t)y_0 = y(t).
      y = X .x.exp(spread(d(:,nr),2,k)*spread(t,1,n))*spread(z_0(:,nr),2,k)

! This is y', derived by differentiating y(t).
      y_prime  = X .x. &
spread(d(:,nr),2,k)*exp(spread(d(:,nr),2,k)*spread(t,1,n))* &
                spread(z_0(:,nr),2,k)

! Check results. Is  y' - Ay = 0?
      err = norm(y_prime-(A .x. y))
      sizes=norm(y_prime)+norm(A)*norm(y)
      if (ALL(err <= sqrt(epsilon(one))*sizes) .and. MP_RANK == 0) &
        write (*,*) 'Parallel Example 4 is correct.'

! See to any error messages and quit MPI.
      MP_NPROCS=MP_SETUP('Final')
```

```
    end
```

EYE

Creates the identity matrix.

Function Return Value

Identity matrix of size $N \times N$ and type real . (Output)

Required Argument

N — Size of output identity matrix. (Input)

FORTRAN 90 Interface

`EYE (N)`

Description

Creates a rank-2 square array whose diagonals are all the value one. The off-diagonals all have value zero.

Examples

Dense Matrix Example (operator_ex07.f90)

```
      use linear_operators

      implicit none

! This is the equivalent of Example 3 (using operators) for LIN_SOL_SELF.

      integer tries
      integer, parameter :: m=8, n=4, k=2
      integer ipivots(n+1)
      real(kind(1d0)) :: one=1.0d0, err
      real(kind(1d0)) a(n,n), b(n,1), c(m,n), x(n,1), &
             e(n), ATEMP(n,n)
      type(d_options) :: iopti(4)

! Generate a random rectangular matrix.
      C = rand(C)

! Generate a random right hand side for use in the inverse
! iteration.
```

```
      b = rand(b)

! Compute the positive definite matrix.
      A = C .tx. C; A = (A+.t.A)/2

! Obtain just the eigenvalues.
      E = EIG(A)

! Use packaged option to reset the value of a small diagonal.
      iopti(4) = 0
      iopti(1) = d_options(d_lin_sol_self_set_small,&
                 epsilon(one)*abs(E(1)))

! Use packaged option to save the factorization.
      iopti(2) = d_lin_sol_self_save_factors

! Suppress error messages and stopping due to singularity
! of the matrix, which is expected.
      iopti(3) = d_lin_sol_self_no_sing_mess

      ATEMP = A

! Compute A-eigenvalue*I as the coefficient matrix.
! Use eigenvalue number k.
      A = A - e(k)*EYE(n)

      do tries=1,2
         call lin_sol_self(A, b, x, &
                    pivots=ipivots, iopt=iopti)
! When code is re-entered, the already computed factorization
! is used.
         iopti(4) = d_lin_sol_self_solve_A

! Reset right-hand side in the direction of the eigenvector.
         B = UNIT(x)
      end do

! Normalize the eigenvector.
      x = UNIT(x)

! Check the results.
      b=ATEMP .x. x
      err =  dot_product(x(1:n,1), b(1:n,1)) - e(k)

! If any result is not accurate, quit with no printing.
      if (abs(err) <= sqrt(epsilon(one))*E(1)) then
        write (*,*) 'Example 3 for LIN_SOL_SELF (operators) is correct.'
      end if

      end
```

FFT

more...

Computes the Discrete Fourier Transform of one complex sequence.

Function Return Value

Complex array containing the Discrete Fourier Transform of X . The result is the complex array of the same shape and rank as X. (Output)

Required Argument

X — Array containing the sequence for which the transform is to be computed. X is an assumed shape complex array of rank 1, 2 or 3. If X is real or double, it is converted to complex internally prior to the computation. (Input)

Optional Arguments, Packaged Options

WORK — A COMPLEX array of the same precision as the data. For rank-1 transforms the size of WORK is $n + 15$. To define this array for each problem, set WORK(1) = 0. Each additional rank adds the dimension of the transform plus 15. Using the optional argument WORK increases the efficiency of the transform.

The option and derived type names are given in the following tables:

Option Names for FFT	Option Value
Options_for_fast_dft	1

Name of Unallocated Option Array to Use for Setting Options	Use	Derived Type
?_fft_options(:)	Use when setting options for calls hereafter.	?_options
?_fft_options_once(:)	Use when setting options for next call only.	?_options

For a description on how to use these options, see *Matrix Optional Data Changes*. See `FAST_DFT` located in *Chapter 6, "Transforms"* for the specific options for this routine.

FORTRAN 90 Interface

FFT (X [, …])

Description

Computes the Discrete Fourier Transform of a complex sequence. This function uses `FAST_DFT`, `FAST_2DFT`, and `FAST_3DFT` from Chapter 6.

Example (operator_ex37.f90)

```
      use rand_gen_int
      use fft_int
      use ifft_int
      use linear_operators

      implicit none

! This is Example 4 for FAST_DFT (using operators).

      integer j
      integer, parameter :: n=40
      real(kind(1e0)) :: err, one=1e0
      real(kind(1e0)), dimension(n) :: a, b, c, yy(n,n)
      complex(kind(1e0)), dimension(n) ::  f, fa, fb

! Generate two random periodic sequences 'a' and 'b'.
      a=rand(a); b=rand(b)

! Compute the convolution 'c' of 'a' and 'b'.
      yy(1:,1)=b
      do j=2,n
        yy(2:,j)=yy(1:n-1,j-1)
        yy(1,j)=yy(n,j-1)
      end do

      c=yy .x. a

! Compute f=inverse(transform(a)*transform(b)).
      fa = fft(a)
```

```
      fb = fft(b)
      f=ifft(fa*fb)

! Check the Convolution Theorem:
! inverse(transform(a)*transform(b)) = convolution(a,b).
      err = norm(c-f)/norm(c)
      if (err <= sqrt(epsilon(one))) then
         write (*,*) 'Example 4 for FAST_DFT (operators) is correct.'
      end if

      end
```

FFT_BOX

more... more...

Computes the Discrete Fourier Transform of several complex or real sequences.

Function Return Value

Complex array containing the Discrete Fourier Transform of the sequences in X . If X is an assumed shape complex array of rank 2, 3 or 4, the result is a complex array of the same shape and rank consisting of the DFT for each of the last rank's indices. (Output)

Required Argument

X — Box containing the sequences for which the transform is to be computed. X is an assumed shape complex array of rank 2, 3 or 4. If X is real or double, it is converted to complex internally prior to the computation. (Input)

Optional Arguments, Packaged Options

WORK — A COMPLEX array of the same precision as the data. For rank-1 transforms the size of WORK is $n + 15$. To define this array for each problem, set WORK(1) = 0. Each additional rank adds the dimension of the transform plus 15. Using the optional argument WORK increases the efficiency of the transform

The option and derived type names are given in the following tables:

Option Names for FFT	Option Value
Options_for_fast_dft	1

Name of Unallocated Option Array to Use for Setting Options	Use	Derived Type
?_fft_box_options(:)	Use when setting options for calls hereafter.	?_options
?_fft_box_options_once(:)	Use when setting options for next call only.	?_options

For a description on how to use these options, see *Matrix Optional Data Changes*. See `FAST_DFT` located in *Chapter 6, "Transforms"* for the specific options for this routine.

FORTRAN 90 Interface

`FFT_BOX (X [, …])`

Description

Computes the Discrete Fourier Transform of a box of complex sequences. This function uses `FAST_DFT`, `FAST_2DFT`, and `FAST_3DFT` from Chapter 6.

Examples

Parallel Example

```
      use rand_gen_int
      use fft_box_int
      use ifft_box_int
      use linear_operators
      use mpi_setup_int

      implicit none

! This is FFT_BOX example.

      integer i,j
      integer, parameter :: n=40, nr=4
      real(kind(1e0)) :: err(nr), one=1e0
      real(kind(1e0)) :: a(n,1,nr), b(n,nr), c(n,1,nr), yy(n,n,nr)
      complex(kind(1e0)), dimension(n,nr) :: f, fa, fb, cc, aa

      real(kind(1e0)),parameter::zero_par=0.e0
      real(kind(1e0))::dummy_par(0)
      integer iseed_par
      type(s_options)::iopti_par(2)


! setup for MPI
      MP_NPROCS = MP_SETUP()

! Set Random Number generator seed
```

```
       iseed_par = 53976279
       iopti_par(1)=s_options(s_rand_gen_generator_seed,zero_par)
       iopti_par(2)=s_options(iseed_par,zero_par)


       call rand_gen(dummy_par,iopt=iopti_par)

 ! Generate two random periodic sequences 'a' and 'b'.
       a=rand(a); b=rand(b)

 ! Compute the convolution 'c' of 'a' and 'b'.
      do i=1,nr
       aa(1:,i) = a(1:,1,i)
       yy(1:,1,i)=b(1:,i)
       do j=2,n
         yy(2:,j,i)=yy(1:n-1,j-1,i)
         yy(1,j,i)=yy(n,j-1,i)
       end do
      end do

       c=yy .x. a

 ! Compute f=inverse(transform(a)*transform(b)).
       fa = fft_box(aa)
       fb = fft_box(b)
       f=ifft_box(fa*fb)

 ! Check the Convolution Theorem:
 ! inverse(transform(a)*transform(b)) = convolution(a,b).
       do i=1,nr
        cc(1:,i) = c(1:,1,i)
       end do
       err = norm(cc-f)/norm(cc)
       if (ALL(err <= sqrt(epsilon(one))) .AND. MP_RANK == 0) then
          write (*,*) 'FFT_BOX is correct.'
       end if

        MP_NPROCS = MP_SETUP('Final')
       end
```

IFFT

more...

Computes the inverse of the Discrete Fourier Transform of one complex sequence.

Function Return Value

Complex array containing the inverse of the Discrete Fourier Transform of `X`. The result is the complex array of the same shape and rank as `X`. (Output)

Required Argument

X — Array containing the sequence for which the inverse transform is to be computed. `X` is an assumed shape complex array of rank 1, 2 or 3. If `X` is real or double, it is converted to complex internally prior to the computation. (Input)

Optional Arguments, Packaged Options

WORK — a `COMPLEX` array of the same precision as the data. For rank-1 transforms the size of `WORK` is $n + 15$. To define this array for each problem, set `WORK(1) = 0`. Each additional rank adds the dimension of the transform plus 15. Using the optional argument `WORK` increases the efficiency of the transform.

The option and derived type names are given in the following tables:

Option Name for IFFT	Option Value
options_for_fast_dft	1

Name of Unallocated Option Array to Use for Setting Options	Use	Derived Type
?_ifft_options(:)	Use when setting options for calls hereafter.	?_options
?_ifft_options_once(:)	Use when setting options for next call only.	?_options

For a description on how to use these options, see *Matrix Optional Data Changes*. See `FAST_DFT` located in *Chapter 6, "Transforms"* for the specific options for this routine.

FORTRAN 90 Interface

IFFT (X [, …])

Description

Computes the inverse of the Discrete Fourier Transform of a complex sequence. This function uses `FAST_DFT`, `FAST_2DFT`, and `FAST_3DFT` from Chapter 6.

Example (operator_ex37.f90)

```
      use rand_gen_int
      use fft_int
      use ifft_int
      use linear_operators

      implicit none

! This is the equivalent of Example 4 for FAST_DFT (using operators).

      integer j
      integer, parameter :: n=40
      real(kind(1e0)) :: err, one=1e0
      real(kind(1e0)), dimension(n) :: a, b, c, yy(n,n)
      complex(kind(1e0)), dimension(n) ::  f, fa, fb

! Generate two random periodic sequences 'a' and 'b'.
      a=rand(a); b=rand(b)

! Compute the convolution 'c' of 'a' and 'b'.
      yy(1:,1)=b
      do j=2,n
        yy(2:,j)=yy(1:n-1,j-1)
        yy(1,j)=yy(n,j-1)
      end do

      c=yy .x. a

! Compute f=inverse(transform(a)*transform(b)).
```

```
       fa = fft(a)
       fb = fft(b)
       f=ifft(fa*fb)

 ! Check the Convolution Theorem:
 ! inverse(transform(a)*transform(b)) = convolution(a,b).
       err = norm(c-f)/norm(c)
       if (err <= sqrt(epsilon(one))) then
          write (*,*) 'Example 4 for FAST_DFT (operators) is correct.'
       end if

       end
```

IFFT_BOX

more...

more...

Computes the inverse Discrete Fourier Transform of several complex or real sequences.

Function Return Value

Complex array containing the inverse of the Discrete Fourier Transform of the sequences in `X`. If `X` is an assumed shape complex array of rank 2, 3 or 4, the result is a complex array of the same shape and rank consisting of the inverse DFT for each of the last rank's indices. (Output)

Required Argument

X — Box containing the sequences for which the inverse transform is to be computed. `X` is an assumed shape complex array of rank 2, 3 or 4. If `X` is real or double, it is converted to complex internally prior to the computation. (Input)

Optional Arguments, Packaged Options

WORK — A `COMPLEX` array of the same precision as the data. For rank-1 transforms the size of `WORK` is $n + 15$. To define this array for each problem, set `WORK(1) = 0`. Each additional rank adds the dimension of the transform plus 15. Using the optional argument `WORK` increases the efficiency of the transform.

The option and derived type names are given in the following tables:

Option Names for IFFT	Option Value
Options_for_fast_dft	1

Name of Unallocated Option Array to Use for Setting Options	Use	Derived Type
?_ifft_box_options(:)	Use when setting options for calls hereafter.	?_options
?_ifft_box_options_once(:)	Use when setting options for next call only.	?_options

For a description on how to use these options, see *Matrix Optional Data Changes*. See `FAST_DFT` located in *Chapter 6, "Transforms"* for the specific options for this routine.

FORTRAN 90 Interface

IFFT_BOX (X [, …])

Description

Computes the inverse of the Discrete Fourier Transform of a box of complex sequences. This function uses `FAST_DFT`, `FAST_2DFT`, and `FAST_3DFT` from Chapter 6.

Parallel Example

```
      use rand_gen_int
      use fft_box_int
      use ifft_box_int
      use linear_operators
      use mpi_setup_int

      implicit none

! This is FFT_BOX example.

      integer i,j
      integer, parameter :: n=40, nr=4
      real(kind(1e0)) :: err(nr), one=1e0
      real(kind(1e0)) :: a(n,1,nr), b(n,nr), c(n,1,nr), yy(n,n,nr)
      complex(kind(1e0)), dimension(n,nr) :: f, fa, fb, cc, aa

      real(kind(1e0)),parameter::zero_par=0.e0
      real(kind(1e0))::dummy_par(0)
      integer iseed_par
      type(s_options)::iopti_par(2)


! setup for MPI
      MP_NPROCS = MP_SETUP()

! Set Random Number generator seed

      iseed_par = 53976279
```

```
      iopti_par(1)=s_options(s_rand_gen_generator_seed,zero_par)
      iopti_par(2)=s_options(iseed_par,zero_par)

      call rand_gen(dummy_par,iopti=iopti_par)

! Generate two random periodic sequences 'a' and 'b'.
      a=rand(a); b=rand(b)

! Compute the convolution 'c' of 'a' and 'b'.
     do i=1,nr
      aa(1:,i) = a(1:,1,i)
      yy(1:,1,i)=b(1:,i)
      do j=2,n
        yy(2:,j,i)=yy(1:n-1,j-1,i)
        yy(1,j,i)=yy(n,j-1,i)
      end do
     end do

      c=yy .x. a

! Compute f=inverse(transform(a)*transform(b)).
      fa = fft_box(aa)
      fb = fft_box(b)
      f=ifft_box(fa*fb)

! Check the Convolution Theorem:
! inverse(transform(a)*transform(b)) = convolution(a,b).
      do i=1,nr
       cc(1:,i) = c(1:,1,i)
      end do
      err = norm(cc-f)/norm(cc)
      if (ALL(err <= sqrt(epsilon(one))) .AND. MP_RANK == 0) then
         write (*,*) 'FFT_BOX is correct.'
      end if

       MP_NPROCS = MP_SETUP('Final')
      end
```

isNaN

Tests for NaN.

Function Return Value

Logical indicating whether or not A contains NaN. The output value tests `.true.` only if there is at least one NaN in the scalar or array. (Output)

Required Argument

A — The argument can be a scalar or array of rank-1, rank-2 or rank-3. The values can be any of the four intrinsic floating-point types. (Input)

FORTRAN 90 Interface

`isNaN(A)`

Description

This is a generic logical function used to test scalars or arrays for occurrence of an IEEE 754 Standard format of floating point (ANSI/IEEE 1985) NaN, or not-a-number. Either *quiet* or *signaling* NaNs are detected without an exception occurring in the test itself. The individual array entries are each examined, with bit manipulation, until the first NaN is located. For non-IEEE formats, the bit pattern tested for single precision is `transfer(not(0),1)`. For double precision numbers `x`, the bit pattern tested is equivalent to assigning the integer array `i(1:2) = not(0)`, then testing this array with the bit pattern of the integer array `transfer(x,i)`. This function is likely to be required whenever there is the possibility that a subroutine blocked the output with NaNs in the presence of an error condition.

Example

```
      use isnan_int
      implicit none

! This is the equivalent of Example 1 for NaN.
      integer, parameter :: n=3
      real(kind(1e0)) A(n,n); real(kind(1d0)) B(n,n)
      real(kind(1e0)), external :: s_NaN
```

```
      real(kind(1d0)), external :: d_NaN

! Assign NaNs to both A and B:
      A = s_Nan(1e0); B = d_Nan(1d0)

! Check that NaNs are noted in both A and B:
      if (isNan(A) .and. isNan(B)) then
         write (*,*) 'Example 1 for NaN is correct.'
      end if

      end
```

NaN

Returns the value for NaN.

Function Return Value

Returns, as a scalar, a value corresponding to the IEEE 754 Standard format of floating point (ANSI/IEEE 1985) for NaN. For other floating point formats a special pattern is returned that tests `.true.` using the function `isNaN`. (Output)

Required Argument

X — Scalar value of the same type and precision as the desired result, NaN. This input value is used only to match the type of output. (Input)

FORTRAN 90 Interface

`NaN(A)`

Description

NaN returns, as a scalar, a value corresponding to the IEEE 754 Standard format of floating point (ANSI/IEEE 1985) for NaN.

The bit pattern used for single precision is `transfer (not(0),1)`. For double precision, the bit pattern for single precision is replicated by assigning the temporary integer array `i(1:2) = not(0)`, and then using the double-precision bit pattern `transfer(i,x)` for the output value.

Example

Arrays are assigned all NaN values, using single and double-precision formats. These are tested using the logical function routine `isNaN`.

```
      use isnan_int
      implicit none

! This is the equivalent of Example 1 for NaN.
      integer, parameter :: n=3
      real(kind(1e0)) A(n,n); real(kind(1d0)) B(n,n)
```

```
       real(kind(1e0)), external :: s_NaN
       real(kind(1d0)), external :: d_NaN

 ! Assign NaNs to both A and B:
       A = s_Nan(1e0); B = d_Nan(1d0)

 ! Check that NaNs are noted in both A and B:
       if (isNan(A) .and. isNan(B)) then

          write (*,*) 'Example 1 for NaN is correct.'
       end if

       end
```

NORM

more...

Computes the norm of an array.

Function Return Value

Norm of A. This is a scalar for the case where A is rank 1 or rank 2. For rank-3 arrays, the norms of each rank-2 array, in dimension 3, are computed. (Output)

Required Argument

A — An array of rank-1, rank-2, or rank-3, containing the values for which the norm is to be computed. It may be real, double, complex, or double complex. (Input)

Optional Arguments, Packaged Options

TYPE —Integer indicating the type of norm to be computed.

$1 = l_1$

$2 = l_2$ (default)

huge(1) = l_∞

Use of the option number `?_reset_default_norm` will switch the default from the l_2 to the l_1 or l_∞ norms. (Input)

The option and derived type names are given in the following tables:

Option Names for `NORM`	Option Value
?_norm_for_lin_sol_svd	1
?_reset_default_norm	2

Name of Unallocated Option Array to Use for Setting Options	Use	Derived Type
?_norm_options(:)	Use when setting options for calls hereafter.	?_options
?_norm_options_once(:)	Use when setting options for next call only.	?_options

For a description on how to use these options, see *Matrix Optional Data Changes*. See `LIN_SOL_SVD` in *Chapter 1, "Linear Systems"* for the specific options for these routines.

FORTRAN 90 Interface

NORM (A [, …])

Description

Computes the l_2, l_1, or l_∞ norm. The l_1 and l_∞ norms are likely to be less expensive to compute than the l_2 norm.

$$\left\|A\right\|_1 = \max_j\left(\sum_{i=1}^{m}|a_{ij}|\right)$$
$$\left\|A\right\|_2 = s_1 = \text{largest singular value}$$
$$\left\|A\right\|_{\infty\leftrightarrow\text{huge}(1)} = \max_i\left(\sum_{j=1}^{n}|a_{ij}|\right)$$

If the l_2 norm is required, this function uses `LIN_SOL_SVD` (see *Chapter 1, "Linear Systems"*), to compute the largest singular value of *A*. For the other norms, Fortran 90 intrinsics are used.

Examples

Example 1

```
Compute three norms of an array

use norm_int
  real (kind(1e0)) A(5), n_1, n_2, n_inf
  A = rand (A)
! I1
  n_1 = norm(A, TYPE=1)
  write (*,*) n_1
! I2
  n_2 = norm(A)
  write (*,*) n_2
```

```
! I infinity
  n_inf = norm(A, TYPE=huge(1))
  write (*,*) n_inf
  end
```

Parallel Example (parallel_ex15.f90)

A "Polar Decomposition" of several matrices are computed. The box data type and the `SVD()` function are used. Orthogonality and small residuals are checked to verify that the results are correct.

```
      use linear_operators
      use mpi_setup_int
      implicit none

! This is Parallel Example 15 using operators and
! functions for a polar decomposition.
      integer, parameter :: n=33, nr=3
      real(kind(1d0)) :: one=1d0, zero=0d0
      real(kind(1d0)),dimension(n,n,nr) :: A, P, Q, &
             S_D(n,nr), U_D, V_D
      real(kind(1d0)) TEMP1(nr), TEMP2(nr)

! Setup for MPI:
      mp_nprocs = mp_setup()

! Generate a random matrix.
      if(mp_rank == 0) A = rand(A)

! Compute the singular value decomposition.
      S_D = SVD(A, U=U_D, V=V_D)

! Compute the (left) orthogonal factor.
      P = U_D .xt. V_D

! Compute the (right) self-adjoint factor.
      Q = V_D .x. diag(S_D) .xt. V_D
! Check the results for orthogonality and
! small residuals.
      TEMP1 = NORM(spread(EYE(n),3,nr) - (p .xt. p))
      TEMP2 = NORM(A -(P .X. Q)) / NORM(A)
      if (ALL(TEMP1 <= sqrt(epsilon(one))) .and. &
          ALL(TEMP2 <= sqrt(epsilon(one)))) then
            if(mp_rank == 0)&
            write (*,*) 'Parallel Example 15 is correct.'
      end if

! See to any error messages and exit MPI.
      mp_nprocs = mp_setup('Final')

      end
```

ORTH

MPI CAPABLE
more...

Orthogonalizes the columns of a matrix.

Function Return Value

Orthogonal matrix Q from the decomposition A=QR. If A is rank-3, Q is rank-3. (Output)

Required Argument

A — Matrix A to be decomposed. Must be an array of rank-2 or rank-3 (box data) of type real, double, complex, or double complex. (Input)

Optional Arguments, Packaged Options

R — Upper-triangular or upper trapezoidal matrix R, from the QR decomposition. If this optional argument is present, the decomposition is complete. If A is rank-3, R is rank-3. (Output)

The option and derived type names are given in the following tables:

Option Name for ORTH	Option Value
Skip_error_processing	5

Name of Unallocated Option Array to Use for Setting Options	Use	Derived Type
?_orth_options(:)	Use when setting options for calls hereafter.	?_options
?_orth_options_once(:)	Use when setting options for next call only.	?_options

For a description on how to use these options, see *Matrix Optional Data Changes*.

FORTRAN 90 Interface

ORTH (A [, …])

Description

Orthogonalizes the columns of a matrix. The decomposition $A = QR$ is computed using a forward and backward sweep of the Modified Gram-Schmidt algorithm.

Examples

Example 1: (Operator_ex19.f90)

```
use linear_operators
      use lin_sol_tri_int
      use rand_int
      use Numerical_Libraries

      implicit none

! This is the equivalent of Example 3 (using operators) for LIN_SOL_TRI.

      integer i, nopt
      integer, parameter :: n=128, k=n/4, ncoda=1, lda=2
      real(kind(1e0)), parameter :: s_one=1e0, s_zero=0e0
      real(kind(1e0)) A(lda,n), EVAL(k)
      type(s_options) :: iopt(2)
      real(kind(1e0)) d(n), b(n), d_t(2*n,k), c_t(2*n,k), perf_ratio, &
           b_t(2*n,k), y_t(2*n,k), eval_t(k), res(n,k)
      logical small

! This flag is used to get the k largest eigenvalues.
      small = .false.

! Generate the main diagonal and the co-diagonal of the
! tridiagonal matrix.
      b=rand(b); d=rand(d)
      A(1,1:)=b; A(2,1:)=d

! Use Numerical Libraries routine for the calculation of k
! largest eigenvalues.
      CALL EVASB (N, K, A, LDA, NCODA, SMALL, EVAL)
      EVAL_T = EVAL

! Use IMSL Fortran Numerical Librarytridiagonal solver for inverse iteration
! calculation of eigenvectors.
      factorization_choice:  do nopt=0,1

! Create k tridiagonal problems, one for each inverse
! iteration system.
         b_t(1:n,1:k) = spread(b,DIM=2,NCOPIES=k)
         c_t(1:n,1:k) = EOSHIFT(b_t(1:n,1:k),SHIFT=1,DIM=1)
         d_t(1:n,1:k) = spread(d,DIM=2,NCOPIES=k) - &
                        spread(EVAL_T,DIM=1,NCOPIES=n)

! Start the right-hand side at random values, scaled downward
```

```
! to account for the expected 'blowup' in the solution.
         y_t=rand(y_t)

! Do two iterations for the eigenvectors.
         do i=1, 2
            y_t(1:n,1:k) = y_t(1:n,1:k)*epsilon(s_one)
            call lin_sol_tri(c_t, d_t, b_t, y_t, &
                        iopt=iopt)
            iopt(nopt+1) = s_lin_sol_tri_solve_only
         end do

! Orthogonalize the eigenvectors.  (This is the most
! intensive part of the computing.)
         y_t(1:n,1:k) = ORTH(y_t(1:n,1:k))


! See if the performance ratio is smaller than the value one.
! If it is not the code will re-solve the systems using Gaussian
! Elimination.  This is an exceptional event.  It is a necessary
! complication for achieving reliable results.

         res(1:n,1:k) = spread(d,DIM=2,NCOPIES=k)*y_t(1:n,1:k) + &
          spread(b,DIM=2,NCOPIES=k)* &
          EOSHIFT(y_t(1:n,1:k),SHIFT=-1,DIM=1) + &
          EOSHIFT(spread(b,DIM=2,NCOPIES=k)*y_t(1:n,1:k),SHIFT=1) &
            -    y_t(1:n,1:k)*spread(EVAL_T(1:k),DIM=1,NCOPIES=n)

! If the factorization method is Cyclic Reduction and perf_ratio is
! larger than one, re-solve using Gaussian Elimination.  If the
! method is already Gaussian Elimination, the loop exits
! and perf_ratio is checked at the end.
         perf_ratio = norm(res(1:n,1:k),1) / &
                      norm(EVAL_T(1:k),1) / &
                         epsilon(s_one) / (5*n)
         if (perf_ratio <= s_one) exit factorization_choice
         iopt(nopt+1) = s_lin_sol_tri_use_Gauss_elim

      end do factorization_choice

      if (perf_ratio <= s_one) then
         write (*,*) 'Example 3 for LIN_SOL_TRI (operators) is correct.'
      end if

      end
```

Parallel Example

```
  use linear_operators
  use mpi_setup_int

  integer, parameter :: N=32, nr=4
  real (kind(1.e0)) A(N,N,nr), Q(N,N,nr)
! Setup for MPI
   mp_nprocs = mp_setup()

  if (mp_rank == 0) then
    A = rand(A)
  end if

  Q = orth(A)

  mp_nprocs = mp_setup ('Final')

  end
```

RAND

Generates a scalar, rank-1, rank-2 or rank-3 array of random numbers.

Function Return Value

Scalar, rank-1, rank-2 or rank-3 array of random numbers. The output function value matches the input argument A in type, kind and rank. For complex arguments, the output values will be real and imaginary parts with random values of the same type, kind, and rank. (Output)

Required Argument

A — The argument must be a scalar, rank-1, rank-2, or rank-3 array of type single, double, complex, or double complex. Used only to determine the type and rank of the output. (Input)

Optional Arguments, Packaged Options

Note: If any of the arrays `s_rand_options(:)`, `s_rand_options_once(:)`, `d_rand_options(:)`, or `d_rand_options_once(:)` are allocated, they are passed as arguments to `rand_gen` using the keyword "`iopt=`".

The option and derived type names are given in the following table:

Name of Unallocated Option Array to Use for Setting Options	Use	Derived Type
?_rand_options(:)	Use when setting options for calls hereafter.	?_options
?_rand_options_once(:)	Use when setting options for next call only.	?_options

FORTRAN 90 Interface

```
RAND(A)
```

Description

Generates a scalar, rank-1, rank-2 or rank-3 array of random numbers. Each component number is positive and strictly less than one in value.

This function uses rand_gen to obtain the number of values required by the argument. The values are then copied using the RESHAPE intrinsic

Example

```
        use show_int
        use rand_int

        implicit none

! This is the equivalent of Example 1 for SHOW.

        integer, parameter :: n=7, m=3
        real(kind(1e0)) s_x(-1:n), s_m(m,n)
        real(kind(1d0)) d_x(n), d_m(m,n)
        complex(kind(1e0)) c_x(n), c_m(m,n)
        complex(kind(1d0)) z_x(n),z_m(m,n)
        integer i_x(n), i_m(m,n)
        type (s_options) options(3)

! The data types printed are real(kind(1e0)), real(kind(1d0)),
! complex(kind(1e0)), complex(kind(1d0)), and INTEGER. Fill with random
! numbers and then print the contents, in each case with a label.
        s_x=rand(s_x); s_m=rand(s_m)
        d_x=rand(d_x); d_m=rand(d_m)
        c_x=rand(c_x); c_m=rand(c_m)
        z_x=rand(z_x); z_m=rand(z_m)
        i_x=100*rand(s_x(1:n)); i_m=100*rand(s_m)

        call show (s_x, 'Rank-1, REAL')
        call show (s_m, 'Rank-2, REAL')
        call show (d_x, 'Rank-1, DOUBLE')
        call show (d_m, 'Rank-2, DOUBLE')
        call show (c_x, 'Rank-1, COMPLEX')
        call show (c_m, 'Rank-2, COMPLEX')
        call show (z_x, 'Rank-1, DOUBLE COMPLEX')
        call show (z_m, 'Rank-2, DOUBLE COMPLEX')
        call show (i_x, 'Rank-1, INTEGER')
        call show (i_m, 'Rank-2, INTEGER')

! Show 7 digits per number and -1 according to the
! natural or declared size of the array.
        options(1)=show_significant_digits_is_7
        options(2)=show_starting_index_is
        options(3)= -1 ! The starting -1 value.
        call show (s_x, &
'Rank-1, REAL with 7 digits, natural indexing', IOPT=options)
        end
```

RANK

MPI CAPABLE
more...

Computes the mathematical rank of a matrix.

Function Return Value

Integer rank of A. The output function value is an integer with a value equal to the number of singular values that are greater than a tolerance. (Output)

Required Argument

A — Matrix for which the rank is to be computed. The argument must be rank-2 or rank-3 (box) array of type single, double, complex, or double complex. (Input)

Optional Arguments, Packaged Options

This function uses `LIN_SOL_SVD` to compute the singular values of the argument. The singular values are then compared with the value of the tolerance to compute the rank.

The option and derived type names are given in the following tables:

Option Names for `RANK`	**Option Value**
?_rank_set_small	1
?_rank_for_lin_sol_svd	2

Name of Unallocated Option Array to Use for Setting Options	**Use**	**Derived Type**
?_rank_options(:)	Use when setting options for calls hereafter.	?_options
?_rank_options_once(:)	Use when setting options for next call only.	?_options

For a description on how to use these options, see *Matrix Optional Data Changes*. See `LIN_SOL_SVD` in *Chapter 1, "Linear Systems"* for the specific options for these routines.

FORTRAN 90 Interface

RANK (A)

Description

Computes the mathematical rank of a rank-2 or rank-3 array. The output function value is an integer with a value equal to the number of singular values that are greater than a tolerance. The default value for this tolerance is $\varepsilon^{1/2}s_1$, where ε is machine precision and s_1 is the largest singular value of the matrix.

Examples

Example 1

```
use linear_operators
real (kind(1e0)) A(5,5)
A = rand (A)
write (*,*) rank(A)
A=1.0
write (*,*) rank(A)
end
```

Output

```
    5
    1
```

Parallel Example

```
use linear_operators
use mpi_setup_int

integer, parameter :: N=3, nr=4
integer  r(nr)
real (kind(1.e0)) s_mat(N,N), s_box(N,N,nr)
! Setup for MPI
 mp_nprocs = mp_setup()

 if (mp_rank == 0) then
     s_mat = reshape((/1.,0.,0.,epsilon(1.0e0)/),(/n,n/))
     s_box = spread(s_mat,dim=3,ncopies=nr)
 end if

     r = rank(s_box)

mp_nprocs = mp_setup ('Final')
```

```
    end
```

SVD

more...

Computes the singular value decomposition of a matrix, $A = USV^T$.

Function Return Value

$m \times n$ diagonal matrix of singular values, S, from the $A = USV^T$ decomposition. (Output)

Required Argument

A — Array of size $m \times n$ to be decomposed. Must be rank-2 or rank-3 array of type single, double, complex, or double complex. (Input)

Optional Arguments, Packaged Options

U — Array of size $m \times m$ containing the singular vectors U. (Output)

V — Array of size $n \times n$ containing the singular vectors V. (Output)

The option and derived type names are given in the following tables:

Option Names for SVD	Option Value
Options_for_lin_svd	1
Options_for_lin_sol_svd	2
skip_error_processing	5

Name of Unallocated Option Array to Use for Setting Options	Use	Derived Type
?_svd_options(:)	Use when setting options for calls hereafter.	?_options
?_svd_options_once(:)	Use when setting options for next call only.	?_options

For a description on how to use these options, see *Matrix Optional Data Changes*. See `LIN_SVD` and `LIN_SOL_SVD` in *Chapter 1, "Linear Systems"* for the specific options for these routines.

FORTRAN 90 Interface

`SVD (A [, …])`

Description

Computes the singular value decomposition of a rank-2 or rank-3 array, $A = USV^T$.

This function uses one of the routines `LIN_SVD` and `LIN_SOL_SVD`. If a complete decomposition is required, `LIN_SVD` is used. If singular values only, or singular values and one of the right and left singular vectors are required, then `LIN_SOL_SVD` is called.

Examples

Example 1: operator_ex14.f90

```
      use linear_operators
      implicit none

! This is the equivalent of Example 2 for LIN_SOL_SVD using operators
! and functions.
      integer, parameter :: n=32
      real(kind(1d0)) :: one=1d0, zero=0d0
      real(kind(1d0)) A(n,n), P(n,n), Q(n,n), &
             S_D(n), U_D(n,n), V_D(n,n)

! Generate a random matrix.
      A = rand(A)

! Compute the singular value decomposition.
      S_D = SVD(A, U=U_D, V=V_D)

! Compute the (left) orthogonal factor.
      P = U_D .xt. V_D
```

```
! Compute the (right) self-adjoint factor.
      Q = V_D .x. diag(S_D) .xt. V_D

! Check the results.
      if (norm( EYE(n) - (P .xt. P)) &
               <= sqrt(epsilon(one))) then
         if (norm(A - (P .x. Q))/norm(A) &
               <= sqrt(epsilon(one))) then
            write (*,*) 'Example 2 for LIN_SOL_SVD (operators) is correct.'
         end if
      end if
      end
```

Parallel Example (parallel_ex14.f90)

Systems of least-squares problems are solved, but now using the `SVD()` function. A box data type is used. This is an example which uses optional arguments and a generic function overloaded for parallel execution of a box data type. Any number of nodes can be used.

```
      use linear_operators
      use mpi_setup_int
      implicit none

! This is the equivalent of Parallel Example 14
! for SVD, .tx. , .x. and NORM.
      integer, parameter :: m=128, n=32, nr=4
      real(kind(1d0)) :: one=1d0, err(nr)
      real(kind(1d0)) A(m,n,nr), b(m,1,nr), x(n,1,nr), U(m,m,nr), &
        V(n,n,nr), S(n,nr), g(m,1,nr)

! Setup for MPI:
      mp_nprocs=mp_setup()

      if(mp_rank == 0) then
! Generate a random matrix and right-hand side.
         A = rand(A); b = rand(b)
      endif

! Compute the least-squares solution matrix of Ax=b.
      S = SVD(A, U = U, V = V)
      g = U .tx. b
      x = V .x. (diag(one/S) .x. g(1:n,:,:))

! Check the results.
      err = norm(A .tx. (b - (A .x. x)))/(norm(A)+norm(x))
      if (ALL(err <= sqrt(epsilon(one)))) then
         if(mp_rank == 0) &
         write (*,*) 'Parallel Example 14 is correct.'
      end if

! See to any error messages and quit MPI
      mp_nprocs = mp_setup('Final')

      end
```

UNIT

Normalizes the columns of a matrix so each has Euclidean length of value one.

Function Return Value

Matrix containing the normalized values of A . The output function value is an array of the same type and kind as A, where each column of each rank-2 principal section has Euclidean length of value one (Output)

Required Argument

A — Matrix to be normalized. The argument must be a rank-2 or rank-3 array of type single, double, complex, or double complex. (Input)

FORTRAN 90 Interface

```
UNIT(A)
```

Description

Normalizes the columns of a rank-2 or rank-3 array so each has Euclidean length of value one.

This function uses a rank-2 Euclidean length subroutine to compute the lengths of the nonzero columns, which are then normalized to have lengths of value one. The subroutine carefully avoids overflow or damaging underflow by rescaling the sums of squares as required.

Example (operator_ex28.f90)

```
use linear_operators

      implicit none

! This is the equivalent of Example 4 (using operators) for LIN_EIG_SELF.

      integer, parameter :: n=64
      real(kind(1e0)), parameter :: one=1d0
      real(kind(1e0)), dimension(n,n) :: A, B, C, D(n), lambda(n), &
                 S(n), vb_d, X, res

! Generate random self-adjoint matrices.
      A = rand(A); A = A + .t.A
      B = rand(B); B = B + .t.B
```

```
! Add a scalar matrix so B is positive definite.
      B = B + norm(B)*EYE(n)

! Get the eigenvalues and eigenvectors for B.
      S = EIG(B,V=vb_d)

! For full rank problems, convert to an ordinary self-adjoint
! problem.  (All of these examples are full rank.)
      if (S(n) > epsilon(one)) then
         D = one/sqrt(S)
         C = diag(D) .x. (vb_d .tx. A .x. vb_d) .x. diag(D)
         C = (C + .t.C)/2

! Get the eigenvalues and eigenvectors for C.
         lambda = EIG(C,v=X)

! Compute and normalize the generalized eigenvectors.
         X = UNIT(vb_d .x. diag(D) .x. X)
         res = (A .x. X) - (B .x. X .x. diag(lambda))

! Check the results.
         if(norm(res)/(norm(A)+norm(B)) <= &
            sqrt(epsilon(one))) then
            write (*,*) 'Example 4 for LIN_EIG_SELF (operators) is correct.'
         end if

      end if

      end
```

Utilities

Routines

11.10 Options Manager

11.11 Line Printer Graphics

11.12 Miscellaneous

Usage Notes for ScaLAPACK Utilities

MPI REQUIRED

For a detailed description of MPI Requirements see "*Dense Matrix Parallelism Using MPI*" in *Chapter 10* of this manual.

This section describes the use of *ScaLAPACK*, a suite of dense linear algebra solvers, applicable when a single problem size is large. We have integrated usage of IMSL Fortran Library with *ScaLAPACK*. However, the *ScaLAPACK* library, including libraries for *BLACS* and *PBLAS*, are not part of this Library. To use *ScaLAPACK* software, the required libraries must be installed on the user's computer system. We adhered to the specification of Blackford, et al. (1997), but use only MPI for communication. The *ScaLAPACK* library includes certain *LAPACK* routines, Anderson, et al. (1995), redesigned for distributed memory parallel computers. It is written in a Single Program, Multiple Data (SPMD) style using explicit message passing for communication. Matrices are laid out in a two-dimensional block-cyclic decomposition. Using High Performance Fortran (HPF) directives, Koelbel, et al. (1994), and a *static* $p \times q$ processor array, and following declaration of the array, `A(*,*)`, this is illustrated by:

```
INTEGER, PARAMETER :: N=500, P= 2, Q=3, MB=32, NB=32
!HPF$ PROCESSORS PROC(P,Q)
!HPF$ DISTRIBUTE A(cyclic(MB), cyclic(NB)) ONTO PROC
```

Our integration work provides modules that describe the interface to the *ScaLAPACK* library. We recommend that users include these modules when using *ScaLAPACK* or ancillary packages, including *BLACS* and *PBLAS*. For the job of distributing data within a user's application to the block-cyclic decomposition required by *ScaLAPACK* solvers, we provide a utility that reads data from an external file and arranges the data within the distributed machines for a computational step. Another utility writes the results into an external file. We also provide similar utilities that map/unmap global arrays to/from local arrays. These utilities are used in our *ScaLAPACK* examples for brevity.

The data types supported for these utilities are **integer**; **single precision, real**; **double precision, real**; **single precision, complex**; and **double precision, complex**.

A *ScaLAPACK* library normally includes routines for:

- the solution of full-rank linear systems of equations,
- general and symmetric, positive-definite, banded linear systems of equations,
- general and symmetric, positive-definite, tri-diagonal, linear systems of equations,
- condition number estimation and iterative refinement for LU and Cholesky factorization,

- matrix inversion,
- full-rank linear least-squares problems,
- orthogonal and generalized orthogonal factorizations,
- orthogonal transformation routines,
- reductions to upper Hessenberg, bidiagonal and tridiagonal form,
- reduction of a symmetric-definite, generalized eigenproblem to standard form,
- the self-adjoint or Hermitian eigenproblem,
- the generalized self-adjoint or Hermitian eigenproblem, and
- the non-symmetric eigenproblem.

ScaLAPACK routines are available in four data types: **single precision**, **real**; **double precision**; **real**, **single precision**, **complex**, and **double precision**, **complex**. At present, the non-symmetric eigenproblem is only available in single and double precision. More background information and user documentation is available on the World Wide Web at location `www.netlib.org/scalapack/slug/scalapack_slug.html`.

For users with rank deficiency or simple constraints in their linear systems or least-squares problem, we have routines for:

- full or deficient rank least-squares problems with non-negativity constraints
- full or deficient rank least-squares problems with simple upper and lower bound constraints

These are available in two data types: **single precision, real**, and **double precision, real**, and they are not part of *ScaLAPACK*. The matrices are distributed in a general block-column layout.

We also provide generic interfaces to a number of *ScaLAPACK* routines through the standard IMSL Library routines. These are listed in in the Introduction of this manual.

The global arrays which are to be distributed across the processor grid for use by the *ScaLAPACK* routines require that an *array descriptor* be defined for each of them. We use the *ScaLAPACK TOOLS* routine `DESCINIT` to set up array descriptors in our examples. A typical call to `DESCINIT`:

```
CALL DESCINIT(DESCA, M, N, MB, NB, IRSRC, ICSRC, ICTXT, LLD, INFO)
```

Where the arguments in the above call are defined as follows for the matrix being described:

DESCA — An input integer vector of length 9 which is to contain the array descriptor information.

M — An input integer which indicates the row size of the global array which is being described.

N — An input integer which indicates the column size of the global array which is being described.

MB — An input integer which indicates the blocking factor used to distribute the rows of the matrix being described.

NB — An input integer which indicates the blocking factor used to distribute the columns of the matrix being described.

IRSRC — An input integer which indicates the processor grid row over which the first row of the array being described is distributed.

ICSRC — An input integer which indicates the processor grid column over which the first column of the array being described is distributed.

ICTXT — An input integer which indicates the BLACS context handle.

LLD — An input integer indicating the leading dimension of the local array which is to be used for storing the local blocks of the array being described

INFO — An output integer indicating whether or not the call was successful. INFO = 0 indicates a successful exit. INFO = –i indicates the i-th argument had an illegal value.

This call is equivalent to the following assignment statements:

```
DESCA(1) = 1                ! This is the descriptor
                            ! type. In this case,  1.
DESCA(2) = ICTXT
DESCA(3) = M
DESCA(4) = N
DESCA(5) = MB
DESCA(6) = NB
DESCA(7) = IRSRC
DESCA(8) = ICSRC
DESCA(9) = LLD
```

The IMSL Library routines which interface with *ScaLAPACK* routines use `IRSRC = 0` and `ICSRC = 0` for the internal calls to `DESCINIT`.

Supporting Modules

We recommend that users needing routines from *ScaLAPACK*, *PBLAS* or *BLACS*, Version 1.4, use modules that describe the interface to individual codes. This practice, including use of the declaration directive, `IMPLICIT NONE`, is a reliable way of writing *ScaLAPACK* application code, since the routines may have lengthy lists of arguments. Using the modules is helpful to avoid the mistakes such as missing arguments or mismatches involving Type, Kind or Rank (TKR). The modules are part of the Fortran Library product. There is a comprehensive module, ScaLAPACK_Support, that includes use of all the modules in the table below. This module decreases the number of lines of code for checking the interface, but at the cost of increasing source compilation time compared with using individual modules.

Module Name	**Contents of the Module**
ScaLAPACK_Support	All of the following modules
ScaLAPACK_Int	All interfaces to *ScaLAPACK* routines
PBLAS_Int	All interfaces to parallel *BLAS*, or *PBLAS*
BLACS_Int	All interfaces to basic linear algebra communication routines, or *BLACS*
TOOLS_Int	Interfaces to ancillary routines used by *ScaLAPACK*, but not in other packages
LAPACK_Int	All interfaces to *LAPACK* routines required by *ScaLAPACK*
ScaLAPACK_IO_Int	All interfaces to ScaLAPACK_READ, ScaLAPACK_WRITE utility routines. See this Chapter.
MPI_Node_Int	The module holding data describing the MPI communicator, MP_LIBRARY_WORLD. See *Dense Matrix Parallelism Using MPI*.
GRIDINFO_Int	The module holding data describing the processor grid and information required to map the target array to the processors. See the Description section of ScaLAPACK_SETUP below.
ScaLAPACK_MAP_Int	The interface to the ScaLAPACK_MAP utility routines.
ScaLAPACK_UNMAP_Int	The interface to the ScaLAPACK_UNMAP utility routines.

ScaLAPACK_SETUP

MPI REQUIRED

For a detailed description of MPI Requirements see "*Using ScaLAPACK Enhanced Routines*" in the Introduction of this manual.

This routine sets up a processor grid and calculates default values for various entities to be used in mapping a global array to the processor grid. All processors in the *BLACS* context call the routine.

Required Arguments

M — The row dimension of the global array for which the local array dimensions are to be calculated. (Input)

N — The column dimension of the global array for which the local array dimensions are to be calculated. (Input)

NSQUARE —Input logical which indicates whether the block used for mapping the global array to the processor grid must be square. If the block must be square, set `NSQUARE` to `.TRUE.`, otherwise, set it to `.FALSE.`. (Input)

GRID1D — Input logical which indicates whether the processor grid is to be one dimensional or two dimensional. Set `GRID1D` to `.TRUE.` if the grid is to be one dimensional. Otherwise, set `GRID1D` to `.FALSE.`. (Input)

FORTRAN 90 Interface

Generic: `CALL ScaLAPACK_SETUP (M, N, NSQUARE, GRID1D)`

Description

Subroutine `ScaLAPACK_SETUP` creates a processor grid based on the number of processors being used and the `GRID1D` logical supplied by the user. The argument, `NSQUARE`, is supplied because some *ScaLAPACK* routines require that the row and column blocking factors be equal. `GRID1D` is supplied for those routines which require that the processor grid be one dimensional. ScaLAPACK_SETUP also establishes values for MP_M, MP_N, MP_NPROW, MP_NPCOL, MP_MB, MP_NB, MP_PIGRID, MP_ICTXT, MP_NSQUARE, and MP_GRID1D in the IMSL Fortran Library module GRIDINFO_INT. The above entities are defined as follows:

MP_M — The row dimension of the primary array which is to be distributed among the processors.

MP_N — The column dimension of the primary array which is to be distributed among the processors.

MP_NPROW — The number of rows in the processor grid.

MP_NPCOL — The number of columns in the processor grid.

MP_MB — The row blocking factor to be used in distributing the array.

MP_NB — The column blocking factor to be used in distributing the array.

MP_PIGRID — The pointer to the processor grid, MP_IGRID.

MP_ICTXT — The *BLACS* context ID associated with the processor grid.

MP_NSQUARE — Logical indicating whether or not the block used for mapping the global array to the processor grid must be square.

MP_GRID1D — Logical indicating whether or not the processor grid must be one dimensional.

GRIDINFO_INT is used by MPI_SETUP_INT so users do not need to explicitly use GRIDINFO_INT since they will be using MPI_SETUP_INT when they use MPI.

Example

See ScaLAPACK_WRITE.

ScaLAPACK_GETDIM

MPI REQUIRED

For a detailed description of MPI Requirements see "*Using ScaLAPACK Enhanced Routines*" in the Introduction of this manual.

This routine calculates the row and column dimensions of a local distributed array based on the size of the array to be distributed and the row and column blocking factors to be used. All processors in the *BLACS* context call the routine.

Required Arguments

M — The row dimension of the global array for which the local array dimensions are to be calculated. (Input)

N — The column dimension of the global array for which the local array dimensions are to be calculated. (Input)

MB — The row blocking factor to be used in distributing the array. (Input)

NB — The column blocking factor to be used in distributing the array. (Input)

MXLDA — The row dimension of the local array. (Output)

MXCOL — The column dimension of the local array. (Output)

FORTRAN 90 Interface

Generic: `CALL ScaLAPACK_GETDIM` (M, N, MB, NB, MXLDA, MXCOL)

Description

Subroutine `ScaLAPACK_GETDIM` calculates the row and column dimensions of a local array by using the ScaLAPACK utility `NUMROC`.

> **Note** that `ScaLAPACK_SETUP` must be called prior to calling this routine because `ScaLAPACK_GETDIM` will use some of the global entities defined by `ScaLAPACK_SETUP`.

Example

See `ScaLAPACK_WRITE`.

ScaLAPACK_READ

MPI REQUIRED

For a detailed description of MPI Requirements see "*Using ScaLAPACK Enhanced Routines*" in the Introduction of this manual.

This routine reads matrix data from a file and transmits it into the two-dimensional block-cyclic form required by *ScaLAPACK* routines. This routine contains a call to a barrier routine so that if one process is writing the file and an alternate process is to read it, the results will be synchronized.

All processors in the *BLACS* context call the routine.

Required Arguments

File_Name — A character variable naming the file containing the matrix data. (Input)
This file is opened with `STATUS="OLD."` If the name is misspelled or the file does not exist, or any access violation occurs, a type = `terminal` error message will occur. After the contents are read, the file is closed. This file is read with a loop logically equivalent to groups of reads:

```
READ() ((BUFFER(I,J), I=1,M), J=1, NB)
```

or (optionally):

```
READ() ((BUFFER(I,J), J=1,N), I=1, MB)
```

DESC_A(*) — The nine integer parameters associated with the *ScaLAPACK* matrix descriptor. Values for NB,MB,LDA are contained in this array. (Input)

A (***LDA***,*) — This is an assumed-size array, with leading dimension `LDA`, that will contain this processor's piece of the block-cyclic matrix. The data type for `A`(*,*) is any of five Fortran intrinsic types: **integer**; **single precision, real**; **double precision, real**; **single precision, complex**; and **double precision, complex**. (Output)

Optional Arguments

Format **—** A character variable containing a format to be used for reading the file containing matrix data. If this argument is not present, an unformatted or list-directed read is used. (Input)

iopt **—** Derived type array with the same precision as the array `A(*,*)`, used for passing optional data to `ScaLAPACK_READ`. (Input)
The options are as follows:

Packaged Options for **`ScaLAPACK_READ`**		
Option Prefix = ?	Option Name	Option Value
`S_, d_`	`ScaLAPACK_READ_UNIT`	1
`S_, d_`	`ScaLAPACK_READ_FROM_PROCESS`	2
`S_, d_`	`ScaLAPACK_READ_BY_ROWS`	3

iopt(IO) = `ScaLAPACK_READ_UNIT`
Sets the unit number to the value in `iopt(IO + 1)%idummy`. The default unit number is the value 11.

iopt(IO) = `ScaLAPACK_READ_FROM_PROCESS`
Sets the process number that reads the named file to the value in `iopt(IO + 1)%idummy`. The default process number is the value 0.

iopt(IO) = `ScaLAPACK_READ_BY_ROWS`
Read the matrix by rows from the named file. By default the matrix is read by columns.

FORTRAN 90 Interface

Generic: `CALL ScaLAPACK_READ (File_Name, DESC_A, A [, …])`

Specific: The specific interface names are `S_ScaLAPACK_READ` and `D_ScaLAPACK_READ`.

Description

Subroutine `ScaLAPACK_READ` reads columns or rows of a problem matrix so that it is usable by a *ScaLAPACK* routine. It uses the two-dimensional block-cyclic array descriptor for the matrix to place the data in the desired assumed-size arrays on the processors. The blocks of data are read, then transmitted and received. The block sizes, contained in the array descriptor, determines the data set size for each blocking send and receive pair. The number of these synchronization points is proportional to $\lceil M \times N / (MB \times NB) \rceil$. A temporary local buffer is allocated for staging the matrix data. It is of size `M` by `NB`, when reading by columns, or `N` by `MB`, when reading by rows.

Example

See ScaLAPACK_WRITE.

ScaLAPACK_WRITE

For a detailed description of MPI Requirements see "`Using ScaLAPACK Enhanced Routines`" in the Introduction of this manual.

This routine writes the matrix data to a file. The data is transmitted from the two-dimensional block-cyclic form used by *ScaLAPACK* routines. This routine contains a call to a barrier routine so that if one process is writing the file and an alternate process is to read it, the results will be synchronized. All processors in the *BLACS* context call the routine.

Required Arguments

File_Name **—** A character variable naming the file to receive the matrix data. (Input)
This file is opened with `"STATUS="UNKNOWN."` If any access violation happens, a type = terminal error message will occur. If the file already exists it will be overwritten. After the contents are written, the file is closed. This file is written with a loop logically equivalent to groups of writes:

```
WRITE() ((BUFFER(I,J), I=1,M), J=1, NB)
```

or (optionally):

```
WRITE() ((BUFFER(I,J), J=1,N), I=1, MB)
```

DESC_A(*) **—** The nine integer parameters associated with the *ScaLAPACK* matrix descriptor. Values for `NB`, `MB`, `LDA` are contained in this array. (Input)

A (***LDA***,*) **—** This is an assumed-size array, with leading dimension `LDA`, containing this processor's piece of the block-cyclic matrix. The data type for `A(*,*)` is any of five Fortran intrinsic types: **integer; single precision, real**; **double precision, real**; **single precision**, **complex**; or **double precision**, **complex**. (Input)

Optional Arguments

Format **—**A character variable containing a format to be used for writing the file that receives matrix data. If this argument is not present, an unformatted or list-directed write is used. (Input)

iopt **—** Derived type array with the same precision as the array A(*,*), used for passing optional data to ScaLAPACK_WRITE. Use single precision when A(*,*) is type INTEGER. (Input)
The options are as follows:

Packaged Options for ScaLAPACK_WRITE		
Option Prefix = ?	Option Name	Option Value
s_, d_	ScaLAPACK_WRITE_UNIT	1
s_, d_	ScaLAPACK_WRITE_FROM_PROCESS	2
s_, d_	ScaLAPACK_WRITE_BY_ROWS	3

iopt(IO) =ScaLAPACK_WRITE_UNIT
Sets the unit number to the integer component of iopt(IO + 1)%idummy. The default unit number is the value 11.

iopt(IO) = ScaLAPACK_WRITE_FROM_PROCESS
Sets the process number that writes the named file to the integer component of iopt(IO + 1)%idummy. The default process number is the value 0.

iopt(IO) = ScaLAPACK_WRITE_BY_ROWS
Write the matrix by rows to the named file. By default the matrix is written by columns.

FORTRAN 90 Interface

Generic: CALL ScaLAPACK_WRITE (File_Name, DESC_A, A [, …])

Specific: The specific interface names are S_ScaLAPACK_WRITE and D_ScaLAPACK_WRITE.

Description

Subroutine ScaLAPACK_WRITE writes columns or rows of a problem matrix output by a *ScaLAPACK* routine. It uses the two-dimensional block-cyclic array descriptor for the matrix to extract the data from the assumed-size arrays on the processors. The blocks of data are transmitted and received, then written. The block sizes, contained in the array descriptor, determines the data set size for each blocking send and receive pair. The number of these synchronization points is proportional to $\lceil M \times N / (MB \times NB) \rceil$. A temporary local buffer is allocated for staging the matrix data. It is of size M by NB, when writing by columns, or N by MB, when writing by rows.

Examples

Example 1: Distributed Transpose of a Matrix, In Place

The program `SCPK_EX1` illustrates an *in-situ* transposition of a matrix. An $m \times n$ matrix, A, is written to a file, by rows. The $n \times m$ matrix, $B = A^T$, overwrites storage for A. Two temporary files are created and deleted. This algorithm for transposing a matrix is not efficient. It is used to illustrate the read and write routines and optional arguments for writing of data by matrix rows.

```
  program scpk_ex1
! This is Example 1 for ScaLAPACK_READ and ScaLAPACK_WRITE.
! It shows in-situ or in-place transposition of a
! block-cyclic matrix.
USE ScaLAPACK_SUPPORT
USE ERROR_OPTION_PACKET
USE MPI_SETUP_INT
IMPLICIT NONE
INCLUDE "mpif.h"
INTEGER, PARAMETER :: M=6, N=6, NIN=10
INTEGER  DESC_A(9), IERROR, INFO, I, J, K, L, MXLDA, MXCOL
LOGICAL :: GRID1D = .TRUE., NSQUARE = .TRUE.
real(kind(1d0)), allocatable :: A(:,:), A0(:,:)
real(kind(1d0)) ERROR
TYPE(d_OPTIONS) IOPT(1)

    MP_NPROCS=MP_SETUP()

!  Set up a 1D processor grid and define its context ID, MP_ICTXT
   CALL SCALAPACK_SETUP(M, N, NSQUARE, GRID1D)
!  Get the array descriptor entities MXLDA, and MXCOL
   CALL SCALAPACK_GETDIM(M, N, MP_MB, MP_NB, MXLDA, MXCOL)
!  Set up the array descriptor
   CALL DESCINIT(DESC_A, M, N, MP_MB, MP_NB, 0, 0, MP_ICTXT, &
   MXLDA, INFO)
!   Allocate space for local arrays
    ALLOCATE(A0(MXLDA,MXCOL))

! A root process is used to create the matrix data for the test.
IF(MP_RANK == 0) THEN
  ALLOCATE(A(M,N))
! Fill array with a pattern that is easy to recognize.
  K=0
  DO
   K=K+1; IF(10**K > N) EXIT
  END DO
  DO J=1,N
    DO I=1,M
! The values will appear, as decimals I.J, where I is
! the row and J is the column.
      A(I,J)=REAL(I)+REAL(J)*10d0**(-K)
    END DO
  END DO

  OPEN(UNIT=NIN, FILE='test.dat', STATUS='UNKNOWN')
! Write the data by columns.
  DO J=1,N,MP_NB
    WRITE(NIN,*) ((A(I,L),I=1,M),L=J,min(N,J+MP_NB-1))
  END DO
  CLOSE(NIN)
  DEALLOCATE(A)
  ALLOCATE(A(N,M))
```

```
END IF

! Read the matrix into the local arrays.
CALL ScaLAPACK_READ('test.dat', DESC_A, A0)
! To transpose, write the matrix by rows as the first step.
! This requires an option since the default is to write
! by columns.
IOPT(1)=ScaLAPACK_WRITE_BY_ROWS
CALL ScaLAPACK_WRITE("TEST.DAT", DESC_A, A0, IOPT=IOPT)

!  Resize the local storage
   DEALLOCATE(A0)
  CALL SCALAPACK_GETDIM(N, M, MP_NB, MP_MB, MXLDA, MXCOL)
!  Set up the array descriptor
!  Reshape the descriptor for the transpose of the matrix.
!  The number of rows and columns are swapped.
  CALL DESCINIT(DESC_A, N, M, MP_NB, MP_MB, 0, 0, MP_ICTXT, &
  MXLDA, INFO

  ALLOCATE(A0(MXLDA,MXCOL))

!  Read the transpose matrix

CALL ScaLAPACK_READ("TEST.DAT", DESC_A, A0)

IF(MP_RANK == 0) THEN

! Open the used files and delete when closed.
  OPEN(UNIT=NIN, FILE='test.dat', STATUS='OLD')
  CLOSE(NIN,STATUS='DELETE')
  OPEN(UNIT=NIN, FILE='TEST.DAT', STATUS='OLD')
  DO J=1,M,MP_MB
    READ(NIN,*) ((A(I,L), I=1,N),L=J,min(M,J+MP_MB-1))
  END DO
  CLOSE(NIN,STATUS='DELETE')
  DO I=1,N
    DO J=1,M
! The values will appear, as decimals I.J, where I is the row
!  and J is the column.
      A(I,J)=REAL(J)+REAL(I)*10d0**(-K) - A(I,J)
    END DO
  END DO
  ERROR=SUM(ABS(A))
 END IF
! See to any error messages.
  call e1pop("Mp_setup")
! Check results on just one process.
IF(ERROR <= SQRT(EPSILON(ERROR)) .and. &
  MP_RANK == 0) THEN
  write(*,*) " Example 1 for BLACS is correct."
END IF

! Deallocate storage arrays and exit from BLACS.
IF(ALLOCATED(A)) DEALLOCATE(A)
IF(ALLOCATED(A0)) DEALLOCATE(A0)
! Exit from using this process grid.
  CALL SCALAPACK_EXIT( MP_ICTXT )
! Shut down MPI
  MP_NPROCS = MP_SETUP(‘FINAL’)
END
```

Output

```
Example 1 for BLACS is correct.
```

Example 2: Distributed Matrix Product with PBLAS

The program `SCPK_EX2` illustrates computation of the matrix product $C_{m \times n} = A_{m \times k} B_{k \times n}$. The matrices on the right-hand side are random. Three temporary files are created and deleted. *BLACS* and *PBLAS* are used. The problem size is such that the results are checked on one process.

```
  program scpk_ex2
! This is Example 2 for ScaLAPACK_READ and ScaLAPACK_WRITE.
! The product of two matrices is computed with PBLAS
! and checked for correctness.

USE ScaLAPACK_SUPPORT
USE MPI_SETUP_INT

IMPLICIT NONE
INCLUDE "mpif.h"

INTEGER, PARAMETER :: K=32, M=33, N=34, NIN=10
INTEGER INFO, IA, JA, IB, JB, IC, JC, MXLDA, MXCOL, MXLDB, &
  MXCOLB, MXLDC, MXCOLC, IERROR, I, J, L,&
  DESC_A(9), DESC_B(9), DESC_C(9)
LOGICAL :: GRID1D = .TRUE., NSQUARE = .TRUE.

 real(kind(1d0)) :: ALPHA, BETA, ERROR=1d0, SIZE_C
 real(kind(1d0)), allocatable, dimension(:,:) :: A,B,C,X(:),&
 A0, B0, C0

 MP_NPROCS=MP_SETUP()

! Set up a 1D processor grid and define its context ID, MP_ICTXT
  CALL SCALAPACK_SETUP(M, N, NSQUARE, GRID1D)
! Get the array descriptor entities
  CALL SCALAPACK_GETDIM(M, K, MP_MB, MP_NB, MXLDA, MXCOL)
  CALL SCALAPACK_GETDIM(K, N, MP_NB, MP_MB, MXLDB, MXCOLB)
  CALL SCALAPACK_GETDIM(M, N, MP_MB, MP_NB, MXLDC, MXCOLC)
! Set up the array descriptors
  CALL DESCINIT(DESC_A, M, K, MP_MB, MP_NB, 0, 0, MP_ICTXT, &
  MXLDA, INFO)
  CALL DESCINIT(DESC_B, K, N, MP_NB, MP_NB, 0, 0, MP_ICTXT, &
  MXLDB, INFO)
  CALL DESCINIT(DESC_C, M, N, MP_MB, MP_NB, 0, 0, MP_ICTXT, &
  MXLDC, INFO)

ALLOCATE(A0(MXLDA,MXCOL), B0(MXLDB,MXCOLB),C0(MXLDC,MXCOLC))

! A root process is used to create the matrix data for the test.
IF(MP_RANK == 0) THEN
  ALLOCATE(A(M,K), B(K,N), C(M,N), X(M))
  CALL RANDOM_NUMBER(A); CALL RANDOM_NUMBER(B)

  OPEN(UNIT=NIN, FILE='Atest.dat', STATUS='UNKNOWN')
! Write the data by columns.
  DO J=1,K,MP_NB
    WRITE(NIN,*) ((A(I,L),I=1,M),L=J,min(K,J+MP_NB-1))
  END DO
  CLOSE(NIN)

  OPEN(UNIT=NIN, FILE='Btest.dat', STATUS='UNKNOWN')
! Write the data by columns.
```

```
    DO J=1,N,MP_NB
      WRITE(NIN,*) ((B(I,L),I=1,K),L=J,min(N,J+MP_NB-1))
    END DO
    CLOSE(NIN)
  END IF

  ! Read the factors into the local arrays.
  CALL ScaLAPACK_READ('Atest.dat', DESC_A, A0)
  CALL ScaLAPACK_READ('Btest.dat', DESC_B, B0)

  ! Compute the distributed product C = A x B.
  ALPHA=1d0; BETA=0d0
  IA=1; JA=1; IB=1; JB=1; IC=1; JC=1
  C0=0
  CALL pdGEMM &
    ("No", "No", M, N, K, ALPHA, A0, IA, JA,&
    DESC_A, B0, IB, JB, DESC_B, BETA,&
    C0, IC, JC, DESC_C )

  ! Put the product back on the root node.
  Call ScaLAPACK_WRITE('Ctest.dat', DESC_C, C0)

  IF(MP_RANK == 0) THEN

  ! Read the residuals and check them for size.
    OPEN(UNIT=NIN, FILE='Ctest.dat', STATUS='OLD')

  ! Read the data by columns.
    DO J=1,N,MP_NB
      READ(NIN,*) ((C(I,L),I=1,M),L=J,min(N,J+MP_NB-1))
    END DO

    CLOSE(NIN,STATUS='DELETE')
    SIZE_C=SUM(ABS(C)); C=C-matmul(A,B)
    ERROR=SUM(ABS(C))/SIZE_C

  ! Open other temporary files and delete them.
    OPEN(UNIT=NIN, FILE='Atest.dat', STATUS='OLD')
    CLOSE(NIN,STATUS='DELETE')
    OPEN(UNIT=NIN, FILE='Btest.dat', STATUS='OLD')
    CLOSE(NIN,STATUS='DELETE')

  END IF

  ! See to any error messages.
  call e1pop("Mp_Setup")
  ! Deallocate storage arrays and exit from BLACS.
  IF(ALLOCATED(A)) DEALLOCATE(A)
  IF(ALLOCATED(B)) DEALLOCATE(B)
  IF(ALLOCATED(C)) DEALLOCATE(C)
  IF(ALLOCATED(X)) DEALLOCATE(X)
  IF(ALLOCATED(A0)) DEALLOCATE(A0)
  IF(ALLOCATED(B0)) DEALLOCATE(B0)
  IF(ALLOCATED(C0)) DEALLOCATE(C0)

  ! Check the results.

  IF(ERROR <= SQRT(EPSILON(ALPHA)) .and. &
    MP_RANK == 0) THEN
    write(*,*) " Example 2 for BLACS and PBLAS is correct."
  END IF

     ! Exit from using this process grid.
       CALL SCALAPACK_EXIT( MP_ICTXT )
    ! Shut down MPI
    MP_NPROCS = MP_SETUP('FINAL')
```

```
END
```

Output

```
Example 2 for BLACS and PBLAS is correct.
```

Example 3: Distributed Linear Solver with ScaLAPACK

The program `SCPK_EX3` illustrates solving a system of linear-algebraic equations, $Ax = B$ by calling a *ScaLAPACK* routine directly. The right-hand side is produced by defining A and y to have random values. Then the matrix-vector product $b = Ay$ is computed. The problem size is such that the residuals, $x–y≈0$ are checked on one process. Three temporary files are created and deleted. *BLACS* are used to define the process grid and provide further information identifying each process. Then a *ScaLAPACK* routine is called directly to compute the approximate solution, x.

```
  program scpk_ex3
! This is Example 3 for ScaLAPACK_READ and ScaLAPACK_WRITE.
! A linear system is solved with ScaLAPACK and checked.
USE ScaLAPACK_SUPPORT
USE ERROR_OPTION_PACKET
USE MPI_SETUP_INT

IMPLICIT NONE

INCLUDE "mpif.h"
INTEGER, PARAMETER :: N=9, NIN=10
INTEGER  INFO, IA, JA, IB, JB, MXLDA,MXCOL,&
  IERROR, I, J, L, DESC_A(9),&
  DESC_B(9), BUFF(3), RBUF(3)

LOGICAL :: COMMUTE = .TRUE., NSQUARE = .TRUE., GRID1D = .TRUE.
INTEGER, ALLOCATABLE :: IPIV0(:)
real(kind(1d0)) :: ERROR=0d0, SIZE_Y
real(kind(1d0)), allocatable, dimension(:,:) :: A, B(:), &
  X(:), Y(:), A0, B0

  MP_NPROCS=MP_SETUP()

! Set up a 1D processor grid and define its context ID, MP_ICTXT
  CALL SCALAPACK_SETUP(N, N, NSQUARE, GRID1D)
! Get the array descriptor entities
  CALL SCALAPACK_GETDIM(N, N, MP_MB, MP_NB, MXLDA, MXCOL)
! Set up the array descriptors
  CALL DESCINIT(DESC_A, N, N, MP_MB, MP_NB, 0, 0, MP_ICTXT, &
  MXLDA, INFO)
  CALL DESCINIT(DESC_B, N, 1, MP_MB, MP_NB, 0, 0, MP_ICTXT, &
  MXLDA, INFO)

! Allocate local space for each array.
  ALLOCATE(A0(MXLDA,MXCOL), B0(MXLDA,1), IPIV0(MXLDA+MP_MB))

! A root process is used to create the matrix data for the test.
IF(MP_RANK == 0) THEN
  ALLOCATE(A(N,N), B(N), X(N), Y(N))
  CALL RANDOM_NUMBER(A); CALL RANDOM_NUMBER(Y)

! Compute the correct result.
  B=MATMUL(A,Y); SIZE_Y=SUM(ABS(Y))
  OPEN(UNIT=NIN, FILE='Atest.dat', STATUS='UNKNOWN')

! Write the data by columns.
```

```
  DO J=1,N,MP_NB
    WRITE(NIN,*) ((A(I,L),I=1,N),L=J,min(N,J+MP_NB-1))
  END DO
  CLOSE(NIN)

  OPEN(UNIT=NIN, FILE='Btest.dat', STATUS='UNKNOWN')
! Write the data by columns.
  WRITE(NIN,*) (B(I),I=1,N)
  CLOSE(NIN)
END IF

! Read the factors into the local arrays.
CALL ScaLAPACK_READ('Atest.dat', DESC_A, A0)
CALL ScaLAPACK_READ('Btest.dat', DESC_B, B0)

! Compute the distributed product solution to A x = b.
IA=1; JA=1; IB=1; JB=1

CALL pdGESV  (N, 1, A0, IA, JA, DESC_A, IPIV0, &
B0, IB, JB, DESC_B, INFO)

! Put the result on the root node.
Call ScaLAPACK_WRITE('Xtest.dat', DESC_B, B0)

IF(MP_RANK == 0) THEN

! Read the residuals and check them for size.
  OPEN(UNIT=NIN, FILE='Xtest.dat', STATUS='OLD')

! Read the approximate solution data.
      READ(NIN,*) X
      B=X-Y

  CLOSE(NIN,STATUS='DELETE')

ERROR=SUM(ABS(B))/SIZE_Y
! Delete temporary files.
  OPEN(UNIT=NIN, FILE='Atest.dat', STATUS='OLD')
  CLOSE(NIN,STATUS='DELETE')
  OPEN(UNIT=NIN, FILE='Btest.dat', STATUS='OLD')
  CLOSE(NIN,STATUS='DELETE')

END IF
! See to any error messages.
call e1pop("Mp_Setup")
! Deallocate storage arrays
IF(ALLOCATED(A)) DEALLOCATE(A)
IF(ALLOCATED(B)) DEALLOCATE(B)
IF(ALLOCATED(X)) DEALLOCATE(X)
IF(ALLOCATED(Y)) DEALLOCATE(Y)
IF(ALLOCATED(A0)) DEALLOCATE(A0)
IF(ALLOCATED(B0)) DEALLOCATE(B0)
IF(ALLOCATED(IPIV0)) DEALLOCATE(IPIV0)
IF(ERROR <= SQRT(EPSILON(ERROR)) .and. MP_RANK == 0) THEN
  write(*,*) &
  " Example 3 for BLACS and ScaLAPACK solver is correct."
END IF

! Exit from using this process grid.
  CALL SCALAPACK_EXIT( MP_ICTXT )
! Shut down MPI
  MP_NPROCS = MP_SETUP('FINAL')
END
```

Output

```
Example 3 for BLACS and ScaLAPACK is correct.
```

ScaLAPACK_MAP

For a detailed description of MPI Requirements see "*Using ScaLAPACK Enhanced Routines*" in the Introduction of this manual.

This routine maps array data from a global array to local arrays in the two-dimensional block-cyclic form required by *ScaLAPACK routines*.

All processors in the *BLACS* context call the routine.

Required Arguments

A **—** Global rank-1 or rank-2 array which is to be mapped to the processor grid. The data type for A is any of five Fortran intrinsic types: **integer**; **single precision, real**; **double precision, real**; **single precision, complex**; **double precision, complex**. Normally, the user defines A to be valid only on the MP_RANK = 0 processor. (Input)

DESC_A **—** An integer vector containing the nine parameters associated with the *ScaLAPACK* matrix descriptor for array `A`. See "*Usage Notes for ScaLAPACK Utilities*" for a description of the nine parameters. (Input)

A0 **—** This is a local rank-1 or rank-2 array that will contain this processor's piece of the block-cyclic array. The data type for `A0` is any of five Fortran intrinsic types: **integer**; **single precision, real**; **double precision, real**; **single precision, complex**; **double precision, complex**. (Output)

Optional Arguments

LDA **—** Leading dimension of `A` as specified in the calling program. If this argument is not present, `SIZE(A,1)` is used. (Input)

COLMAP **—** Input logical which indicates whether the global array should be mapped in column major form or row major form. COLMAP set to .TRUE. will result in the array being mapped in column-major form while setting COLMAP to .FALSE. will result in the array being mapped in row major form. The default value of COLMAP is .TRUE.. (Input)

FORTRAN 90 Interface

Generic: CALL ScaLAPACK_MAP (A, DESC_A, A0 [, …])

Description

Subroutine ScaLAPACK_MAP maps columns or rows of a global array on MP_RANK = 0 to local distributed arrays so that the problem array is usable by a *ScaLAPACK* routine. It uses the two-dimensional block-cyclic array descriptor for the matrix to place the data in the desired assumed-size arrays on the processors. The block sizes, contained in the array descriptor, determine the data set size for each blocking send and receive pair. The number of these synchronization points is proportional to $\lceil M \times N / (MB \times NB) \rceil$. A temporary local buffer is allocated for staging the array data. It is of size M by NB, when mapping by columns, or N by MB, when mapping by rows.

Example

See ScaLAPACK_UNMAP.

ScaLAPACK_UNMAP

For a detailed description of MPI Requirements see "*Using ScaLAPACK Enhanced Routines*" in the Introduction of this manual.

This routine unmaps array data from local distributed arrays to a global array. The data in the local arrays must have been stored in the two-dimensional block-cyclic form required by *ScaLAPACK* routines. All processors in the *BLACS* context call the routine.

Required Arguments

A0 — This is a local rank-1 or rank-2 array that contains this processor's piece of the block-cyclic array. The data type for `A0` is any of five Fortran intrinsic types: **integer**; **single precision, real**; **double precision, real**; **single precision, complex**; **double precision, complex**. (Input)

DESC_A — An integer vector containing the nine parameters associated with the *ScaLAPACK* matrix descriptor for array `A`. See "*Usage Notes for ScaLAPACK Utilities*" for a description of the nine parameters. (Input)

A — Global rank-1 or rank-2 array which is to receive the array which had been mapped to the processor grid. The data type for A is any of five Fortran intrinsic types: **integer**; **single precision, real**; **double precision, real**; **single precision, complex**; **double precision, complex**. `A` is only valid on `MP_RANK` = 0 after `ScaLAPACK_UNMAP` has been called. (Output)

Optional Arguments

LDA — Leading dimension of `A` as specified in the calling program. If this argument is not present, `size(A,1)` is used. (Input)

COLMAP — Input logical which indicates whether the global array should be mapped in column major form or row major form. COLMAP set to `.TRUE.` will result in the array being mapped in column major form while setting COLMAP to `.FALSE.` will result in the array being mapped in row major form. The default value of COLMAP is `.TRUE.`. (Input)

FORTRAN 90 Interface

Generic: `CALL ScaLAPACK_UNMAP (A0, DESC_A, A , [, …])`

Description

Subroutine `ScaLAPACK_UNMAP` unmaps columns or rows of local distributed arrays to a global array on `MP_RANK = 0`. It uses the two-dimensional block-cyclic array descriptor for the matrix to retrieve the data from the assumed-size arrays on the processors. The block sizes, contained in the array descriptor, determine the data set size for each blocking send and receive pair. The number of these synchronization points is proportional to $\lceil M \times N / (MB \times NB) \rceil$. A temporary local buffer is allocated for staging the array data. It is of size `M` by `NB`, when mapping by columns, or `N` by `MB`, when mapping by rows.

Example: Distributed Linear Solver with IMSL ScaLAPACK Interface

The program `SCPKMP_EX1` illustrates solving a system of linear-algebraic equations, *Ax* = *b*, by calling routine `LSLRG`, an IMSL routine which interfaces with a *ScaLAPACK* routine. The right-hand side is produced by defining *A* and *y* to have random values. Then the matrix-vector product *b* = *Ay* is computed. The problem size is such that the residuals, *x*−*y*≈0, are checked on MP_RANK = 0. IMSL routine `ScaLAPACK_SETUP` is called to define the process grid and provide further information identifying each process. IMSL routine `ScaLAPACK_MAP` is called to map the global arrays to local distributed arrays. Then `LSLRG` is called to compute the approximate solution, *x*.

```
  program scpkmp_ex1
! This is Example 1 for ScaLAPACK_MAP and ScaLAPACK_UNMAP.
! A linear system is solved with an IMSL routine which
! interfaces with ScaLAPACK and is checked.
USE ScaLAPACK_SUPPORT
USE ERROR_OPTION_PACKET
USE MPI_SETUP_INT

USE LSLRG_INT

IMPLICIT NONE

INCLUDE "mpif.h"
INTEGER, PARAMETER :: N=9
INTEGER MXLDA, MXCOL, INFO, DESC_A(9), DESC_X(9)

LOGICAL :: GRID1D = .TRUE., NSQUARE = .TRUE.
real(kind(1d0)) :: ERROR=0d0, SIZE_Y
real(kind(1d0)), allocatable, dimension(:,:) :: A, B(:), &
  X(:), Y(:), A0, B0(:), X0(:)

  MP_NPROCS=MP_SETUP()

! Set up a 1D processor grid and define its context ID, MP_ICTXT
  CALL SCALAPACK_SETUP(N, N, NSQUARE, GRID1D)
! Get the array descriptor entities MXLDA, and MXCOL
  CALL SCALAPACK_GETDIM(N, N, MP_MB, MP_NB, MXLDA, MXCOL)
! Set up the array descriptors
  CALL DESCINIT(DESC_A, N, N, MP_MB, MP_NB, 0, 0, MP_ICTXT, &
```

```
  MXLDA, INFO)
  CALL DESCINIT(DESC_X, N, 1, MP_MB, 1, 0, 0, MP_ICTXT, &
  MXLDA, INFO)
! Allocate space for local arrays
  ALLOCATE(A0(MXLDA,MXCOL), B0(MXLDA), X0(MXLDA))

! A root process is used to create the matrix data for the test.
IF(MP_RANK == 0) THEN
  ALLOCATE(A(N,N), B(N), X(N), Y(N))
  CALL RANDOM_NUMBER(A); CALL RANDOM_NUMBER(Y)

! Compute the correct result.
  B=MATMUL(A,Y); SIZE_Y=SUM(ABS(Y))
END IF

! Map the input arrays to the processor grid
  CALL SCALAPACK_MAP(A, DESC_A, A0)
  CALL SCALAPACK_MAP(B, DESC_X, B0)

! Compute the distributed product solution to A x = b.
  CALL LSLRG(A0, B0, X0)

! Put the result on the root node.
  Call ScaLAPACK_UNMAP(X0, DESC_X, X)

IF(MP_RANK == 0) THEN
! Check the residuals for size.
  B=X-Y
  ERROR=SUM(ABS(B))/SIZE_Y
END IF
! See to any error messages.
  call e1pop("Mp_Setup")
IF(ERROR <= SQRT(EPSILON(ERROR)) .and. MP_RANK == 0) THEN
  write(*,*) &
  " Example 1 for ScaLAPACK_MAP and ScaLAPACK_UNMAP is correct."
END IF

! Deallocate storage arrays.
  IF (MP_RANK == 0) DEALLOCATE(A, B, X, Y)
  DEALLOCATE(A0, B0, X0)

! Exit from using this process grid.
  CALL SCALAPACK_EXIT( MP_ICTXT )
! Shut down MPI
  MP_NPROCS = MP_SETUP('FINAL')
  END
```

Output

```
Example 1 for ScaLAPACK_MAP and ScaLAPACK_UNMAP is correct.
```

ScaLAPACK_EXIT

MPI REQUIRED

For a detailed description of MPI Requirements see "*Using ScaLAPACK Enhanced Routines*" in the Introduction of this manual.

This routine exits *ScaLAPACK* mode for the IMSL Library routines. All processors in the *BLACS* context call the routine.

Required Arguments

ICTXT — The BLACS context ID to which the processor grid is associated. (Input)

FORTRAN 90 Interface

Generic: `CALL ScaLAPACK_EXIT (ICTXT)`

Description

Subroutine `ScaLAPACK_EXIT` exits `ScaLAPACK` mode for the IMSL Library routines. The following actions occur when this routine is called:

- `BLACS_GRIDEXIT` is called with the input BLACS context ID.
- The pointer to the grid ID, `MP_PIGRID` is nullified.
- If the grid, `MP_IGRID`, has been allocated, it is deallocated.
- `MP_ICTXT` is reset to its default value, `HUGE(1)`.

ERROR_POST

Prints error messages that are generated by IMSL routines using EPACK.

Required Argument

EPACK — (Input [/Output])

Derived type array of size *p* containing the array of message numbers and associated data for the messages. The definition of this derived type is packaged within the modules used as interfaces for each suite of routines. The declaration is:

```
type ?_error
integer idummy; real(kind(?_)) rdummy
end type
```

The choice of "`?_`" is either "`s_`" or "`d_`" depending on the accuracy of the data. This array gets additional messages and data from each routine that uses the "`epack=`" optional argument, provided *p* is large enough to hold data for a new message. The value *p* = 8 is sufficient to hold the longest single *terminal*, *fatal*, or *warning* message that an IMSL Fortran Library routine generates.

The location at entry `epack(1)%idummy` contains the number of data items for all messages. When the `error_post` routine exits, this value is set to zero. Locations in array positions `(2:)` `%idummy` contain groups of integers consisting of a message number, the *error severity level*, then the required integer data for the message. Floating-point data, if required in the message, is passed in locations`(:)%rdummy` matched with the starting point for integer data. The extent of the data for each message is determined by the requirements of the larger of each group of integer or floating-point values.

Optional Arguments

new_unit = `nunit` (Input)

Unit number, of type integer, associated for reading the direct-access file of error messages for the IMSL Fortran 90 routines.

Default: `nunit` = 4

new_path = `path` (Input)

Pathname in the local file space, of type character*64, needed for reading the direct-access file of error messages. Default string for `path` is defined during the installation procedure for certain IMSL Fortran Library routines.

FORTRAN 90 Interface

Generic: `CALL ERROR_POST (EPACK [, …])`

Specific: The specific interface names are `S_ERROR_POST` and `D_ERROR_POST`.

Description

A default direct-access error message file (.daf file) is supplied with this product. This file is read by error_post using the contents of the derived type argument epack, containing the message number, error severity level, and associated data. The message is converted into character strings accepted by the error processor and then printed. The number of pending messages that print depends on the settings of the parameters `PRINT` and `STOP` in the *Reference Material*. These values are initialized to defaults such that any Level 5 or Level 4 message causes a `STOP` within the error processor after a print of the text. To change these defaults so that more than one error message prints, use the routine `ERSET` documented and illustrated with examples in the *Reference Material*. The method of using a message file to store the messages is required to support "shared-memory parallelism."

Managing the Message File

For most applications of this product, there will be no need to manage this file. However, there are a few situations which may require changing or adding messages:

- New system-wide messages have been developed for applications using this Library.
- All or some of the existing messages need to be translated to another language
- A subset of users need to add a specific message file for their applications using this Library.

Following is information on changing the contents of the message file, and information on how to create and access a message file for a private application.

Changing Messages

In order to change messages, two files are required:

- An editable message glossary, messages.gls, supplied with this product.
- A source program, `prepmess.f`, used to generate an executable which builds `messages.daf` from `messages.gls`.

To change messages, first make a backup copy of `messages.gls`. Use a text editor to edit `messages.gls`. The format of this file is a series of pairs of statements:

- message_number=<nnnn>
- message='message string'

(Note that neither of these lines should begin with a tab.)

The variable `<nnnn>` is an integer message number (see below for ranges and reserved message numbers).

The `'message string'` is any valid message string not to exceed 255 characters. If a message line is too long for a screen, the standard Fortran 90 concatenation operator `//` with the line continuation character `&` may be used to wrap the text.

Most strings have substitution parameters embedded within them. These may be in the following forms:

- %(i<n>) for an integer substitution, where n is the nth integer output in this message.
- %(r<n>) for single precision real number substitution, where n is the nth real number output in this message.
- %(d<n>) for double precision real number substitution, where n is the nth double precision number output in this message.

New messages added to the system-wide error message file should be placed at the end of the file. Message numbers 5000 through 10000 have been reserved for user-added messages. Currently, messages 1 through 1400 are used by IMSL. Gaps in message number ranges are permitted; however, the message numbers must be in ascending order within the file. The message numbers used for each IMSL Fortran Library subroutine are documented in this manual and in online help.

If existing messages are being edited or translated, make sure not to alter the message_number lines. (This prevents conflicts with any new messages.gls file supplied with future versions of this Library.)

Building a New Direct-access Message File

The `prepmess` executable must be available to complete the message changing process. For information on building the `prepmess` executable from `prepmess.f`, consult the installation guide for this product.

Once new messages have been placed in the `messages.gls` file, make a backup copy of the `messages.daf` file. Then remove `messages.daf` from the current directory. Now enter the following command:

```
prepmess > prepmess_output
```

A new `messages.daf` file is created. Edit the `prepmess_output` file and look near the end of the file for the new error messages. The `prepmess` program processes each message through the error message system as a validity check. There should be no `FATAL` error announcement within the `prepmess_output` file.

Private Message Files

Users can create a private message file within their own messages. This file would generally be used by an application that calls this Library. Follow the steps outlined above to create a private `messages.gls` file. The user should then be given a copy of the `prepmess` executable. In the application code, call the `error_post` subprogram with the `new_unit/new_path` optional arguments. The new path should point to the directory in which the private `messages.daf` file resides.

SHOW

Prints rank-1 or rank-2 arrays of numbers in a readable format.

Required Arguments

X — Rank-1 or rank-2 array containing the numbers to be printed. (Input)

Optional Arguments

text = `CHARACTER` (Input)
`CHARACTER(LEN=*)` string used for labeling the array.

image = `buffer` (Output)
`CHARACTER(LEN=*)` string used for an internal write buffer. With this argument present the output is converted to characters and packed. The lines are separated by an end-of-line sequence. The length of `buffer` is estimated by the line width in effect, time the number of lines for the array.

iopt = `iopt(:)` (Input)
Derived type array with the same precision as the input array; used for passing optional data to the routine. Use the `REAL(KIND(1E0))` precision for output of `INTEGER` arrays. The options are as follows:

Packaged Options for **SHOW**		
Prefix is blank	Option Name	Option Value
	show_significant_digits_is_4	1
	show_significant_digits_is_7	2
	show_significant_digits_is_16	3
	show_line_width_is_44	4
	show_line_width_is_72	5
	show_line_width_is_128	6
	show_end_of_line_sequence_is	7
	show_starting_index_is	8
	show_starting_row_index_is	9
	show_starting_col_index_is	10

```
iopt(IO) = show_significant_digits_is_4
```

`iopt(IO) = show_significant_digits_is_7`

`iopt(IO) = show_significant_digits_is_16`

These options allow more precision to be displayed. The default is 4D for each value. The other possible choices display 7D or 16D.

`iopt(IO) = show_line_width_is_44`

`iopt(IO) = show_line_width_is_72`

`iopt(IO) = show_line_width_is_128`

These options allow varying the output line width. The default is 72 characters per line. This allows output on many work stations or terminals to be read without wrapping of lines.

`iopt(IO) = show_end-of_line_sequence_is`

The sequence of characters ending a line when it is placed into the internal character buffer corresponding to the optional argument `'IMAGE = buffer'`. The value of `iopt(IO+1)%idummy` is the number of characters. These are followed, starting at `iopt(IO+2)%idummy`, by the *ASCII* codes of the characters themselves. The default is the single character, *ASCII* value 10 or *New Line*.

`iopt(IO) = show_starting_index_is`

This are used to reset the starting index for a rank-1 array to a value different from the default value, which is 1.

`iopt(IO) = show_starting_row_index_is`

`iopt(IO) = show_starting_col_index_is`

These are used to reset the starting row and column indices to values different from their defaults, each 1.

FORTRAN 90 Interface

Generic: `CALL SHOW (X [, …])`

Specific: The specific interface names are `S_SHOW` and `D_SHOW`.

Description

The `show` routine is a generic subroutine interface to separate low-level subroutines for each data type and array shape. Output is directed to the unit number `IUNIT`. That number is obtained with the subroutine `UMACH`. Thus the user must open this unit in the calling program if it desired to be different from the standard output unit. If the optional argument `'IMAGE = buffer'` is present, the output is not sent to a file but to a character string within `buffer`. These characters are available to output or be used in the application.

Fatal and Terminal Error Messages

See the `messages.gls` file for error messages for `SHOW`. These error messages are numbered 601−606; 611−617; 621−627; 631−636; 641−646.

Examples

Example1: Printing an Array

Array of random numbers for all the intrinsic data types are printed. For `REAL(KIND(1E0))` rank-1 arrays, the number of displayed digits is reset from the default value of 4 to the value 7 and the subscripts for the array are reset so they match their declared extent when printed. The output is not shown.

```
    use show_int
    use rand_int

    implicit none

! This is Example 1 for SHOW.

    integer, parameter :: n=7, m=3
    real(kind(1e0)) s_x(-1:n), s_m(m,n)
    real(kind(1d0)) d_x(n), d_m(m,n)
    complex(kind(1e0)) c_x(n), c_m(m,n)
    complex(kind(1d0)) z_x(n),z_m(m,n)
    integer i_x(n), i_m(m,n)
        type (s_options) options(3)

! The data types printed are real(kind(1e0)), real(kind(1d0)),
! complex(kind(1e0)),  complex(kind(1d0)), and INTEGER.
! Fill with randsom numbers and then print the contents,
! in each case with a label.
    s_x=rand(s_x); s_m=rand(s_m)
    d_x=rand(d_x); d_m=rand(d_m)
    c_x=rand(c_x); c_m=rand(c_m)
    z_x=rand(z_x); z_m=rand(z_m)
    i_x=100*rand(s_x(1:n)); i_m=100*rand(s_m)

    call show (s_x, 'Rank-1, REAL')
    call show (s_m, 'Rank-2, REAL')
    call show (d_x, 'Rank-1, DOUBLE')
    call show (d_m, 'Rank-2, DOUBLE')
    call show (c_x, 'Rank-1, COMPLEX')
    call show (c_m, 'Rank-2, COMPLEX')
    call show (z_x, 'Rank-1, DOUBLE COMPLEX')
    call show (z_m, 'Rank-2, DOUBLE COMPLEX')
    call show (i_x, 'Rank-1, INTEGER')
    call show (i_m, 'Rank-2, INTEGER')

! Show 7 digits per number and  according to the
! natural or declared size of the array.
        options(1)=show_significant_digits_is_7
        options(2)=show_starting_index_is
        options(3)= -1 ! The starting  value.
        call show (s_x, &
'Rank-1, REAL with 7 digits, natural indexing', IOPT=options)
        end
```

Output

Example 1 for SHOW is correct.

Example 2: Writing an Array to a Character Variable

This example prepares a rank-1 array for further processing, in this case delayed writing to the standard output unit. The indices and the amount of precision are reset from their defaults, as in Example 1. An end-of-line sequence of the characters CR-NL (*ASCII* 10,13) is used in place of the standard *ASCII* 10. This is not required for writing this array, but is included for an illustration of the option.

```
        use show_int
        use rand_int

        implicit none

! This is Example 2 for SHOW.
        integer, parameter :: n=7
        real(kind(1e0)) s_x(-1:n)
        type (s_options) options(7)
        CHARACTER (LEN=(72+2)*4) BUFFER
! The data types printed are real(kind(1e0)) random numbers.
        s_x=rand(s_x)


! Show 7 digits per number and  according to the
! natural or declared size of the array.
! Prepare the output lines in array BUFFER.
! End each line with ASCII sequence CR-NL.
        options(1)=show_significant_digits_is_7

        options(2)=show_starting_index_is
        options(3)= -1 ! The starting  value.

        options(4)=show_end_of_line_sequence_is
        options(5)=  2 ! Use 2 EOL characters.
        options(6)= 10 ! The ASCII code for CR.
        options(7)= 13 ! The ASCII code for NL.

        BUFFER= ' '    ! Blank out the buffer.

! Prepare the output in BUFFER.
 call show (s_x, &
 'Rank-1, REAL with 7 digits, natural indexing '//&
 'internal BUFFER, CR-NL EOLs.',&
 IMAGE=BUFFER,  IOPT=options)

! Display BUFFER as a CHARACTER array. Discard blanks
! on the ends.
        WRITE(*,'(1x,A)') TRIM(BUFFER)

        end
```

Output

```
Example 2 for SHOW is correct.
```

WRRRN

Prints a real rectangular matrix with integer row and column labels.

Required Arguments

TITLE — Character string specifying the title. (Input)
`TITLE` set equal to a blank character(s) suppresses printing of the title. Use "% /" within the title to create a new line. Long titles are automatically wrapped.

A — `NRA` by `NCA` matrix to be printed. (Input)

Optional Arguments

NRA — Number of rows. (Input)
Default: `NRA` = `size` (A,1).

NCA — Number of columns. (Input)
Default: `NCA` = `size` (A,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement in the calling program. (Input)
Default: `LDA` = `size` (A,1).

ITRING — Triangle option. (Input)
Default: `ITRING` = 0.

ITRING	Action
0	Full matrix is printed.
1	Upper triangle of `A` is printed, including the diagonal.
2	Upper triangle of `A` excluding the diagonal of `A` is printed.
−1	Lower triangle of `A` is printed, including the diagonal.
−2	Lower triangle of `A` excluding the diagonal of `A` is printed.

FORTRAN 90 Interface

Generic: `CALL WRRRN (TITLE, A [, …])`

Specific: The specific interface names are S_WRRRN and D_WRRRN for two dimensional arrays, and S_WRRRN1D and D_WRRRN1D for one dimensional arrays.

FORTRAN 77 Interface

Single: CALL WRRRN (TITLE, NRA, NCA, A, LDA, ITRING)

Double: The double precision name is DWRRRN.

Description

Routine WRRRN prints a real rectangular matrix with the rows and columns labeled 1, 2, 3, and so on. WRRRN can restrict printing to the elements of the upper or lower triangles of matrices via the ITRING option. Generally, ITRING $\neq 0$ is used with symmetric matrices.

In addition, one-dimensional arrays can be printed as column or row vectors. For a column vector, set NRA to the length of the array and set NCA = 1. For a row vector, set NRA = 1 and set NCA to the length of the array. In both cases, set LDA = NRA and set ITRING = 0.

Comments

1. A single D, E, or F format is chosen automatically in order to print 4 significant digits for the largest element of A in absolute value. Routine WROPT can be used to change the default format.

2. Horizontal centering, a method for printing large matrices, paging, printing a title on each page, and many other options can be selected by invoking WROPT.

3. A page width of 78 characters is used. Page width and page length can be reset by invoking PGOPT .

4. Output is written to the unit specified by UMACH (see the *Reference Material*).

Example

The following example prints all of a 3×4 matrix A where $a_{ij} = i + j/10$.

```
      USE WRRRN_INT

        IMPLICIT   NONE
        INTEGER    ITRING, LDA, NCA, NRA
        PARAMETER  (ITRING=0, LDA=10, NCA=4, NRA=3)
!
        INTEGER    I, J
        REAL       A(LDA,NCA)
!
        DO 20  I=1, NRA
           DO 10  J=1, NCA
              A(I,J) = I + J*0.1
```

```
   10    CONTINUE
   20 CONTINUE
!                                   Write A matrix.
      CALL WRRRN ('A', A, NRA=NRA)
      END
```

Output

```
                   A
        1       2       3       4
 1   1.100   1.200   1.300   1.400
 2   2.100   2.200   2.300   2.400
 3   3.100   3.200   3.300   3.400
```

WRRRL

Print a real rectangular matrix with a given format and labels.

Required Arguments

TITLE — Character string specifying the title. (Input)
TITLE set equal to a blank character(s) suppresses printing of the title.

A — NRA by NCA matrix to be printed. (Input)

RLABEL — CHARACTER * (*) vector of labels for rows of A. (Input)
If rows are to be numbered consecutively 1, 2, …, NRA, use RLABEL(1) = 'NUMBER'. If no row labels are desired, use RLABEL(1) = 'NONE'. Otherwise, RLABEL is a vector of length NRA containing the labels.

CLABEL — CHARACTER * (*) vector of labels for columns of A. (Input)
If columns are to be numbered consecutively 1, 2, …, NCA, use CLABEL(1) = 'NUMBER'. If no column labels are desired, use CLABEL(1) = 'NONE'. Otherwise, CLABEL(1) is the heading for the row labels, and either CLABEL(2) must be 'NUMBER' or 'NONE', or CLABEL must be a vector of length NCA + 1 with CLABEL(1 + *j*) containing the column heading for the *j*-th column.

Optional Arguments

NRA — Number of rows. (Input)
Default: NRA = size (A,1).

NCA — Number of columns. (Input)
Default: NCA = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement in the calling program. (Input)
Default: LDA = size (A,1).

ITRING — Triangle option. (Input)
Default: ITRING = 0.

ITRING	Action
0	Full matrix is printed.
1	Upper triangle of A is printed, including the diagonal.
2	Upper triangle of A excluding the diagonal of A is printed.
−1	Lower triangle of A is printed, including the diagonal.
−2	Lower triangle of A excluding the diagonal of A is printed.

FMT — Character string containing formats. (Input)
If FMT is set to a blank character(s), the format used is specified by WROPT. Otherwise, FMT must contain exactly one set of parentheses and one or more edit descriptors. For example, FMT = '(F10.3)' specifies this F format for the entire matrix. FMT = '(2E10.3, 3F10.3)' specifies an E format for columns 1 and 2 and an F format for columns 3, 4 and 5. If the end of FMT is encountered and if some columns of the matrix remain, format control continues with the first format in FMT. Even though the matrix A is real, an I format can be used to print the integer part of matrix elements of A. The most useful formats are special formats, called the V and W formats, that can be used to specify pretty formats automatically. Set FMT = '(V10.4)' if you want a single D, E, or F format selected automatically with field width 10 and with 4 significant digits. Set FMT = '(W10.4)' if you want a single D, E, F, or I format selected automatically with field width 10 and with 4 significant digits. While the V format prints trailing zeroes and a trailing decimal point, the W format does not. See Comment 4 for general descriptions of the V and W formats. FMT may contain only D, E, F, G, I, V, or W edit descriptors, e.g., the X descriptor is not allowed.
Default: FMT = ' '.

FORTRAN 90 Interface

Generic: CALL WRRRL (TITLE, A, RLABEL, CLABEL [, …])

Specific: The specific interface names are S_WRRRL and D_WRRRL for two dimensional arrays, and S_WRRRL1D and D_WRRRL1D for one dimensional arrays.

FORTRAN 77 Interface

Single: CALL WRRRL (TITLE, NRA, NCA, A, LDA, ITRING, FMT, RLABEL, CLABEL)

Double:The double precision name is DWRRRL.

Description

Routine WRRRL prints a real rectangular matrix (stored in *A*) with row and column labels (specified by RLABEL and CLABEL, respectively) according to a given format (stored in FMT). WRRRL can restrict printing to the elements of upper or lower triangles of matrices via the ITRING option. Generally, ITRING $\neq 0$ is used with symmetric matrices.

In addition, one-dimensional arrays can be printed as column or row vectors. For a column vector, set NRA to the length of the array and set NCA = 1. For a row vector, set NRA = 1 and set NCA to the length of the array. In both cases, set LDA = NRA, and set ITRING = 0.

Comments

1. Workspace may be explicitly provided, if desired, by use of W2RRL/DW2RRL. The reference is:

   CALL W2RRL (TITLE, NRA, NCA, A, LDA, ITRING, FMT, RLABEL, CLABEL, CHWK)

   The additional argument is:

   CHWK — CHARACTER * 10 work vector of length NCA. This workspace is referenced only if all three conditions indicated at the beginning of this comment are met. Otherwise, CHWK is not referenced and can be a CHARACTER * 10 vector of length one.

2. The output appears in the following form:

   TITLE

CLABEL(1)	CLABEL(2)	CLABEL(3)	CLABEL(4)
RLABEL(1)	Xxxxx	Xxxxx	Xxxxx
RLABEL(2)	Xxxxx	Xxxxx	Xxxxx

3. Use “% /” within titles or labels to create a new line. Long titles or labels are automatically wrapped.

4. For printing numbers whose magnitudes are unknown, the G format in FORTRAN is useful; however, the decimal points will generally not be aligned when printing a column of numbers. The V and W formats are special formats used by this routine to select a D, E, F, or I format so that the decimal points will be aligned. The V and W formats are specified as *Vn.d* and *Wn.d*. Here, *n* is the field width and *d* is the number of significant digits generally printed. Valid values for *n* are 3, 4,…, 40. Valid values for *d* are 1, 2, …, $n - 2$. If FMT specifies one format and that format is a V or W format, all elements of the matrix A are examined to determine one FORTRAN format for printing. If FMT specifies more than one format, FORTRAN formats are generated separately from each V or W format.

5. A page width of 78 characters is used. Page width and page length can be reset by invoking PGOPT .

6. Horizontal centering, method for printing large matrices, paging, method for printing NaN (not a number), printing a title on each page, and many other options can be selected by invoking WROPT .

7. Output is written to the unit specified by UMACH (see *Reference Material*).

Example

The following example prints all of a 3 $\times$ 4 matrix A where $a_{ij} = (i + j/10)10^{j-3}$.

```
      USE WRRRL_INT

      IMPLICIT   NONE
      INTEGER    ITRING, LDA, NCA, NRA
      PARAMETER  (ITRING=0, LDA=10, NCA=4, NRA=3)
!
      INTEGER    I, J
      REAL       A(LDA,NCA)
      CHARACTER  CLABEL(5)*5, FMT*8, RLABEL(3)*5
!
      DATA FMT/'(W10.6)'/
      DATA CLABEL/'    ', 'Col 1', 'Col 2', 'Col 3', 'Col 4'/
      DATA RLABEL/'Row 1', 'Row 2', 'Row 3'/
!
      DO 20  I=1, NRA
         DO 10  J=1, NCA
            A(I,J) = (I+J*0.1)*10.0**(J-3)
   10    CONTINUE
   20 CONTINUE
!                                   Write A matrix.
      CALL WRRRL ('A', A, RLABEL, CLABEL, NRA=NRA, FMT=FMT)
      END
```

Output

```
                                A
            Col 1       Col 2       Col 3        Col 4
Row 1       0.011       0.120       1.300       14.000
Row 2       0.021       0.220       2.300       24.000
Row 3       0.031       0.320       3.300       34.000
```

WRIRN

Prints an integer rectangular matrix with integer row and column labels.

Required Arguments

TITLE — Character string specifying the title. (Input)
TITLE set equal to a blank character(s) suppresses printing of the title. Use "%/" within the title to create a new line. Long titles are automatically wrapped.

MAT — NRMAT by NCMAT matrix to be printed. (Input)

Optional Arguments

NRMAT — Number of rows. (Input)
Default: NRMAT = size (MAT,1).

NCMAT — Number of columns. (Input)
Default: NCMAT = size (MAT,2).

LDMAT — Leading dimension of MAT exactly as specified in the dimension statement in the calling program. (Input)
Default: LDMAT = size (MAT,1).

ITRING — Triangle option. (Input)
Default: ITRING = 0.

ITRING	Action
0	Full matrix is printed.
1	Upper triangle of MAT is printed, including the diagonal.
2	Upper triangle of MAT excluding the diagonal of MAT is printed.
−1	Lower triangle of MAT is printed, including the diagonal.
−2	Lower triangle of MAT excluding the diagonal of MAT is printed.

FORTRAN 90 Interface

Generic: ***CALL WRIRN*** (TITLE, MAT [, …])

Specific: The specific interface name is S_WRIRN.

FORTRAN 77 Interface

Single: CALL WRIRN (TITLE, NRMAT, NCMAT, MAT, LDMAT, ITRING)

Description

Routine WRIRN prints an integer rectangular matrix with the rows and columns labeled 1, 2, 3, and so on. WRIRN can restrict printing to elements of the upper and lower triangles of matrices via the ITRING option. Generally, ITRING $\neq$ 0 is used with symmetric matrices.

In addition, one-dimensional arrays can be printed as column or row vectors. For a column vector, set NRMAT to the length of the array and set NCMAT = 1. For a row vector, set NRMAT = 1 and set NCMAT to the length of the array. In both cases, set LDMAT = NRMAT and set ITRING = 0.

Comments

1. All the entries in MAT are printed using a single I format. The field width is determined by the largest absolute entry.
2. Horizontal centering, a method for printing large matrices, paging, printing a title on each page, and many other options can be selected by invoking WROPT.
3. A page width of 78 characters is used. Page width and page length can be reset by invoking PGOPT .
4. Output is written to the unit specified by UMACH (see *Reference Material*).

Example

The following example prints all of a 3 $\times$ 4 matrix A = MAT where $a_{ij} = 10i + j$.

```
      USE WRIRN_INT

      IMPLICIT   NONE
      INTEGER    ITRING, LDMAT, NCMAT, NRMAT
      PARAMETER  (ITRING=0, LDMAT=10, NCMAT=4, NRMAT=3)
!
      INTEGER    I, J, MAT(LDMAT,NCMAT)
!
      DO 20  I=1, NRMAT
         DO 10  J=1, NCMAT
            MAT(I,J) = I*10 + J
   10    CONTINUE
   20 CONTINUE
!                                  Write MAT matrix.
      CALL WRIRN ('MAT', MAT, NRMAT=NRMAT)
      END
```

Output

```
           MAT
      1     2     3     4
 1   11    12    13    14
 2   21    22    23    24
 3   31    32    33    34
```

WRIRL

Print an integer rectangular matrix with a given format and labels.

Required Arguments

TITLE — Character string specifying the title. (Input)
TITLE set equal to a blank character(s) suppresses printing of the title.

MAT — NRMAT by NCMAT matrix to be printed. (Input)

RLABEL — CHARACTER * (*) vector of labels for rows of MAT. (Input)
If rows are to be numbered consecutively 1, 2, …, NRMAT, use RLABEL(1) = 'NUMBER'. If no row labels are desired, use RLABEL(1) = 'NONE'. Otherwise, RLABEL is a vector of length NRMAT containing the labels.

CLABEL — CHARACTER * (*) vector of labels for columns of MAT. (Input)
If columns are to be numbered consecutively 1, 2, …, NCMAT, use CLABEL(1) = 'NUMBER'. If no column labels are desired, use CLABEL(1) = 'NONE'. Otherwise, CLABEL(1) is the heading for the row labels, and either CLABEL(2) must be 'NUMBER' or 'NONE', or CLABEL must be a vector of length

NCMAT + 1 with CLABEL(1 + *j*) containing the column heading for the *j*-th column.

Optional Arguments

NRMAT — Number of rows. (Input)
Default: NRMAT = size (MAT,1).

NCMAT — Number of columns. (Input)
Default: NCMAT = size (MAT,2).

LDMAT — Leading dimension of MAT exactly as specified in the dimension statement in the calling program. (Input)
Default: LDMAT = size (MAT,1).

ITRING — Triangle option. (Input)
Default: ITRING = 0.

ITRING	Action
0	Full matrix is printed.
1	Upper triangle of MAT is printed, including the diagonal.
2	Upper triangle of MAT excluding the diagonal of MAT is printed.
−1	Lower triangle of MAT is printed, including the diagonal.
−2	Lower triangle of MAT excluding the diagonal of MAT is printed.

FMT — Character string containing formats. (Input)
If FMT is set to a blank character(s), the format used is a single I format with field width determined by the largest absolute entry. Otherwise, FMT must contain exactly one set of parentheses and one or more I edit descriptors. For example, FMT = ′(I10)′ specifies this I format for the entire matrix. FMT = ′(2I10, 3I5)′ specifies an I10 format for columns 1 and 2 and an I5 format for columns 3, 4 and 5. If the end of FMT is encountered and if some columns of the matrix remain, format control continues with the first format in FMT. FMT may only contain the I edit descriptor, e.g., the X edit descriptor is not allowed.
Default: FMT = ‘‘.

FORTRAN 90 Interface

Generic: CALL WRIRL (TITLE, MAT, RLABEL, CLABEL [, …])

Specific: The specific interface name is S_WRIRL.

FORTRAN 77 Interface

Single: CALL WRIRL (TITLE, NRMAT, NCMAT, MAT, LDMAT, ITRING, FMT, RLABEL, CLABEL)

Description

Routine WRIRL prints an integer rectangular matrix (stored in MAT) with row and column labels (specified by RLABEL and CLABEL, respectively), according to a given format (stored in FMT). WRIRL can restrict printing to the elements of upper or lower triangles of matrices via the ITRING option. Generally, ITRING $\neq$ 0 is used with symmetric matrices. In addition, one-dimensional arrays can be printed as column or row vectors. For a column vector, set NRMAT to the length of the array and set NCMAT = 1. For a row vector, set NRMAT = 1 and set NCMAT to the length of the array. In both cases, set LDMAT = NRMAT, and set ITRING = 0.

Comments

1. The output appears in the following form:

TITLE

CLABEL(1)	CLABEL(2)	CLABEL(3)	CLABEL 4)
RLABEL(1)	Xxxxx	xxxxx	xxxxx
RLABEL(2)	Xxxxx	xxxxx	xxxxx

2. Use “% /” within titles or labels to create a new line. Long titles or labels are automatically wrapped.
3. A page width of 78 characters is used. Page width and page length can be reset by invoking `PGOPT`.
4. Horizontal centering, a method for printing large matrices, paging, printing a title on each page, and many other options can be selected by invoking `WROPT`.
5. Output is written to the unit specified by `UMACH` (see the *Reference Material*).

Example

The following example prints all of a 3 × 4 matrix A = `MAT` where $a_{ij} = 10i + j$.

```
      USE WRIRL_INT

      IMPLICIT   NONE
      INTEGER    ITRING, LDMAT, NCMAT, NRMAT

      PARAMETER  (ITRING=0, LDMAT=10, NCMAT=4, NRMAT=3)
!
      INTEGER    I, J, MAT(LDMAT,NCMAT)
      CHARACTER  CLABEL(5)*5, FMT*8, RLABEL(3)*5
!
      DATA FMT/'(I2)'/
      DATA CLABEL/'     ', 'Col 1', 'Col 2', 'Col 3', 'Col 4'/
      DATA RLABEL/'Row 1', 'Row 2', 'Row 3'/
!
      DO 20  I=1, NRMAT
         DO 10  J=1, NCMAT
            MAT(I,J) = I*10 + J
   10    CONTINUE
   20 CONTINUE
!                                  Write MAT matrix.
      CALL WRIRL ('MAT', MAT, RLABEL, CLABEL, NRMAT=NRMAT)
      END
```

Output

```
                     MAT
         Col 1  Col 2  Col 3  Col 4
Row 1      11     12     13     14
Row 2      21     22     23     24
Row 3      31     32     33     34
```

WRCRN

Prints a complex rectangular matrix with integer row and column labels.

Required Arguments

TITLE — Character string specifying the title. (Input)
`TITLE` set equal to a blank character(s) suppresses printing of the title. Use "% /" within the title to create a new line. Long titles are automatically wrapped.

A — Complex `NRA` by `NCA` matrix to be printed. (Input)

Optional Arguments

NRA — Number of rows. (Input)
Default: `NRA` = `size` (A,1).

NCA — Number of columns. (Input)
Default: `NCA` = `size` (A,2).

LDA — Leading dimension of `A` exactly as specified in the dimension statement in the calling program. (Input)
Default: `LDA` = `size` (A,1).

ITRING — Triangle option. (Input)
Default: `ITRING` = 0.

ITRING	Action
0	Full matrix is printed.
1	Upper triangle of `A` is printed, including the diagonal.
2	Upper triangle of `A` excluding the diagonal of `A` is printed.
−1	Lower triangle of `A` is printed, including the diagonal.
−2	Lower triangle of `A` excluding the diagonal of `A` is printed.

FORTRAN 90 Interface

Generic: `CALL WRCRN (TITLE, A [, …])`

Specific: The specific interface names are S_WRCRN and D_WRCRN for two dimensional arrays, and S_WRCRN1D and D_WRCRN1D for one dimensional arrays.

FORTRAN 77 Interface

Single: CALL WRCRN (TITLE, NRA, NCA, A, LDA, ITRING)

Double:The double precision name is DWRCRN.

Description

Routine WRCRN prints a complex rectangular matrix with the rows and columns labeled 1, 2, 3, and so on. WRCRN can restrict printing to the elements of the upper or lower triangles of matrices via the ITRING option. Generally, ITRING $\neq$ 0 is used with Hermitian matrices.

In addition, one-dimensional arrays can be printed as column or row vectors. For a column vector, set NRA to the length of the array, and set NCA = 1. For a row vector, set NRA = 1, and set NCA to the length of the array. In both cases, set LDA = NRA, and set ITRING = 0.

Comments

1. A single D, E, or F format is chosen automatically in order to print 4 significant digits for the largest real or imaginary part in absolute value of all the complex numbers in A. Routine WROPT can be used to change the default format.
2. Horizontal centering, a method for printing large matrices, paging, method for printing NaN (not a number), and printing a title on each page can be selected by invoking WROPT.
3. A page width of 78 characters is used. Page width and page length can be reset by invoking subroutine PGOPT .
4. Output is written to the unit specified by UMACH (see *Reference Material*).

Example

This example prints all of a 3 × 4 complex matrix *A* with elements

$$a_{mn} = m + ni, \text{where } i = \sqrt{-1}$$

```
      USE WRCRN_INT

      IMPLICIT   NONE
      INTEGER    ITRING, LDA, NCA, NRA
```

```
      PARAMETER  (ITRING=0, LDA=10, NCA=4, NRA=3)
!
      INTEGER    I, J
      COMPLEX    A(LDA,NCA), CMPLX
      INTRINSIC  CMPLX
!
      DO 20  I=1, NRA
         DO 10  J=1, NCA
            A(I,J) = CMPLX(I,J)
   10    CONTINUE
   20 CONTINUE
!                                  Write A matrix.
      CALL WRCRN ('A', A, NRA=NRA)
      END
```

Output

```
                                  A
                 1                 2                 3                 4
1  ( 1.000, 1.000)  ( 1.000, 2.000)  ( 1.000, 3.000)  ( 1.000, 4.000)
2  ( 2.000, 1.000)  ( 2.000, 2.000)  ( 2.000, 3.000)  ( 2.000, 4.000)
3  ( 3.000, 1.000)  ( 3.000, 2.000)  ( 3.000, 3.000)  ( 3.000, 4.000)
```

WRCRL

Prints a complex rectangular matrix with a given format and labels.

Required Arguments

TITLE — Character string specifying the title. (Input)
TITLE set equal to a blank character(s) suppresses printing of the title.

A — Complex NRA by NCA matrix to be printed. (Input)

RLABEL — CHARACTER * (*) vector of labels for rows of A. (Input)
If rows are to be numbered consecutively 1, 2, …, NRA, use RLABEL(1) = 'NUMBER'. If no row labels are desired, use RLABEL(1) = 'NONE'. Otherwise, RLABEL is a vector of length NRA containing the labels.

CLABEL — CHARACTER * (*) vector of labels for columns of A. (Input)
If columns are to be numbered consecutively 1, 2, …, NCA, use CLABEL(1) = 'NUMBER'. If no column labels are desired, use CLABEL(1) = 'NONE'. Otherwise, CLABEL(1) is the heading for the row labels, and either CLABEL(2) must be 'NUMBER' or 'NONE', or CLABEL must be a vector of length NCA + 1 with CLABEL(1 + *j*) containing the column heading for the *j*-th column.

Optional Arguments

NRA — Number of rows. (Input)
Default: NRA = size (A,1).

NCA — Number of columns. (Input)
Default: NCA = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement in the calling program. (Input)
Default: LDA = size (A,1).

ITRING — Triangle option. (Input)
Default: ITRING = 0.

ITRING	Action
0	Full matrix is printed.
1	Upper triangle of A is printed, including the diagonal.
2	Upper triangle of A excluding the diagonal of A is printed.
−1	Lower triangle of A is printed, including the diagonal.
−2	Lower triangle of A excluding the diagonal of A is printed.

FMT — Character string containing formats. (Input)
If FMT is set to a blank character(s), the format used is specified by WROPT. Otherwise, FMT must contain exactly one set of parentheses and one or more edit descriptors. Because a complex number consists of two parts (a real and an imaginary part), two edit descriptors are used for printing a single complex number. FMT = '(E10.3, F10.3)' specifies an E format for the real part and an F format for the imaginary part. FMT = '(F10.3)' uses an F format for both the real and imaginary parts. If the end of FMT is encountered and if all columns of the matrix have not been printed, format control continues with the first format in FMT. Even though the matrix A is complex, an I format can be used to print the integer parts of the real and imaginary components of each complex number. The most useful formats are special formats, called the "V and W formats," that can be used to specify pretty formats automatically. Set FMT = '(V10.4)' if you want a single D, E, or F format selected automatially with field width 10 and with 4 significant digits. Set FMT = '(W10.4)' if you want a single D, E, F, or I format selected automatically with field width 10 and with 4 significant digits. While the V format prints trailing zeroes and a trailing decimal point, the W format does not. See Comment 4 for general descriptions of the V and W formats. FMT may contain only D, E, F, G, I, V, or W edit descriptors, e.g., the X descriptor is not allowed.
Default: FMT = ' '.

FORTRAN 90 Interface

Generic: CALL WRCRL (TITLE, A, RLABEL, CLABEL [, …])

Specific: The specific interface names are S_WRCRL and D_WRCRL for two dimensional arrays, and S_WRCRL1D and D_WRCRL1D for one dimensional arrays.

FORTRAN 77 Interface

Single: CALL WRCRL (TITLE, NRA, NCA, A, LDA, ITRING, FMT, RLABEL, CLABEL)

Double: The double precision name is DWRCRL.

Description

Routine WRCRL prints a complex rectangular matrix (stored in *A*) with row and column labels (specified by RLABEL and CLABEL, respectively) according to a given format (stored in FMT). Routine WRCRL can restrict printing to the elements of upper or lower triangles of matrices via the ITRING option. Generally, the ITRING $\neq 0$ is used with Hermitian matrices.

In addition, one-dimensional arrays can be printed as column or row vectors. For a column vector, set NRA to the length of the array, and set NCA = 1. For a row vector, set NRA = 1, and set NCA to the length of the array. In both cases, set LDA = NRA, and set ITRING = 0.

Comments

1. Workspace may be explicitly provided, if desired, by use of W2CRL/DW2CRL. The reference is:

   CALL W2CRL (TITLE, NRA, NCA, A, LDA, ITRING, FMT, RLABEL, CLABEL, CHWK)

   The additional argument is:

   CHWK — CHARACTER * 10 work vector of length 2 * NCA. This workspace is referenced only if all three conditions indicated at the beginning of this comment are met. Otherwise, CHWK is not referenced and can be a CHARACTER * 10 vector of length one.

2. The output appears in the following form:

   TITLE

CLABEL(1)	CLABEL(2)	CLABEL(3)	CLABEL(4)
RLABEL(1)	(xxxxx,xxxxx)	(xxxxx,xxxxx)	(xxxxx,xxxxx)
RLABEL(2)	(xxxxx,xxxxx)	(xxxxx,xxxxx)	(xxxxx,xxxxx)

3. Use “% /” within titles or labels to create a new line. Long titles or labels are automatically wrapped.

4. For printing numbers whose magnitudes are unknown, the G format in FORTRAN is useful; however, the decimal points will generally not be aligned when printing a column of numbers. The V and W formats are special formats used by this routine to select a D, E, F, or I format so that the decimal points will be aligned. The V and W formats are specified as *Vn.d* and *Wn.d*. Here, *n* is the field width, and *d* is the number of significant digits generally printed. Valid values for *n* are 3, 4, …, 40. Valid values for *d* are 1, 2, …, $n - 2$. If FMT specifies one format and that format is a V or W format, all elements of the matrix A are examined to determine one FORTRAN format for printing. If FMT specifies more than one format, FORTRAN formats are generated separately from each V or W format.

5. A page width of 78 characters is used. Page width and page length can be reset by invoking `PGOPT`.

6. Horizontal centering, a method for printing large matrices, paging, method for printing NaN (not a number), printing a title on each page, and may other options can be selected by invoking `WROPT`.

7. Output is written to the unit specified by `UMACH` (see the *Reference Material*).

Example

The following example prints all of a 3 × 4 matrix *A* with elements

$$a_{mn} = (m + .123456) + ni, \text{where } i = \sqrt{-1}$$

```
      USE WRCRL_INT

      IMPLICIT   NONE

      INTEGER    ITRING, LDA, NCA, NRA
      PARAMETER  (ITRING=0, LDA=10, NCA=4, NRA=3)
!
      INTEGER    I, J
      COMPLEX    A(LDA,NCA), CMPLX
      CHARACTER  CLABEL(5)*5, FMT*8, RLABEL(3)*5
      INTRINSIC  CMPLX
!
      DATA FMT/'(W12.6)'/
      DATA CLABEL/'    ', 'Col 1', 'Col 2', 'Col 3', 'Col 4'/
      DATA RLABEL/'Row 1', 'Row 2', 'Row 3'/
!
      DO 20  I=1, NRA
         DO 10  J=1, NCA
            A(I,J) = CMPLX(I,J) + 0.123456
   10    CONTINUE
   20 CONTINUE
!                                Write A matrix.
      CALL WRCRL ('A', A, RLABEL, CLABEL, NRA=NRA, FMT=FMT)
      END
```

Output

```
                                A
                              Col 1                             Col 2
 Row 1  (      1.12346,      1.00000)  (      1.12346,      2.00000)
 Row 2  (      2.12346,      1.00000)  (      2.12346,      2.00000)
 Row 3  (      3.12346,      1.00000)  (      3.12346,      2.00000)
                              Col 3                             Col 4
 Row 1  (      1.12346,      3.00000)  (      1.12346,      4.00000)
 Row 2  (      2.12346,      3.00000)  (      2.12346,      4.00000)
 Row 3  (      3.12346,      3.00000)  (      3.12346,      4.00000)
```

WROPT

Sets or retrieves an option for printing a matrix.

Required Arguments

IOPT — Indicator of option type. (Input)

IOPT	Description of Option Type
−1, 1	Horizontal centering or left justification of matrix to be printed
−2, 2	Method for printing large matrices
−3, 3	Paging
−4, 4	Method for printing NaN (not a number), and negative and positive machine infinity.
−5, 5	Title option
−6, 6	Default format for real and complex numbers
−7, 7	Spacing between columns
−8, 8	Maximum horizontal space reserved for row labels
−9, 9	Indentation of continuation lines for row labels
−10, 10	Hot zone option for determining line breaks for row labels
−11, 11	Maximum horizontal space reserved for column labels
−12, 12	Hot zone option for determining line breaks for column labels
−13, 13	Hot zone option for determining line breaks for titles
−14, 14	Option for the label that appears in the upper left hand corner that can be used as a heading for the row numbers or a label for the column headings for WR**N routines
−15, 15	Option for skipping a line between invocations of WR**N routines, provided a new page is not to be issued
−16, 16	Option for vertical alignment of the matrix values relative to the associated row labels that occupy more than one line
0	Reset all the current settings saved in internal variables back to their last setting made with an invocation of WROPT with ISCOPE = 1. (This option is used internally by routines printing a matrix and is not useful otherwise.)

If IOPT is negative, ISETNG and ISCOPE are input and are saved in internal variables. If IOPT is positive, ISETNG is output and receives the currently active setting for the option (if ISCOPE = 0) or the last global setting for the option (if ISCOPE = 1).
If IOPT = 0, ISETNG and ISCOPE are not referenced.

ISETNG — Setting for option selected by IOPT. (Input, if IOPT is negative; output, if IOPT is positive; not referenced if IOPT = 0)

IOPT	ISETNG	Meaning
−1, 1	0	Matrix is left justified
	1	Matrix is centered horizontally on page
−2, 2	0	A complete row is printed before the next row is printed. Wrapping is used if necessary.
	m	Here, m is a positive integer. Let n_1 be the maximum number of columns beginning with column 1 that fit across the page (as determined by the widths of the printing formats). First, columns 1 through n_1 are printed for rows 1 through m. Let n_2 be the maximum number of columns beginning with column n_1 + 1 that fit across the page. Second, columns n_1 + 1 through n_1 + n_2 are printed for rows 1 through m. This continues until the last columns are printed for rows 1 through m. Printing continues in this fashion for the next m rows, etc.
−3, 3	−2	Printing begins on the next line, and no paging occurs.
	−1	Paging is on. Every invocation of a WR*** routine begins on a new page, and paging occurs within each invocation as is needed
	0	Paging is on. The first invocation of a WR*** routine begins on a new page, and subsequent paging occurs as is needed. With this option, every invocation of a WR*** routine ends with a call to WROPT to reset this option to k, a positive integer giving the number of lines printed on the current page.
	k	Here, k is a positive integer. Paging is on, and k lines have been printed on the current page. If k is less than the page length IPAGE (see PGOPT), then IPAGE – k lines are printed before a new page instruction is issued. If k is greater than or equal to IPAGE, then the first invocation of a WR*** routine begins on a new page. In any case, subsequent paging occurs as is needed. With this option, every invocation of a WR*** routine ends with a call to WROPT to reset the value of k.
−4, 4	0	NaN is printed as a series of decimal points, negative machine infinity is printed as a series of minus signs, and positive machine infinity is printed as a series of plus signs.
	1	NaN is printed as a series of blank characters, negative machine infinity is printed as a series of minus signs, and positive machine infinity is printed as a series of plus signs.
	2	NaN is printed as “NaN,” negative machine infinity is printed as “-Inf” and positive machine infinity is printed as “Inf.”

IOPT	ISETNG	Meaning
	3	NaN is printed as a series of blank characters, negative machine infinity is printed as “-Inf,” and positive machine infinity is printed as “Inf.”
−5, 5	0	Title appears only on first page.
	1	Title appears on the first page and all continuation pages.
−6, 6	0	Format is (W10.4). See Comment 2.
	1	Format is (W12.6). See Comment 2.
	2	Format is (1PE12.5).
	3	Format is Vn.4 where the field width n is determined. See Comment 2.
	4	Format is *V*n.6 where the field width *n* is determined. See Comment 2.
	5	Format is 1PEn.d where n = d + 7, and d + 1 is the maximum number of significant digits.
−7, 7	K_1	Number of characters left blank between columns. K_1 must be between 0 and 5, inclusively.
−8, 8	K_2	Maximum width (in characters) reserved for row labels. $K_2 = 0$ means use the default.
−9, 9	K_3	Number of characters used to indent continuation lines for row labels. K_3 must be between 0 and 10, inclusively.
−10, 10	K_4	Width (in characters) of the hot zone where line breaks in row labels can occur. $K_4 = 0$ means use the default. K_4 must not exceed 50.
−11, 11	K_5	Maximum width (in characters) reserved for column labels. $K_5 = 0$ means use the default.
−12, 12	K_6	Width (in characters) of the hot zone where line breaks in column labels can occur. $K_6 = 0$ means use the default. K_6 must not exceed 50.
−13, 13	K_7	Width (in characters) of the hot zone where line breaks in titles can occur. K_7 must be between 1 and 50, inclusively.
−14	0	There is no label in the upper left hand corner.
	1	The label in the upper left hand corner is “Component” if a row vector or column vector is printed; the label is “Row/Column” if both the number of rows and columns are greater than one; otherwise, there is no label.
−15	0	A blank line is printed on each invocation of a WR**N routine before the matrix title provided a new page is not to be issued.
	1	A blank line is not printed on each invocation of a WR**N routine before the matrix title.
−16, 16	0	The matrix values are aligned vertically with the last line of the associated row label for the case IOPT = 2 and ISET is positive.
	1	The matrix values are aligned vertically with the first line of the associated row label.

ISCOPE — Indicator of the scope of the option. (Input if IOPT is nonzero; not referenced if IOPT = 0)

ISCOPE	Action
0	Setting is temporarily active for the next invocation of a WR*** matrix printing routine.
1	Setting is active until it is changed by another invocation of WROPT.

FORTRAN 90 Interface

Generic: CALL WROPT (IOPT, ISETNG, ISCOPE)

Specific: The specific interface name is WROPT.

FORTRAN 77 Interface

Single: CALL WROPT (IOPT, ISETNG, ISCOPE)

Description

Routine WROPT allows the user to set or retrieve an option for printing a matrix. The options controlled by WROPT include the following: horizontal centering, a method for printing large matrices, paging, method for printing NaN (not a number) and positive and negative machine infinities, printing titles, default formats for numbers, spacing between columns, maximum widths reserved for row and column labels, indentation of row labels that continue beyond one line, widths of hot zones for breaking of labels and titles, the default heading for row labels, whether to print a blank line between invocations of routines, and vertical alignment of matrix entries with respect to row labels continued beyond one line. (NaN and positive and negative machine infinities can be retrieved by AMACH and DMACH that are documented in the section "*Machine-Dependent Constants*" in the Reference Material.) Options can be set globally (ISCOPE = 1) or temporarily for the next call to a printing routine (ISCOPE = 0).

Comments

1. This program can be invoked repeatedly before using a WR*** routine to print a matrix. The matrix printing routines retrieve these settings to determine the printing options. It is not necessary to call WROPT if a default value of a printing option is desired. The defaults are as follows.

IOPT	**Default Value for ISET**	**Meaning**
1	0	Left justified
2	1000000	Number lines before wrapping
3	−2	No paging
4	2	NaN is printed as “NaN,” negative machine infinity is printed as “−Inf” and positive machine infinity is printed as “Inf.”
5	0	Title only on first page.
6	3	Default format is Vn.4.
7	2	2 spaces between columns.
8	0	Maximum row label width MAXRLW = 2 * IPAGEW/3 if matrix has one column; MAXRLW = IPAGEW/4 otherwise.
9	3	3 character indentation of row labels continued beyond one line.
10	0	Width of row label hot zone is MAXRLW/3 characters.
11	0	Maximum column label width MAXCLW = min{max (NW + NW/2, 15), 40} for integer and real matrices, where NW is the field width for the format corresponding to the particular column. MAXCLW = min{max(NW + NW/2, 15), 83} for complex matrices, where NW is the sum of the two field widths for the formats corresponding to the particular column plus 3.
12	0	Width of column label hot zone is MAXCLW/3 characters.
13	10	Width of hot zone for titles is 10 characters.
14	0	There is no label in the upper left hand corner.
15	0	Blank line is printed.
16	0	The matrix values are aligned vertically with the last line of the associated row label.

For IOPT = 8, the default depends on the current value for the page width, IPAGEW (see PGOPT).

2. The V and W formats are special formats that can be used to select a D, E, F, or I format so that the decimal points will be aligned. The V and W formats are specified as *Vn.d* and *Wn.d*. Here, *n* is the field width and *d* is the number of significant digits generally printed. Valid values for *n* are 3, 4, …, 40. Valid values for *d* are 1, 2, …, *n* − 2. While the V format prints trailing zeroes and a trailing decimal point, the W format does not.

Example

The following example illustrates the effect of `WROPT` when printing a 3 × 4 real matrix *A* with `WRRRN` where $a_{ij} = i + j/10$. The first call to `WROPT` sets horizontal printing so that the matrix is first printed horizontally centered on the page. In the next invocation of `WRRRN`, the left-justification option has been set via routine `WROPT` so the matrix is left justified when printed. Finally, because the scope of left justification was only for the next call to a printing routine, the last call to `WRRRN` results in horizontally centered printing.

```
      USE WROPT_INT
      USE WRRRN_INT

      IMPLICIT   NONE
      INTEGER    ITRING, LDA, NCA, NRA
      PARAMETER  (ITRING=0, LDA=10, NCA=4, NRA=3)
!
      INTEGER    I, IOPT, ISCOPE, ISETNG, J
      REAL       A(LDA,NCA)
!
      DO 20  I=1, NRA
         DO 10  J=1, NCA
            A(I,J) = I + J*0.1
   10    CONTINUE
   20 CONTINUE
!                                 Activate centering option.
!                                 Scope is global.
      IOPT   = -1
      ISETNG = 1
      ISCOPE = 1
!
      CALL WROPT (IOPT, ISETNG, ISCOPE)
!                                 Write A matrix.
      CALL WRRRN ('A', A, NRA=NRA)
!                                 Activate left justification.
!                                 Scope is local.
      IOPT   = -1
      ISETNG   = 0
      ISCOPE = 0
      CALL WROPT (IOPT, ISETNG, ISCOPE)
      CALL WRRRN ('A', A, NRA=NRA)
      CALL WRRRN ('A', A, NRA=NRA)
      END
```

Output

```
                                          A
                                1        2        3        4
                        1   1.100    1.200    1.300    1.400
                        2   2.100    2.200    2.300    2.400
                        3   3.100    3.200    3.300    3.400
                 A
       1        2        3        4
1   1.100    1.200    1.300    1.400
2   2.100    2.200    2.300    2.400
3   3.100    3.200    3.300    3.400
                                          A
                                1        2        3        4
                        1   1.100    1.200    1.300    1.400
                        2   2.100    2.200    2.300    2.400
                        3   3.100    3.200    3.300    3.400
```

PGOPT

Sets or retrieves page width and length for printing.

Required Arguments

IOPT — Page attribute option. = (Input)

IOPT	Description of Attribute
−1, 1	Page width.
−2, 2	Page length.

Negative values of IOPT indicate the setting IPAGE is input. Positive values of IOPT indicate the setting IPAGE is output.

IPAGE — Value of page attribute. = (Input, if IOPT is negative; output, if IOPT is positive.)

IOPT	Description of Attribute	Settings for IPAGE
−1, 1	Page width (in characters)	10, 11, …
−2, 2	Page length (in lines) =	10, 11, …

FORTRAN 90 Interface

Generic: CALL PGOPT (IOPT, IPAGE)

Specific: The specific interface name is PGOPT.

FORTRAN 77 Interface

Single: CALL PGOPT (IOPT, IPAGE)

Description

Routine PGOPT is used to set or retrieve the page width or the page length for routines that perform printing.

Example

The following example illustrates the use of PGOPT to set the page width at 20 characters. Routine WRRRN is then used to print a 3 × 4 matrix *A* where $a_{ij} = i + j/10$.

```
      USE PGOPT_INT
```

```
      USE WRRRN_INT

      IMPLICIT   NONE
      INTEGER    ITRING, LDA, NCA, NRA
      PARAMETER  (ITRING=0, LDA=3, NCA=4, NRA=3)
!
      INTEGER    I, IOPT, IPAGE, J
      REAL       A(LDA,NCA)
!
      DO 20  I=1, NRA
         DO 10  J=1, NCA
            A(I,J) = I + J*0.1
   10    CONTINUE
   20 CONTINUE
!                                  Set page width.
      IOPT  = -1
      IPAGE = 20
      CALL PGOPT (IOPT, IPAGE)
!                                  Print the matrix A.
      CALL WRRRN ('A', A)
      END
```

Output

```
          A
         1       2
1   1.100   1.200
2   2.100   2.200
3   3.100   3.200

         3       4
1   1.300   1.400
2   2.300   2.400
3   3.300   3.400
```

PERMU

Rearranges the elements of an array as specified by a permutation.

Required Arguments

X — Real vector of length N containing the array to be permuted. (Input)

IPERMU — Integer vector of length N containing a permutation IPERMU(1), …, IPERMU(N) of the integers 1, …, N. (Input)

XPERMU — Real vector of length N containing the array X permuted. (Output)
If X is not needed, X and XPERMU can share the same storage locations.

Optional Arguments

N — Length of the arrays X and XPERMU. (Input)
Default: N = size (IPERMU,1).

IPATH — Integer flag. (Input)
Default: IPATH = 1.
IPATH = 1 means IPERMU represents a forward permutation, i.e., X(IPERMU(I)) is moved to XPERMU(I). IPATH = 2 means IPERMU represents a backward permutation, i.e., X(I) is moved to XPERMU (IPERMU(I)).

FORTRAN 90 Interface

Generic: CALL PERMU (X, IPERMU, XPERMU [, …])

Specific: The specific interface names are S_PERMU and D_PERMU.

FORTRAN 77 Interface

Single: CALL PERMU (N, X, IPERMU, IPATH, XPERMU)

Double: The double precision name is DPERMU.

Description

Routine PERMU rearranges the elements of an array according to a permutation vector. It has the option to do both forward and backward permutations.

Example

This example rearranges the array *X* using IPERMU; forward permutation is performed.

```
      USE PERMU_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    IPATH, N
      PARAMETER  (IPATH=1, N=4)
!
      INTEGER    IPERMU(N), J, NOUT
      REAL       X(N), XPERMU(N)
!                                 Set values for  X, IPERMU
!
!                           X = ( 5.0  6.0  1.0  4.0 )
!                           IPERMU = ( 3 1 4 2 )
!
      DATA X/5.0, 6.0, 1.0, 4.0/, IPERMU/3, 1, 4, 2/
!                                 Permute X into XPERMU
      CALL PERMU (X, IPERMU, XPERMU)
!                                 Get output unit number
      CALL UMACH (2, NOUT)
!                                 Print results
      WRITE (NOUT,99999) (XPERMU(J),J=1,N)
!
99999 FORMAT ('  The output vector is:', /, 10(1X,F10.2))
      END
```

Output

```
The Output vector is:
1.00       5.00       4.00       6.00
```

PERMA

Permutes the rows or columns of a matrix.

Required Arguments

A — NRA by NCA matrix to be permuted. (Input)

IPERMU — Vector of length K containing a permutation IPERMU(1), …, IPERMU(K) of the integers 1, …, K where K = NRA if the rows of A are to be permuted and K = NCA if the columns of A are to be permuted. (Input)

APER — NRA by NCA matrix containing the permuted matrix. (Output)
If A is not needed, A and APER can share the same storage locations.

Optional Arguments

NRA — Number of rows. (Input)
Default: NRA = size (A,1).

NCA — Number of columns. (Input)
Default: NCA = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

IPATH — Option parameter. (Input)
IPATH = 1 means the rows of A will be permuted. IPATH = 2 means the columns of A will be permuted.
Default: IPATH = 1.

LDAPER — Leading dimension of APER exactly as specified in the dimension statement of the calling program. (Input)
Default: LDAPER = size (APER,1).

FORTRAN 90 Interface

Generic: CALL PERMA (A, IPERMU, APER [, …])

Specific: The specific interface names are S_PERMA and D_PERMA.

FORTRAN 77 Interface

Single: CALL PERMA (NRA, NCA, A, LDA, IPERMU, IPATH, APER, LDAPER)

Double: The double precision name is DPERMA.

Description

Routine PERMA interchanges the rows or columns of a matrix using a permutation vector such as the one obtained from routines SVRBP or SVRGP.

The routine PERMA permutes a column (row) at a time by calling PERMU. This process is continued until all the columns (rows) are permuted. On completion, let B = APER and p_i = IPERMU(I), then

$$B_{ij} = A_{p_i j}$$

for all i, j.

Comments

1. Workspace may be explicitly provided, if desired, by use of P2RMA/DP2RMA. The reference is:

   CALL P2RMA (NRA, NCA, A, LDA, IPERMU, IPATH, APER, LDAPER, WORK)

   The additional argument is:

   WORK — Real work vector of length NCA.

Example

This example permutes the columns of a matrix A.

```
      USE PERMA_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    IPATH, LDA, LDAPER, NCA, NRA
      PARAMETER  (IPATH=2, LDA=3, LDAPER=3, NCA=5, NRA=3)
!
      INTEGER    I, IPERMU(5), J, NOUT

!                                 Set values for  A, IPERMU
!                                 A = ( 3.0  5.0  1.0  2.0  4.0 )
!                                     ( 3.0  5.0  1.0  2.0  4.0 )
!                                     ( 3.0  5.0  1.0  2.0  4.0 )
!
!                                 IPERMU = ( 3 4 1 5 2 )
!
      DATA A/3*3.0, 3*5.0, 3*1.0, 3*2.0, 3*4.0/, IPERMU/3, 4, 1, 5, 2/
!                                 Perform column permutation on A,
!                                 giving APER
```

```
      CALL PERMA (A, IPERMU, APER, IPATH=IPATH)
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Print results
      WRITE (NOUT,99999) ((APER(I,J),J=1,NCA),I=1,NRA)
!
99999 FORMAT ('  The output matrix is:', /, 3(5F8.1,/))
      END
```

Output

```
The Output matrix is:
1.0     2.0     3.0     4.0     5.0
1.0     2.0     3.0     4.0     5.0
1.0     2.0     3.0     4.0     5.0
```

SORT_REAL

Sorts a rank-1 array of real numbers x so the y results are algebraically nondecreasing, $y_1 \le y_2 \le \ldots y_n$.

Required Arguments

X — Rank-1 array containing the numbers to be sorted. (Output)

Y — Rank-1 array containing the sorted numbers. (Output)

Optional Arguments

nsize = `n` (Input)
Uses the sub-array of size `n` for the numbers.
Default value: `n` = `size`(`x`)

iperm = `iperm` (Input/Output)
Applies interchanges of elements that occur to the entries of `iperm(:)`. If the values `iperm(i)=i,i=1,n` are assigned prior to call, then the output array is moved to its proper order by the subscripted array assignment `y = x(iperm(1:n))`.

icycle = `icycle` (Output)
Permutations applied to the input data are converted to cyclic interchanges. Thus, the output array `y` is given by the following elementary interchanges, where `:=:` denotes a swap:

j = icycle(i)
y(j) :=: y(i), i = 1,n

iopt = `iopt(:)` (Input)
Derived type array with the same precision as the input matrix; used for passing optional data to the routine. The options are as follows:

Packaged Options for SORT_REAL		
Option Prefix = ?	Option Name	Option Value
s_, d_	`Sort_real_scan_for_NaN`	1

`iopt(IO) = ?_options(?_sort_real_scan_for_NaN, ?_dummy)`
Examines each input array entry to find the first value such that `isNaN(x(i)) == .true.`

See the `isNaN()` function, *Chapter 10*.
Default: Does not scan for NaNs.

FORTRAN 90 Interface

Generic: `CALL SORT_REAL (X, Y [, …])`

Specific: The specific interface names are `S_SORT_REAL` and `D_SORT_REAL`.

Description

For a detailed description, see the "*Description*" section of routine `SVRGN`, which appears later in this chapter.

Fatal and Terminal Error Messages

See the *messages.gls* file for error messages for `SORT_REAL`. These error messages are numbered 561–567; 581–587.

Examples

Example 1: Sorting an Array

An array of random numbers is obtained. The values are sorted so they are nondecreasing.

```
      use sort_real_int
      use rand_gen_int

      implicit none

! This is Example 1 for SORT_REAL.

      integer, parameter :: n=100
      real(kind(1e0)), dimension(n) :: x, y

! Generate random data to sort.
      call rand_gen(x)

! Sort the data so it is non-decreasing.
      call sort_real(x, y)

! Check that the sorted array is not decreasing.
      if (count(y(1:n-1) > y(2:n)) == 0) then
         write (*,*) 'Example 1 for SORT_REAL is correct.'
      end if

      end
```

Output

```
Example 1 for SORT_REAL is correct.
```

Example 2: Sort and Final Move with a Permutation

A set of n random numbers is sorted so the results are nonincreasing. The columns of an $n \times n$ random matrix are moved to the order given by the permutation defined by the interchange of the entries. Since the routine sorts the results to be algebraically nondecreasing, the array of negative values is used as input. Thus, the negative value of the sorted output order is nonincreasing. The optional argument “`iperm=`” records the final order and is used to move the matrix columns to that order. This example illustrates the principle of sorting record *keys*, followed by direct movement of the records to sorted order.

```
      use sort_real_int
      use rand_gen_int

      implicit none

! This is Example 2 for SORT_REAL.

      integer i
      integer, parameter :: n=100
      integer ip(n)
      real(kind(1e0)) a(n,n), x(n), y(n), temp(n*n)

! Generate a random array and matrix of values.
      call rand_gen(x)
      call rand_gen(temp)
      a = reshape(temp,(/n,n/))

! Initialize permutation to the identity.
      do i=1, n
         ip(i) = i
      end do

! Sort using negative values so the final order is
! non-increasing.
      call sort_real(-x, y, iperm=ip)

! Final movement of keys and matrix columns.
      y = x(ip(1:n))
      a = a(:,ip(1:n))

! Check the results.
      if (count(y(1:n-1) < y(2:n)) == 0) then
         write (*,*) 'Example 2 for SORT_REAL is correct.'
      end if

      end
```

Output

```
Example 2 for SORT_REAL is correct.
```

SVRGN

Sorts a real array by algebraically increasing value.

Required Arguments

RA — Vector of length N containing the array to be sorted. (Input)

RB — Vector of length N containing the sorted array. (Output)
If RA is not needed, RA and RB can share the same storage locations.

Optional Arguments

N — Number of elements in the array to be sorted. (Input)
Default: N = size (RA,1).

FORTRAN 90 Interface

Generic: CALL SVRGN (RA, RB [, …])

Specific:The specific interface names are S_SVRGN and D_SVRGN.

FORTRAN 77 Interface

Single: CALL SVRGN (N, RA, RB)

Double: The double precision name is DSVRGN.

Description

Routine SVRGN sorts the elements of an array, A, into ascending order by algebraic value. The array A is divided into two parts by picking a central element T of the array. The first and last elements of A are compared with T and exchanged until the three values appear in the array in ascending order. The elements of the array are rearranged until all elements greater than or equal to the central element appear in the second part of the array and all those less than or equal to the central element appear in the first part. The upper and lower subscripts of one of the segments are saved, and the process continues iteratively on the other segment. When one segment is finally sorted, the process begins again by retrieving the subscripts of another unsorted portion of the array. On completion, $A_j \le A_i$ for $j < i$. For more details, see Singleton (1969), Griffin and Redish (1970), and Petro (1970).

Example

This example sorts the 10-element array RA algebraically.

```
      USE SVRGN_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                  Declare variables
      INTEGER    N, NOUT, J
      PARAMETER  (N=10)
      REAL       RA(N), RB(N)
!                                  Set values for  RA
!     RA = ( -1.0  2.0  -3.0  4.0  -5.0  6.0  -7.0  8.0  -9.0  10.0 )
!
      DATA RA/-1.0, 2.0, -3.0, 4.0, -5.0, 6.0, -7.0, 8.0, -9.0, 10.0/
!                                  Sort RA by algebraic value into RB
      CALL SVRGN (RA, RB)
!                                  Print results
      CALL UMACH (2,NOUT)
      WRITE (NOUT, 99999) (RB(J),J=1,N)
!
99999 FORMAT ('  The output vector is:', /, 10(1X,F5.1))
      END
```

Output

```
The Output vector is:
-9.0  -7.0  -5.0  -3.0  -1.0   2.0   4.0   6.0   8.0  10.0
```

SVRGP

Sorts a real array by algebraically increasing value and return the permutation that rearranges the array.

Required Arguments

RA — Vector of length N containing the array to be sorted. (Input)

RB — Vector of length N containing the sorted array. (Output)
If RA is not needed, RA and RB can share the same storage locations.

IPERM — Vector of length N. (Input/Output)
On input, IPERM should be initialized to the values 1, 2, …, N. On output, IPERM contains a record of permutations made on the vector RA.

Optional Arguments

N — Number of elements in the array to be sorted. (Input)
Default: N = size (IPERM,1).

FORTRAN 90 Interface

Generic: CALL SVRGP (RA, RB, IPERM [, …])

Specific: The specific interface names are S_SVRGP and D_SVRGP.

FORTRAN 77 Interface

Single: CALL SVRGP (N, RA, RB, IPERM)

Double: The double precision name is DSVRGP.

Description

Routine SVRGP sorts the elements of an array, A, into ascending order by algebraic value, keeping a record in P of the permutations to the array A. That is, the elements of P are moved in the same manner as are the elements in A as A is being sorted. The routine SVRGP uses the algorithm discussed in SVRGN. On completion, $A_j \le A_i$ for $j < i$.

Comments

1. For wider applicability, integers (1, 2, ..., N) that are to be associated with RA(I) for I = 1, 2, …, N may be entered into IPERM(I) in any order. Note that these integers must be unique.

Example

This example sorts the 10-element array RA algebraically.

```
      USE SVRGP_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER    N, NOUT, J
      PARAMETER  (N=10)
      REAL       RA(N), RB(N)
      INTEGER    IPERM(N)
!                                 Set values for  RA and IPERM
!     RA    = ( 10.0  -9.0  8.0  -7.0  6.0  5.0  4.0  -3.0  -2.0  -1.0 )
!
!     IPERM = ( 1  2  3  4  5  6  7  8  9  10)
!
      DATA RA/10.0, -9.0, 8.0, -7.0, 6.0, 5.0, 4.0, -3.0, -2.0, -1.0/
      DATA IPERM/1, 2, 3, 4, 5, 6, 7, 8, 9, 10/
!                                 Sort RA by algebraic value into RB
      CALL SVRGP (RA, RB, IPERM)
!                                 Print results
      CALL UMACH (2,NOUT)
      WRITE (NOUT, 99998) (RB(J),J=1,N)
      WRITE (NOUT, 99999) (IPERM(J),J=1,N)
!
99998 FORMAT ('  The output vector is:', /, 10(1X,F5.1))
99999 FORMAT ('  The permutation vector is:', /, 10(1X,I5))
      END
```

Output

```
The output vector is:
-9.0  -7.0  -3.0  -2.0  -1.0   4.0   5.0   6.0   8.0  10.0

The permutation vector is:
2     4     8     9    10     7     6     5     3     1
```

SVIGN

Sorts an integer array by algebraically increasing value.

Required Arguments

IA — Integer vector of length N containing the array to be sorted. (Input)

IB — Integer vector of length N containing the sorted array. (Output)
If IA is not needed, IA and IB can share the same storage locations.

Optional Arguments

N — Number of elements in the array to be sorted. (Input)
Default: N = size (IA,1).

FORTRAN 90 Interface

Generic: CALL SVIGN (IA, IB [, …])

Specific: The specific interface name is S_SVIGN .

FORTRAN 77 Interface

Single: CALL SVIGN (N, IA, IB)

Description

Routine SVIGN sorts the elements of an integer array, *A*, into ascending order by algebraic value. The routine SVIGN uses the algorithm discussed in SVRGN. On completion, $A_j \leq A_i$ for $j < i$.

Example

This example sorts the 10-element array IA algebraically.

```
      USE SVIGN_INT
      USE UMACH_INT

      IMPLICIT   NONE
```

```
!                                  Declare variables
      INTEGER    N, NOUT, J
      PARAMETER  (N=10)
      INTEGER    IA(N), IB(N)
!                                  Set values for  IA
!     IA = ( -1  2  -3  4  -5  6  -7  8  -9  10 )
!
      DATA IA/-1, 2, -3, 4, -5, 6, -7, 8, -9, 10/
!                                  Sort IA by algebraic value into IB
      CALL SVIGN (IA, IB)
!                                  Print results
      CALL UMACH (2,NOUT)
      WRITE (NOUT, 99999) (IB(J),J=1,N)
!
99999 FORMAT ('  The output vector is:', /, 10(1X,I5))
      END
```

Output

```
The Output vector is:
-9    -7    -5    -3    -1     2     4     6     8    10
```

SVIGP

Sorts an integer array by algebraically increasing value and return the permutation that rearranges the array.

Required Arguments

IA — Integer vector of length `N` containing the array to be sorted. (Input)

IB — Integer vector of length `N` containing the sorted array. (Output)
If `IA` is not needed, `IA` and `IB` can share the same storage locations.

IPERM — Vector of length `N`. (Input/Output)
On input, `IPERM` should be initialized to the values 1, 2, …, `N`. On output, `IPERM` contains a record of permutations made on the vector `IA`.

Optional Arguments

N — Number of elements in the array to be sorted. (Input)
Default: `N` = `size` (`IPERM`,1).

FORTRAN 90 Interface

Generic: `CALL SVIGP (IA, IB, IPERM [, …])`

Specific: The specific interface name is `S_SVIGP`.

FORTRAN 77 Interface

Single: `CALL SVIGP (N, IA, IB, IPERM)`

Description

Routine `SVIGP` sorts the elements of an integer array, *A*, into ascending order by algebraic value, keeping a record in *P* of the permutations to the array *A*. That is, the elements of *P* are moved in the same manner as are the elements in *A* as *A* is being sorted. The routine `SVIGP` uses the algorithm discussed in `SVRGN`. On completion, $A_j \le A_i$ for $j < i$.

Comments

1. For wider applicability, integers (1, 2, …, `N`) that are to be associated with `IA(I)` for `I` = 1, 2, …, `N` may be entered into `IPERM(I)` in any order. Note that these integers must be unique.

Example

This example sorts the 10-element array `IA` algebraically.

```
      USE SVIGP_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER N, J, NOUT
      PARAMETER  (N=10)
      INTEGER    IA(N), IB(N), IPERM(N)
!                                 Set values for  IA and IPERM
!     IA    = ( 10  -9  8  -7  6  5  4  -3  -2  -1 )
!
!     IPERM = ( 1, 2, 3, 4, 5, 6, 7, 8, 9, 10 )
!
      DATA IA/10, -9, 8, -7, 6, 5, 4, -3, -2, -1/
      DATA IPERM/1, 2, 3, 4, 5, 6, 7, 8, 9, 10/
!                                 Sort IA by algebraic value into IB
      CALL SVIGP (IA, IB, IPERM)
!                                 Print results
      CALL UMACH (2,NOUT)
      WRITE (NOUT, 99998) (IB(J),J=1,N)
      WRITE (NOUT, 99999) (IPERM(J),J=1,N)
!
99998 FORMAT (' The output vector is:', /, 10(1X,I5))
99999 FORMAT (' The permutation vector is:', /, 10(1X,I5))
      END
```

Output

```
The Output vector is:
-9     -7     -3     -2     -1      4      5      6      8     10

The permutation vector is:
2      4      8      9     10      7      6      5      3      1
```

SVRBN

Sorts a real array by nondecreasing absolute value.

Required Arguments

RA — Vector of length N containing the array to be sorted. (Input)

RB — Vector of length N containing the sorted array. (Output)
If RA is not needed, RA and RB can share the same storage locations.

Optional Arguments

N — Number of elements in the array to be sorted. (Input)
Default: N = size (RA,1).

FORTRAN 90 Interface

Generic: CALL SVRBN (RA, RB [, …])

Specific: The specific interface names are S_SVRBN and D_SVRBN.

FORTRAN 77 Interface

Single: CALL SVRBN (N, RA, RB)

Double: The double precision name is DSVRBN.

Description

Routine SVRBN sorts the elements of an array, A, into ascending order by absolute value. The routine SVRBN uses the algorithm discussed in SVRGN. On completion, $|A_j| \le |A_i|$ for $j < i$.

Example

This example sorts the 10-element array RA by absolute value.

```
USE SVRBN_INT
USE UMACH_INT
```

```
      IMPLICIT   NONE
!                                  Declare variables
      INTEGER N, J, NOUT
      PARAMETER  (N=10)
      REAL       RA(N), RB(N)
!                                  Set values for  RA
!        RA = ( -1.0  3.0  -4.0  2.0  -1.0  0.0  -7.0  6.0  10.0  -7.0 )
!
      DATA RA/-1.0, 3.0, -4.0, 2.0, -1.0, 0.0, -7.0, 6.0, 10.0, -7.0/
!                                  Sort RA by absolute value into RB
      CALL SVRBN (RA, RB)
!                                  Print results
      CALL UMACH (2,NOUT)
      WRITE (NOUT, 99999) (RB(J),J=1,N)
!
99999 FORMAT ('  The output vector is :', /, 10(1X,F5.1))
      END
```

Output

```
The Output vector is :
0.0  -1.0  -1.0   2.0   3.0  -4.0   6.0  -7.0  -7.0  10.0
```

SVRBP

Sorts a real array by nondecreasing absolute value and return the permutation that rearranges the array.

Required Arguments

RA — Vector of length N containing the array to be sorted. (Input)

RB — Vector of length N containing the sorted array. (Output)
If RA is not needed, RA and RB can share the same storage locations.

IPERM — Vector of length N. (Input/Output)
On input, IPERM should be initialized to the values 1, 2, …, N. On output, IPERM contains a record of permutations made on the vector IA.

Optional Arguments

N — Number of elements in the array to be sorted. (Input)
Default: N = size (IPERM,1).

FORTRAN 90 Interface

Generic: CALL SVRBP (RA, RB, IPERM [, …])

Specific: The specific interface names are S_SVRBP and D_SVRBP.

FORTRAN 77 Interface

Single: CALL SVRBP (N, RA, RB, IPERM)

Double: The double precision name is DSVRBP.

Description

Routine SVRBP sorts the elements of an array, A, into ascending order by absolute value, keeping a record in P of the permutations to the array A. That is, the elements of P are moved in the same manner as are the elements in A as A is being sorted. The routine SVRBP uses the algorithm discussed in SVRGN. On completion, $A_j \le A_i$ for $j < i$.

Comments

1. For wider applicability, integers (1, 2, …, N) that are to be associated with RA(I) for I = 1, 2, …, N may be entered into IPERM(I) in any order. Note that these integers must be unique.

Example

This example sorts the 10-element array RA by absolute value.

```
      USE SVRBP_INT
      USE UMACH_INT

      IMPLICIT   NONE
!                                 Declare variables
      INTEGER N, J, NOUT, I
      PARAMETER  (N=10)
      REAL       RA(N), RB(N)
      INTEGER    IPERM(N)
!                                 Set values for  RA and IPERM
!     RA     = ( 10.0  9.0  8.0  7.0  6.0  5.0  -4.0  3.0  -2.0  1.0 )
!
!     IPERM = ( 1  2  3  4  5  6  7  8  9  10 )
!
      DATA RA/10.0, 9.0, 8.0, 7.0, 6.0, 5.0, -4.0, 3.0, -2.0, 1.0/
      DATA IPERM/1, 2, 3, 4, 5, 6, 7, 8, 9, 10/
!                                 Sort RA by absolute value into RB
      CALL SVRBP (RA, RB, IPERM)
!                                 Print results
      CALL UMACH (2,NOUT)
      WRITE (NOUT, 99998) (RB(J),J=1,N)
      WRITE (NOUT, 99999) (IPERM(I),I=1,N)
!
99998 FORMAT ('  The output vector is:', /, 10(1X,F5.1))
99999 FORMAT ('  The permutation vector is:', /, 10(1X,I5))
      END
```

Output

```
The output vector is:
1.0  -2.0   3.0  -4.0   5.0   6.0   7.0   8.0   9.0  10.0
The permutation vector is:
10     9     8     7     6     5     4     3     2     1
```

SVIBN

Sorts an integer array by nondecreasing absolute value.

Required Arguments

IA — Integer vector of length `N` containing the array to be sorted. (Input)

IB — Integer vector of length `N` containing the sorted array. (Output)
If `IA` is not needed, `IA` and `IB` can share the same storage locations.

Optional Arguments

N — Number of elements in the array to be sorted. (Input)
Default: `N` = `size` (`IA`,1).

FORTRAN 90 Interface

Generic: `CALL SVIBN (IA, IB [, …])`

Specific: The specific interface name is `S_SVIBN`.

FORTRAN 77 Interface

Single: `CALL SVIBN (N, IA, IB)`

Description

Routine `SVIBN` sorts the elements of an integer array, A, into ascending order by absolute value. This routine `SVIBN` uses the algorithm discussed in `SVRGN`. `On completion`, $A_j \le A_i$ for $j < i$.

Example

This example sorts the 10-element array `IA` by absolute value.

```
      USE SVIBN_INT
      USE UMACH_INT

      IMPLICIT   NONE
```

```
!                                  Declare variables
      INTEGER I, J, NOUT, N


!                                  Set values for  IA
!     IA = ( -1  3  -4  2  -1  0  -7  6  10  -7)
!
      DATA IA/-1, 3, -4, 2, -1, 0, -7, 6, 10, -7/
!                                  Sort IA by absolute value into IB
      CALL SVIBN (IA, IB)
!                                  Print results
      CALL UMACH (2,NOUT)
      WRITE (NOUT, 99999) (IB(J),J=1,N)
!
99999 FORMAT ('  The output vector is:', /, 10(1X,I5))
      END
```

Output

```
The Output vector is:
0    -1    -1     2     3    -4     6    -7    -7    10
```

SVIBP

Sorts an integer array by nondecreasing absolute value and return the permutation that rearranges the array.

Required Arguments

IA — Integer vector of length `N` containing the array to be sorted. (Input)

IB — Integer vector of length `N` containing the sorted array. (Output)
If `IA` is not needed, `IA` and `IB` can share the same storage locations.

IPERM — Vector of length `N`. (Input/Output)
On input, `IPERM` should be initialized to the values 1, 2, …, `N`. On output, `IPERM` contains a record of permutations made on the vector `IA`.

Optional Arguments

N — Number of elements in the array to be sorted. (Input)
Default: `N` = `size` (`IA`,1).

FORTRAN 90 Interface

Generic: `CALL SVIBP (IA, IB, IPERM [, …])`

Specific: The specific interface name is `S_SVIBP`.

FORTRAN 77 Interface

Single: `CALL SVIBP (N, IA, IB, IPERM)`

Description

Routine `SVIBP` sorts the elements of an integer array, A, into ascending order by absolute value, keeping a record in P of the permutations to the array A. That is, the elements of P are moved in the same manner as are the elements in A as A is being sorted. The routine `SVIBP` uses the algorithm discussed in `SVRGN`. On completion, $A_j \le A_i$ for $j < i$.

Comments

1. For wider applicability, integers (1, 2, …, N) that are to be associated with IA(I) for I = 1, 2, …, N may be entered into IPERM(I) in any order. Note that these integers must be unique.

Example

This example sorts the 10-element array IA by absolute value.

```
      USE SVIBP_INT
      USE UMACH_INT



PARAMETER  (N=10)
      INTEGER    IA(N), IB(N), IPERM(N)
!                                Set values for  IA
!     IA    = ( 10  9  8  7  6  5  -4  3  -2  1 )
!
!     IPERM = ( 1  2  3  4  5  6  7  8  9  10 )
!
      DATA IA/10, 9, 8, 7, 6, 5, -4, 3, -2, 1/
      DATA IPERM/1, 2, 3, 4, 5, 6, 7, 8, 9, 10/
!                                Sort IA by absolute value into IB
      CALL SVIBP (IA, IB, IPERM)
!                                Print results
      CALL UMACH (2,NOUT)
      WRITE (NOUT, 99998) (IB(J),J=1,N)
      WRITE (NOUT, 99999) (IPERM(J),J=1,N)
!
99998 FORMAT ('  The output vector is:', /, 10(1X,I5))
99999 FORMAT ('  The permutation vector is:', /, 10(1X,I5))
      END
```

Output

```
The Output vector is:
1    -2     3    -4     5     6     7     8     9    10

The permutation vector is:
10     9     8     7     6     5     4     3     2     1
```

SRCH

Searches a sorted vector for a given scalar and return its index.

Required Arguments

VALUE — Scalar to be searched for in Y. (Input)

X — Vector of length N * INCX. (Input)
Y is obtained from X for I = 1, 2, …, N by Y(I) = X(1 + (I − 1) * INCX). Y(1), Y(2), …, Y(N) must be in ascending order.

INDEX — Index of Y pointing to VALUE. (Output)
If INDEX is positive, VALUE is found in Y. If INDEX is negative, VALUE is not found in Y.

INDEX	Location of VALUE
1 thru N	VALUE = Y(INDEX)
−1	VALUE < Y(1) or N = 0
−N thru −2	Y(−INDEX −1) < VALUE < Y(−INDEX)
−(N + 1)	VALUE > Y(N)

Optional Arguments

N — Length of vector Y. (Input)
Default: N = (size (X,1)) / INCX.

INCX — Displacement between elements of X. (Input)
INCX must be greater than zero.
Default: INCX = 1.

FORTRAN 90 Interface

Generic: CALL SRCH (VALUE, X, INDEX [, …])

Specific: The specific interface names are S_SRCH and D_SRCH.

FORTRAN 77 Interface

Single: CALL SRCH (N, VALUE, X, INCX, INDEX)

Double: The double precision name is DSRCH.

Description

Routine SRCH searches a real vector x (stored in X), whose n elements are sorted in ascending order for a real number c (stored in VALUE). If c is found in x, its index i (stored in INDEX) is returned so that $x_i = c$. Otherwise, a negative number i is returned for the index. Specifically,

if $1 \le i \le n$	then $x_i = c$
if $i = -1$	then $c < x_1$ or $n = 0$
if $-n \le I \le -2$	then $x_{-i-1} < c < x_{-i}$
if $i = -(n + 1)$	then $c > x_n$

The argument INCX is useful if a row of a matrix, for example, row number I of a matrix X, must be searched. The elements of row I are assumed to be in ascending order. In this case, set INCX equal to the leading dimension of X exactly as specified in the dimension statement in the calling program. With X declared

REAL X(LDX,N)

the invocation

CALL SRCH (N, VALUE, X(I,1), LDX, INDEX)

returns an index that will reference a column number of X.

Routine SRCH performs a binary search. The routine is an implementation of algorithm *B* discussed by Knuth (1973, pages 407−411).

Example

This example searches a real vector sorted in ascending order for the value 653.0. The problem is discussed by Knuth (1973, pages 407−409).

```
      USE SRCH_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    N
      PARAMETER  (N=16)
!
      INTEGER    INDEX, NOUT
```

```
      REAL       VALUE, X(N)
!
      DATA X/61.0, 87.0, 154.0, 170.0, 275.0, 426.0, 503.0, 509.0, &
          512.0, 612.0, 653.0, 677.0, 703.0, 765.0, 897.0, 908.0/
!
      VALUE = 653.0
      CALL SRCH (VALUE, X, INDEX)
!
      CALL UMACH (2, NOUT)
      WRITE (NOUT,*) 'INDEX = ', INDEX
      END
```

Output

```
INDEX =   11
```

ISRCH

Searches a sorted integer vector for a given integer and return its index.

Required Arguments

IVALUE — Scalar to be searched for in IY. (Input)

IX — Vector of length N * INCX. (Input)
IY is obtained from IX for I = 1, 2, ..., N by IY(I) = IX(1 + (I − 1) * INCX). IY(1), IY(2), ..., IY(N) must be in ascending order.

INDEX — Index of IY pointing to IVALUE. (Output)
If INDEX is positive, IVALUE is found in IY. If INDEX is negative, IVALUE is not found in IY.

INDEX	Location of IVALUE
1 thru N	IVALUE = IY(INDEX)
−1	IVALUE < IY(1) or N = 0
−N thru −2	IY(−INDEX −1) < IVALUE < IY(−INDEX)
−(N + 1)	IVALUE > Y(N)

Optional Arguments

N — Length of vector IY. (Input)
Default: N = size (IX,1) / INCX.

INCX — Displacement between elements of IX. (Input)
INCX must be greater than zero.
Default: INCX = 1.

FORTRAN 90 Interface

Generic: CALL ISRCH (IVALUE, IX, INDEX [, …])

Specific: The specific interface name is S_ISRCH.

FORTRAN 77 Interface

Single: CALL ISRCH (N, IVALUE, IX, INCX, INDEX)

Description

Routine ISRCH searches an integer vector x (stored in IX), whose n elements are sorted in ascending order for an integer c (stored in IVALUE). If c is found in x, its index i (stored in INDEX) is returned so that $x_i = c$. Otherwise, a negative number i is returned for the index. Specifically,

if $1 \le i \le n$	Then $x_i = c$
if $i = -1$	Then $c < x_1$ or $n = 0$
if $-n \le i \le -2$	Then $x_{-i-1} < c < x_{-i}$
if $i = -(n + 1)$	Then $c > x_n$

The argument INCX is useful if a row of a matrix, for example, row number I of a matrix IX, must be searched. The elements of row I are assumed to be in ascending order. Here, set INCX equal to the leading dimension of IX exactly as specified in the dimension statement in the calling program. With IX declared

INTEGER IX(LDIX,N)

the invocation

CALL ISRCH (N, IVALUE, IX(I,1), LDIX, INDEX)

returns an index that will reference a column number of IX.

The routine ISRCH performs a binary search. The routine is an implementation of algorithm *B* discussed by Knuth (1973, pages 407−411).

Example

This example searches an integer vector sorted in ascending order for the value 653. The problem is discussed by Knuth (1973, pages 407−409).

```
      USE ISRCH_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    N
      PARAMETER  (N=16)
!
      INTEGER    INDEX, NOUT
      INTEGER    IVALUE, IX(N)
!
```

```
      DATA IX/61, 87, 154, 170, 275, 426, 503, 509, 512, 612, 653, 677, &
             703, 765, 897, 908/
!
      IVALUE = 653
      CALL ISRCH (IVALUE, IX, INDEX)
!
      CALL UMACH (2, NOUT)
      WRITE (NOUT,*) 'INDEX = ', INDEX
      END
```

Output

```
INDEX =   11
```

SSRCH

Searches a character vector, sorted in ascending ASCII order, for a given string and return its index.

Required Arguments

N — Length of vector CHY. (Input)
Default: N = size (CHX,1) / INCX.

STRING — Character string to be searched for in CHY. (Input)

CHX — Vector of length N * INCX containing character strings. (Input)
CHY is obtained from CHX for I = 1, 2, …, N by CHY(I) = CHX(1 + (I − 1) * INCX).
CHY(1), CHY(2), …, CHY(N) must be in ascending ASCII order.

INCX — Displacement between elements of CHX. (Input)
INCX must be greater than zero.
Default: INCX = 1.

INDEX — Index of CHY pointing to STRING. (Output)
If INDEX is positive, STRING is found in CHY. If INDEX is negative, STRING is not found in CHY.

INDEX	**Location of STRING**
1 thru N	STRING = CHY(INDEX)
−1	STRING < CHY(1) or N = 0
−N thru −2	CHY(−INDEX − 1) < STRING < CHY(−INDEX)
−(N + 1)	STRING > CHY(N)

FORTRAN 90 Interface

Generic: CALL SSRCH (N, STRING, CHX, INCX, INDEX)

Specific: The specific interface name is SSRCH.

FORTRAN 77 Interface

Single: CALL SSRCH (N, STRING, CHX, INCX, INDEX)

Description

Routine `SSRCH` searches a vector of character strings *x* (stored in `CHX`), whose *n* elements are sorted in ascending ASCII order, for a character string *c* (stored in `STRING`). If *c* is found in *x*, its index *i* (stored in `INDEX`) is returned so that $x_i = c$. Otherwise, a negative number *i* is returned for the index.

Specifically,

if $1 \le i \le n$	Then $x_i = c$
if $i = -1$	Then $c < x_1$ or $n = 0$
if $-n \le i \le -2$	Then $x_{-i-1} < c < x_{-i}$
if $i = -(n + 1)$	Then $c > x_n$

Here, "<" and ">" are in reference to the ASCII collating sequence. For comparisons made between character strings *c* and x_i with different lengths, the shorter string is considered as if it were extended on the right with blanks to the length of the longer string. (`SSRCH` uses FORTRAN intrinsic functions `LLT` and `LGT`.)

The argument `INCX` is useful if a row of a matrix, for example, row number `I` of a matrix `CHX`, must be searched. The elements of row `I` are assumed to be in ascending ASCII order. In this case, set `INCX` equal to the leading dimension of `CHX` exactly as specified in the dimension statement in the calling program. With `CHX` declared

`CHARACTER * 7 CHX(LDCHX,N)`

the invocation

`CALL SSRCH(N, STRING, CHX(I,1), LDCHX, INDEX)`

returns an index that will reference a column number of `CHX`.

The routine `SSRCH` performs a binary search. The routine is an implementation of algorithm *B* discussed by Knuth (1973, pages 407−411).

Example

This example searches a `CHARACTER * 2` vector containing 9 character strings, sorted in ascending ASCII order, for the value `'CC'`.

```
      USE SSRCH_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    N, INCX
      PARAMETER  (N=9)
```

```
!
      INTEGER    INDEX, NOUT
      CHARACTER  CHX(N)*2, STRING*2
!
      DATA CHX/'AA', 'BB', 'CC', 'DD', 'EE', 'FF', 'GG', 'HH', &
          'II'/
!
      INCX   = 1
      STRING = 'CC'
      CALL SSRCH (N, STRING, CHX, INCX, INDEX)
!
      CALL UMACH (2, NOUT)
      WRITE (NOUT,*) 'INDEX = ', INDEX
      END
```

Output

```
INDEX =   3
```

ACHAR

This function returns a character given its ASCII value.

Function Return Value

ACHAR — CHARACTER * 1 string containing the character in the I-th position of the ASCII collating sequence. (Output)

Required Arguments

I — Integer ASCII value of the character desired. (Input)
I must be greater than or equal to zero and less than or equal to 127.

FORTRAN 90 Interface

Generic: ACHAR (I)

Specific: The specific interface name is ACHAR.

FORTRAN 77 Interface

Single: ACHAR (I)

Description

Routine ACHAR returns the character of the input ASCII value. The input value should be between 0 and 127. If the input value is out of range, the value returned in ACHAR is machine dependent.

Example

This example returns the character of the ASCII value 65.

```
      USE ACHAR_INT
      USE UMACH_INT

!     IMPLICIT   NONE
      INTEGER    I, NOUT
!
      CALL UMACH (2, NOUT)
```

```
!                                  Get character for ASCII value
!                                  of 65 ('A')
      I = 65
      WRITE (NOUT,99999) I, ACHAR(I)
!
99999 FORMAT (' For the ASCII value of ', I2, ', the character is : ', &
            A1)
      END
```

Output

```
For the ASCII value of 65, the character is : A
```

IACHAR

This function returns the integer ASCII value of a character argument.

Function Return Value

IACHAR — Integer ASCII value for `CH`. (Output)
The character `CH` is in the `IACHAR`-th position of the ASCII collating sequence.

Required Arguments

CH — Character argument for which the integer ASCII value is desired. (Input)

FORTRAN 90 Interface

Generic: `IACHAR (CH)`

Specific: The specific interface name is `IACHAR`.

FORTRAN 77 Interface

Single: `IACHAR (CH)`

Description

Routine `IACHAR` returns the ASCII value of the input character.

Example

This example gives the ASCII value of character A.

```
      USE IACHAR_INT

      IMPLICIT   NONE
      INTEGER    NOUT
      CHARACTER  CH
!
      CALL UMACH (2, NOUT)
!                                 Get ASCII value for the character
!                                 'A'.
      CH = 'A'
      WRITE (NOUT,99999) CH, IACHAR(CH)
```

```
!
99999 FORMAT (' For the character  ', A1, '  the ASCII value is : ', &
            I3)
      END
```

Output

```
For the character  A  the ASCII value is :  65
```

ICASE

This function returns the ASCII value of a character converted to uppercase.

Function Return Value

ICASE — Integer ASCII value for CH without regard to the case of CH. (Output)
Routine ICASE returns the same value as IACHAR for all but lowercase letters. For these, it returns the IACHAR value for the corresponding uppercase letter.

Required Arguments

CH — Character to be converted. (Input)

FORTRAN 90 Interface

Generic: ICASE (CH)

Specific: The specific interface name is ICASE.

FORTRAN 77 Interface

Single: ICASE (CH)

Description

Routine ICASE converts a character to its integer ASCII value. The conversion is case insensitive; that is, it returns the ASCII value of the corresponding uppercase letter for a lowercase letter.

Example

This example shows the case insensitive conversion.

```
      USE ICASE_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    NOUT
      CHARACTER  CHR
!                                  Get output unit number
```

```
      CALL UMACH (2, NOUT)
!                                Get ASCII value for the character
!                                'a'.
      CHR = 'a'
      WRITE (NOUT,99999) CHR, ICASE(CHR)
!
99999 FORMAT (' For the character  ', A1, '  the ICASE value is : ', &
            I3)
      END
```

Output

```
For the character  a  the ICASE value is :  65
```

IICSR

This function compares two character strings using the ASCII collating sequence but without regard to case.

Function Return Value

IICSR — Comparison indicator. (Output)

Let `USTR1` and `USTR2` be the uppercase versions of `STR1` and `STR2`, respectively. The following table indicates the relationship between `USTR1` and `USTR2` as determined by the ASCII collating sequence.

IICSR	Meaning
−1	USTR1 precedes USTR2
0	USTR1 equals USTR2
1	USTR1 follows USTR2

Required Arguments

STR1 — First character string. (Input)

STR2 — Second character string. (Input)

FORTRAN 90 Interface

Generic: `IICSR (STR1, STR2)`

Specific: The specific interface name is `IICSR`.

FORTRAN 77 Interface

Single: `IICSR (STR1, STR2)`

Description

Routine `IICSR` compares two character strings. It returns −1 if the first string is less than the second string, 0 if they are equal, and 1 if the first string is greater than the second string. The comparison is case insensitive.

Comments

1. If the two strings, `STR1` and `STR2`, are of unequal length, the shorter string is considered as if it were extended with blanks to the length of the longer string.

Example

This example shows different cases on comparing two strings.

```
      USE IICSR_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    NOUT
      CHARACTER  STR1*6, STR2*6
!                                 Get output unit number
      CALL UMACH (2, NOUT)
!                                 Compare String1 and String2
!                                 String1 is 'bigger' than String2
      STR1 = 'ABc 1'
      STR2 = ' '
      WRITE (NOUT,99999) STR1, STR2, IICSR(STR1,STR2)
!
!                                 String1 is 'equal' to String2
      STR1 = 'AbC'
      STR2 = 'ABc'
      WRITE (NOUT,99999) STR1, STR2, IICSR(STR1,STR2)
!
!                                 String1 is 'smaller' than String2
      STR1 = 'ABc'
      STR2 = 'aBC 1'
      WRITE (NOUT,99999) STR1, STR2, IICSR(STR1,STR2)
!
99999 FORMAT (' For String1 = ', A6, 'and String2 = ', A6, &
            ' IICSR = ', I2, /)
      END
```

Output

```
For String1 = ABc 1 and String2 =        IICSR =  1

For String1 = AbC   and String2 = ABc    IICSR =  0

For String1 = ABc   and String2 = aBC 1  IICSR = -1
```

IIDEX

This funcion determines the position in a string at which a given character sequence begins without regard to case.

Function Return Value

IIDEX — Position in `CHRSTR` where `KEY` begins. (Output)
If `KEY` occurs more than once in `CHRSTR`, the starting position of the first occurrence is returned. If `KEY` does not occur in `CHRSTR`, then `IIDEX` returns a zero.

Required Arguments

CHRSTR — Character string to be searched. (Input)

KEY — Character string that contains the key sequence. (Input)

FORTRAN 90 Interface

Generic: `IIDEX` (`CHRSTR`, `KEY`)

Specific: The specific interface name is `IIDEX`.

FORTRAN 77 Interface

Single: `IIDEX` (`CHRSTR`, `KEY`)

Description

Routine `IIDEX` searches for a key string in a given string and returns the index of the starting element at which the key character string begins. It returns 0 if there is no match. The comparison is case insensitive. For a case-sensitive version, use the FORTRAN 77 intrinsic function `INDEX`.

Comments

1. If the length of `KEY` is greater than the length `CHRSTR`, `IIDEX` returns a zero.

Example

This example locates a key string.

```
      USE IIDEX_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    NOUT
      CHARACTER  KEY*5, STRING*10
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Locate KEY in STRING
      STRING = 'a1b2c3d4e5'
      KEY    = 'C3d4E'
      WRITE (NOUT,99999) STRING, KEY, IIDEX(STRING,KEY)
!
      KEY = 'F'
      WRITE (NOUT,99999) STRING, KEY, IIDEX(STRING,KEY)
!
99999 FORMAT (' For STRING = ', A10, ' and KEY = ', A5, ' IIDEX = ', I2, &
            /)
      END
```

Output

```
For STRING = a1b2c3d4e5 and KEY = C3d4E IIDEX =  5

For STRING = a1b2c3d4e5 and KEY = F     IIDEX =  0
```

CVTSI

Converts a character string containing an integer number into the corresponding integer form.

Required Arguments

STRING — Character string containing an integer number. (Input)

NUMBER — The integer equivalent of `STRING`. (Output)

FORTRAN 90 Interface

Generic: `CALL CVTSI (STRING, NUMBER)`

Specific: The specific interface name is `CVTSI`.

FORTRAN 77 Interface

Single: `CALL CVTSI (STRING, NUMBER)`

Description

Routine `CVTSI` converts a character string containing an integer to an `INTEGER` variable. Leading and trailing blanks in the string are ignored. If the string contains something other than an integer, a terminal error is issued. If the string contains an integer larger than can be represented by an `INTEGER` variable as determined from routine `IMACH` (see the *Reference Material*), a terminal error is issued.

Example

The string "12345" is converted to an `INTEGER` variable.

```
      USE CVTSI_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    NOUT, NUMBER
      CHARACTER  STRING*10
!
      DATA STRING/'12345'/
!
      CALL CVTSI (STRING, NUMBER)
!
      CALL UMACH (2, NOUT)
```

```
      WRITE (NOUT,*) 'NUMBER = ', NUMBER
      END
```

Output

```
NUMBER =   12345
```

CPSEC

This function returns CPU time used in seconds.

Function Return Value

CPSEC — CPU time used (in seconds) since first call to `CPSEC`. (Output)

Required Arguments

None

FORTRAN 90 Interface

Generic: `CPSEC` ()

Specific: The specific interface name is `CPSEC`.

FORTRAN 77 Interface

Single: `CPSEC` (1)

Comments

1. The first call to `CPSEC` returns 0.0.
2. The accuracy of this routine depends on the hardware and the operating system. On some systems, identical runs can produce timings differing by more than 10 percent.

TIMDY

Gets time of day.

Required Arguments

IHOUR — Hour of the day. (Output)
`IHOUR` is between 0 and 23 inclusive.

MINUTE — Minute within the hour. (Output)
`MINUTE` is between 0 and 59 inclusive.

ISEC — Second within the minute. (Output)
`ISEC` is between 0 and 59 inclusive.

FORTRAN 90 Interface

Generic: `CALL TIMDY (IHOUR, MINUTE, ISEC)`

Specific: The specific interface name is `TIMDY`.

FORTRAN 77 Interface

Single: `CALL TIMDY (IHOUR, MINUTE, ISEC)`

Description

Routine `TIMDY` is used to retrieve the time of day.

Example

The following example uses `TIMDY` to return the current time. Obviously, the output is dependent upon the time at which the program is run.

```
      USE TIMDY_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    IHOUR, IMIN, ISEC, NOUT
!
      CALL TIMDY (IHOUR, IMIN, ISEC)
      CALL UMACH (2, NOUT)
```

```
      WRITE (NOUT,*) 'Hour:Minute:Second = ', IHOUR, ':', IMIN, &
                     ':', ISEC
      IF (IHOUR .EQ. 0) THEN
         WRITE (NOUT,*) 'The time is ', IMIN, ' minute(s), ', ISEC, &
                        ' second(s) past midnight.'
      ELSE IF (IHOUR .LT. 12) THEN
         WRITE (NOUT,*) 'The time is ', IMIN, ' minute(s), ', ISEC, &
                        ' second(s) past ', IHOUR, ' am.'
      ELSE IF (IHOUR .EQ. 12) THEN
         WRITE (NOUT,*) 'The time is ', IMIN, ' minute(s), ', ISEC, &
                        ' second(s) past noon.'
      ELSE
         WRITE (NOUT,*) 'The time is ', IMIN, ' minute(s), ', ISEC, &
                        ' second(s) past ', IHOUR-12, ' pm.'
      END IF
      END
```

Output

```
Hour:Minute:Second =  14 : 34 : 30
The time is  34  minute(s),  30  second(s) past  2  pm.
```

TDATE

Gets today's date.

Required Arguments

IDAY — Day of the month. (Output)
IDAY is between 1 and 31 inclusive.

MONTH — Month of the year. (Output)
MONTH is between 1 and 12 inclusive.

IYEAR — Year. (Output)
For example, IYEAR = 1985.

FORTRAN 90 Interface

Generic: CALL TDATE (IDAY, MONTH, IYEAR)

Specific: The specific interface name is TDATE.

FORTRAN 77 Interface

Single: CALL TDATE (IDAY, MONTH, IYEAR)

Description

Routine TDATE is used to retrieve today's date. Obviously, the output is dependent upon the date the program is run.

Example

The following example uses TDATE to return today's date.

```
      USE TDATE_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    IDAY, IYEAR, MONTH, NOUT
!
      CALL TDATE (IDAY, MONTH, IYEAR)
      CALL UMACH (2, NOUT)
```

```
      WRITE (NOUT,*) 'Day-Month-Year = ', IDAY, '-', MONTH, &
                     '-', IYEAR
      END
```

Output

```
Day-Month-Year =  7 - 7 - 2006
```

NDAYS

This function computes the number of days from January 1, 1900, to the given date.

Function Return Value

NDAYS — Function value. (Output)
If `NDAYS` is negative, it indicates the number of days prior to January 1, 1900.

Required Arguments

IDAY — Day of the input date. (Input)

MONTH — Month of the input date. (Input)

IYEAR — Year of the input date. (Input)
1950 would correspond to the year 1950 A.D. and 50 would correspond to year 50 A.D.

FORTRAN 90 Interface

Generic: `NDAYS (IDAY, MONTH, IYEAR)`

Specific: The specific interface name is `NDAYS`.

FORTRAN 77 Interface

Single: `NDAYS (IDAY, MONTH, IYEAR)`

Description

Function `NDAYS` returns the number of days from January 1, 1900, to the given date. The function `NDAYS` returns negative values for days prior to January 1, 1900. A negative `IYEAR` can be used to specify B.C. Input dates in year 0 and for October 5, 1582, through October 14, 1582, inclusive, do not exist; consequently, in these cases, `NDAYS` issues a terminal error.

Comments

1. Informational error

Type	Code	Description
1	1	The Julian calendar, the first modern calendar, went into use in 45 B.C. No calendar prior to 45 B.C. was as universally used nor as accurate as the Julian. Therefore, it is assumed that the Julian calendar was in use prior to 45 B.C.

2. The number of days from one date to a second date can be computed by two references to `NDAYS` and then calculating the difference.

3. The beginning of the Gregorian calendar was the first day after October 4, 1582, which became October 15, 1582. Prior to that, the Julian calendar was in use. `NDAYS` makes the proper adjustment for the change in calendars.

Example

The following example uses `NDAYS` to compute the number of days from January 15, 1986, to February 28, 1986:

```
      USE NDAYS_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    IDAY, IYEAR, MONTH, NDAY0, NDAY1, NOUT
!
      IDAY  = 15
      MONTH = 1
      IYEAR = 1986
      NDAY0 = NDAYS(IDAY,MONTH,IYEAR)
      IDAY  = 28
      MONTH = 2
      IYEAR = 1986
      NDAY1 = NDAYS(IDAY,MONTH,IYEAR)
      CALL UMACH (2, NOUT)
      WRITE (NOUT,*) 'Number of days = ', NDAY1 - NDAY0
      END
```

Output

```
Number of days =   44
```

NDYIN

Gives the date corresponding to the number of days since January 1, 1900.

Required Arguments

NDAYS — Number of days since January 1, 1900. (Input)

IDAY — Day of the input date. (Output)

MONTH — Month of the input date. (Output)

IYEAR — Year of the input date. (Output)
1950 would correspond to the year 195 A.D. and −50 would correspond to year 50 B.C.

FORTRAN 90 Interface

Generic: `CALL NDYIN (NDAYS, IDAY, MONTH, IYEAR)`

Specific: The specific interface name is `NDYIN`.

FORTRAN 77 Interface

Single: `CALL NDYIN (NDAYS, IDAY, MONTH, IYEAR)`

Description

Routine `NDYIN` computes the date corresponding to the number of days since January 1, 1900. For an input value of `NDAYS` that is negative, the date computed is prior to January 1, 1900. The routine `NDYIN` is the inverse of `NDAYS`.

Comments

1. The beginning of the Gregorian calendar was the first day after October 4, 1582, which became October 15, 1582. Prior to that, the Julian calendar was in use. Routine `NDYIN` makes the proper adjustment for the change in calendars.

Example

The following example uses NDYIN to compute the date for the 100th day of 1986. This is accomplished by first using NDAYS to get the “day number” for December 31, 1985.

```
      USE NDYIN_INT
      USE NDAYS_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    IDAY, IYEAR, MONTH, NDAYO, NOUT, NDAY0
!
      NDAY0 = NDAYS(31,12,1985)
      CALL NDYIN (NDAY0+100, IDAY, MONTH, IYEAR)
      CALL UMACH (2, NOUT)
      WRITE (NOUT,*) 'Day 100 of 1986 is (day-month-year) ', IDAY, &
                  '-', MONTH, '-', IYEAR
      END
```

Output

```
Day 100 of 1986 is (day-month-year)   10-   4-   1986
```

IDYWK

This function computes the day of the week for a given date.

Function Return Value

IDYWK — Function value. (Output)
The value of `IDYWK` ranges from 1 to 7, where 1 corresponds to Sunday and 7 corresponds to Saturday.

Required Arguments

IDAY — Day of the input date. (Input)

MONTH — Month of the input date. (Input)

IYEAR — Year of the input date. (Input)
1950 would correspond to the year 1950 A.D. and 50 would correspond to year 50 A.D.

FORTRAN 90 Interface

Generic: `IDYWK (IDAY, MONTH, IYEAR)`

Specific: The specific interface name is `IDYWK`.

FORTRAN 77 Interface

Single: `IDYWK (IDAY, MONTH, IYEAR)`

Description

Function `IDYWK` returns an integer code that specifies the day of week for a given date. Sunday corresponds to 1, Monday corresponds to 2, and so forth.

A negative `IYEAR` can be used to specify B.C. Input dates in year 0 and for October 5, 1582, through October 14, 1582, inclusive, do not exist; consequently, in these cases, `IDYWK` issues a terminal error.

Comments

1. Informational error

Type	Code	Description
1	1	The Julian calendar, the first modern calendar, went into use in 45 B.C. No calendar prior to 45 B.C. was as universally used nor as accurate as the Julian. Therefore, it is assumed that the Julian calendar was in use prior to 45 B.C.

2. The beginning of the Gregorian calendar was the first day after October 4, 1582, which became October 15, 1582. Prior to that, the Julian calendar was in use. Function `IDYWK` makes the proper adjustment for the change in calendars.

Example

The following example uses `IDYWK` to return the day of the week for February 24, 1963.

```
      USE IDYWK_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    IDAY, IYEAR, MONTH, NOUT
!
      IDAY  = 24
      MONTH = 2
      IYEAR = 1963
      CALL UMACH (2, NOUT)
      WRITE (NOUT,*) 'IDYWK (index for day of week) = ', &
                     IDYWK(IDAY,MONTH,IYEAR)
      END
```

Output

```
IDYWK (index for day of week) =   1
```

VERML

This function obtains IMSL MATH/LIBRARY-related version and system information.

Function Return Value

VERML — CHARACTER string containing information. (Output)

Required Arguments

ISELCT — Option for the information to retrieve. (Input)

ISELCTVERML

1 IMSL MATH/LIBRARY version number

2 Operating system (and version number) for which the library was produced.

3 Fortran compiler (and version number) for which the library was produced.

FORTRAN 90 Interface

Generic: VERML (ISELCT)

Specific: The specific interface name is VERML.

FORTRAN 77 Interface

Single: VERML (ISELCT)

Example

In this example, we print all of the information returned by VERML on a particular machine. The output is omitted because the results are system dependent.

```
      USE UMACH_INT
      USE VERML_INT

      IMPLICIT   NONE
      INTEGER    ISELCT, NOUT
      CHARACTER  STRING(3)*50, TEMP*32
!
      STRING(1) = '('' IMSL MATH/LIBRARY Version Number:  '', A)'
```

```
      STRING(2) = '('' Operating System ID Number:  '', A)'
      STRING(3) = '('' Fortran Compiler Version Number:  '', A)'
!                                 Print the versions and numbers.
      CALL UMACH (2, NOUT)
      DO 10  ISELCT=1, 3
         TEMP = VERML(ISELCT)
         WRITE (NOUT,STRING(ISELCT)) TEMP
   10 CONTINUE
      END
```

Output

```
 IMSL MATH/LIBRARY Version Number: IMSL Fortran Numerical Library, Version 6.0.0
 Operating System ID Number:  Solaris Version 10
 Fortran Compiler Version Number:  Sun Fortran 95 8.1 2005/01/07 (Workshop 10.0)
```

RAND_GEN

Generates a rank-1 array of random numbers. The output array entries are positive and less than 1 in value.

Required Argument

X — Rank-1 array containing the random numbers. (Output)

Optional Arguments

IRND = IRND (Output)
Rank-1 integer array. These integers are the internal results of the Generalized Feedback Shift Register (GFSR) algorithm. The values are scaled to yield the floating-point array X. The output array entries are between 1 and $2^{31} - 1$ in value.

ISTATE_IN = ISTATE_IN (Input)
Rank-1 integer array of size $3p + 2$, where $p = 521$, that defines the ensuing state of the GFSR generator. It is used to reset the internal tables to a previously defined state. It is the result of a previous use of the "ISTATE_OUT=" optional argument.

ISTATE_OUT = ISTATE_OUT (Output)
Rank-1 integer array of size $3p + 2$ that describes the current state of the GFSR generator. It is normally used to later reset the internal tables to the state defined following a return from the GFSR generator. It is the result of a use of the generator without a user initialization, or it is the result of a previous use of the optional argument "ISTATE_IN=" followed by updates to the internal tables from newly generated values. Example 2 illustrates use of ISTATE_IN and ISTATE_OUT for setting and then resetting RAND_GEN so that the sequence of integers, irnd, is repeatable.

IOPT = IOPT(:) (Input[/Output])
Derived type array with the same precision as the array x; used for passing optional data to RAND_GEN. The options are as follows:

Packaged Options for **RAND_GEN**		
Option Prefix = ?	Option Name	Option Value
s_, d_	Rand_gen_generator_seed	1
s_, d_	Rand_gen_LCM_modulus	2
s_, d_	Rand_gen_use_Fushimi_start	3

IOPT(IO) = `?_options(?_rand_gen_generator_seed, ?_dummy)`

Sets the initial values for the GFSR. The present value of the seed, obtained by default from the real-time clock as described below, swaps places with
`iopt(IO + 1)%idummy`. If the seed is set before any current usage of `RAND_GEN`, the exchanged value will be zero.

IOPT(IO) = `?_options(?_rand_gen_LCM_modulus, ?_dummy)`

IOPT(IO+1) = `?_options(modulus, ?_dummy)`

Sets the initial values for the GFSR. The present value of the LCM, with default value ***k*** = 16807, swaps places with ***iopt(IO+1)%idummy***.

IOPT(IO) = `?_options(?_rand_gen_use_Fushimi_start, ?_dummy)`

Starts the GFSR sequence as suggested by Fushimi (1990). The default starting sequence is with the LCM recurrence described below.

FORTRAN 90 Interface

Generic: `CALL RAND_GEN (X [, …])`

Specific: The specific interface names are `S_RAND_GEN` and `D_RAND_GEN`.

Description

This GFSR algorithm is based on the recurrence

$$x_t = x_{t-3p} \oplus x_{t-3p}$$

where $a \oplus b$ is the exclusive `OR` operation on two integers a and b. This operation is performed until `SIZE`(***x***) numbers have been generated. The subscripts in the recurrence formula are computed modulo 3*p*. These numbers are converted to floating point by effectively multiplying the positive integer quantity

$$x_t \cup 1$$

by a scale factor slightly smaller than 1./(*huge*(1)). The values $p = 521$ and $q = 32$ yield a sequence with a period approximately

$$2^p > 10^{156.8}$$

The default initial values for the sequence of integers $\{x_t\}$ are created by a congruential generator starting with an odd integer seed

$$m = v + \left| count \cap \left(2^{bit\_size(1)} - 1 \right) \right| \cup 1$$

obtained by the Fortran 90 real-time clock routine:

CALL SYSTEM_CLOCK(COUNT=count,CLOCK_RATE=CLRATE)

An error condition is noted if the value of `CLRATE=0`. This indicates that the processor does not have a functioning real-time clock. In this exceptional case a starting seed must be provided by the user with the optional argument "`iopt=`" and option number `?_rand_generator_seed`. The value *v* is the current clock for this day, in milliseconds. This value is obtained using the date routine:

CALL DATE_AND_TIME(VALUES=values)

and converting `values(5:8)` to milliseconds.

The LCM generator initializes the sequence $\{x_t\}$ using the following recurrence:

$$m \leftarrow m \times k, \ \mathrm{mod}(huge(1)/2)$$

The default value of k = 16807. Using the optional argument "`iopt=`" and the packaged option number `?_rand_gen_LCM_modulus`, k can be given an alternate value. The option number `?_rand_gen_generator_seed` can be used to set the initial value of m instead of using the asynchronous value given by the system clock. This is illustrated in Example 2. If the default choice of m results in an unsatisfactory starting sequence or it is necessary to duplicate the sequence, then it is recommended that users set the initial seed value to one of their own choosing. Resetting the seed complicates the usage of the routine.

This software is based on Fushimi (1990), who gives a more elaborate starting sequence for the $\{x_t\}$. The starting sequence suggested by Fushimi can be used with the option number `?_rand_gen_use_Fushimi_start`. Fushimi's starting process is more expensive than the default method, and it is equivalent to starting in another place of the sequence with period 2^p.

Fatal and Terminal Error Messages

See the *messages.gls* file for error messages for `RAND_GEN`. These error messages are numbered 521−528; 541−548.

Examples

Example 1: Running Mean and Variance

An array of random numbers is obtained. The sample mean and variance are computed. These values are compared with the same quantities computed using a stable method for the running means and variances, sequentially moving through the data. Details about the running mean and variance are found in Henrici (1982, pp. 21–23).

```
      use rand_gen_int

      implicit none

! This is Example 1 for RAND_GEN.

      integer i
      integer, parameter :: n=1000
      real(kind(1e0)), parameter :: one=1e0, zero=0e0
      real(kind(1e0)) x(n), mean_1(0:n), mean_2(0:n), s_1(0:n), s_2(0:n)

! Obtain random numbers.
      call rand_gen(x)

! Calculate each partial mean.
      do i=1,n
        mean_1(i) = sum(x(1:i))/i
      end do

! Calculate each partial variance.
      do i=1,n
        s_1(i)=sum((x(1:i)-mean_1(i))**2)/i
      end do

      mean_2(0)=zero
      mean_2(1)=x(1)
      s_2(0:1)=zero

! Alternately calculate each running mean and variance,
! handling the random numbers once.
      do i=2,n
       mean_2(i)=((i-1)*mean_2(i-1)+x(i))/i
       s_2(i)   = (i-1)*s_2(i-1)/i+(mean_2(i)-x(i))**2/(i-1)
      end do

! Check that the two sets of means and variances agree.
      if (maxval(abs(mean_1(1:)-mean_2(1:))/mean_1(1:)) <= &
              sqrt(epsilon(one))) then
         if (maxval(abs(s_1(2:)-s_2(2:))/s_1(2:)) <= &
              sqrt(epsilon(one))) then
            write (*,*) 'Example 1 for RAND_GEN is correct.'
         end if
      end if

      end
```

Output

```
Example 1 for RAND_GEN is correct.
```

Example 2: Seeding, Using, and Restoring the Generator

```
      use rand_gen_int

      implicit none

! This is Example 2 for RAND_GEN.

      integer i
      integer, parameter :: n=34, p=521
      real(kind(1e0)), parameter :: one=1.0e0, zero=0.0e0
      integer irndi(n), i_out(3*p+2), hidden_message(n)

type(s_options) :: iopti(2)=s_options(0,zero)
      character*34 message, returned_message

! This is the message to be hidden.
      message = 'SAVE YOURSELF.  WE ARE DISCOVERED!'

! Start the generator with a known seed.
      iopti(1) = s_options(s_rand_gen_generator_seed,zero)
      iopti(2) = s_options(123,zero)
      call rand_gen(x, iopt=iopti)

! Save the state of the generator.
      call rand_gen(x, istate_out=i_out)

! Get random integers.
      call rand_gen(y, irnd=irndi)

! Hide text using collating sequence subtracted from integers.
      do i=1, n
         hidden_message(i) = irndi(i) - ichar(message(i:i))
      end do

! Reset generator to previous state and generate the previous
! random integers.
      call rand_gen(x, irnd=irndi, istate_in=i_out)

! Subtract hidden text from integers and convert to character.
      do i=1, n
         returned_message(i:i) = char(irndi(i) - hidden_message(i))
      end do

! Check the results.
      if (returned_message == message) then



         write (*,*) 'Example 2 for RAND_GEN is correct.'
      end if

      end
```

Output

```
Example 2 for RAND_GEN is correct.
```

Example 3: Generating Strategy with a Histogram

We generate random integers but with the frequency as in a histogram with n_{bins} slots. The generator is initially used a large number of times to demonstrate that it is making choices with the same shape as the histogram. This is not required to generate samples. The program next generates a summary set of integers according to the histogram. These are not repeatable and are representative of the histogram in the sense of looking at 20 integers during generation of a large number of samples.

```
      use rand_gen_int
      use show_int

      implicit none

! This is Example 3 for RAND_GEN.

      integer i, i_bin, i_map, i_left, i_right
      integer, parameter :: n_work=1000
      integer, parameter :: n_bins=10
      integer, parameter :: scale=1000
      integer, parameter :: total_counts=100
      integer, parameter :: n_samples=total_counts*scale
      integer, dimension(n_bins) :: histogram=  &
        (/4,  6,  8, 14, 20, 17, 12,  9,  7,  3 /)
      integer, dimension(n_work) :: working=0
      integer, dimension(n_bins) :: distribution=0
      integer break_points(0:n_bins)
      real(kind(1e0)) rn(n_samples)
      real(kind(1e0)), parameter :: tolerance=0.005


      integer, parameter :: n_samples_20=20
      integer rand_num_20(n_samples_20)
      real(kind(1e0)) rn_20(n_samples_20)

! Compute the normalized cumulative distribution.
      break_points(0)=0
      do i=1,n_bins
        break_points(i)=break_points(i-1)+histogram(i)
      end do

      break_points=break_points*n_work/total_counts

! Obtain uniform random numbers.
        call rand_gen(rn)


! Set up the secondary mapping array.
      do i_bin=1,n_bins
        i_left=break_points(i_bin-1)+1
        i_right=break_points(i_bin)
        do i=i_left, i_right
          working(i)=i_bin
        end do
      end do

! Map the random numbers into the 'distribution' array.
! This is made approximately proportional to the histogram.
      do i=1,n_samples
        i_map=nint(rn(i)*(n_work-1)+1)
        distribution(working(i_map))=  &
          distribution(working(i_map))+1
      end do
```

```
! Check the agreement between the distribution of the
! generated random numbers and the original histogram.
       write (*, '(A)', advance='no') 'Original: '
       write (*, '(10I6)') histogram*scale
       write (*, '(A)', advance='no') 'Generated:'
       write (*, '(10I6)') distribution

      if (maxval(abs(histogram(1:)*scale-distribution(1:))) &
            <= tolerance*n_samples) then
        write(*, '(A/)') 'Example 3 for RAND_GEN is correct.'
      end if

! Generate 20 integers in 1, 10 according to the distribution
! induced by the histogram.
        call rand_gen(rn_20)

! Map from the uniform distribution to the induced distribution.
      do i=1,n_samples_20
        i_map=nint(rn_20(i)*(n_work-1)+1)
        rand_num_20(i)=working(i_map)
      end do

        call show(rand_num_20,&
'Twenty integers generated according to the histogram:')
      end
```

Output

```
Example 3 for RAND_GEN is correct.
```

RNGET

Retrieves the current value of the seed used in the IMSL random number generators.

Required Arguments

ISEED — The seed of the random number generator. (Output)
ISEED is in the range (1, 2147483646).

FORTRAN 90 Interface

Generic: CALL RNGET (ISEED)

Specific: The specific interface name is RNGET.

FORTRAN 77 Interface

Single: CALL RNGET (ISEED)

Description

Routine RNGET retrieves the current value of the "seed" used in the IMSL random number generators. A reason for doing this would be to restart a simulation, using RNSET to reset the seed.

Example

The following FORTRAN statements illustrate the use of RNGET:

```
      INTEGER ISEED
!                             Call RNSET to initialize the seed.
      CALL RNSET(123457)
!                             Do some simulations.
         ...
         ...
      CALL RNGET(ISEED)
!                             Save ISEED.  If the simulation is to be continued
!                             in a different program, ISEED should be output,
!                             possibly to a file.
         ...
         ...
!                             When the simulations begun above are to be
!                             restarted, restore ISEED to the value obtained
!                             above and use as input to RNSET.
      CALL RNSET(ISEED)
```

```
 !                        Now continue the simulations.
          ...
          ...
```

RNSET

Initializes a random seed for use in the IMSL random number generators.

Required Arguments

ISEED — The seed of the random number generator. (Input)
ISEED must be in the range (0, 2147483646). If ISEED is zero, a value is computed using the system clock; and, hence, the results of programs using the IMSL random number generators will be different at different times.

FORTRAN 90 Interface

Generic: CALL RNSET (ISEED)

Specific: The specific interface name is RNSET .

FORTRAN 77 Interface

Single: CALL RNSET (ISEED)

Description

Routine RNSET is used to initialize the seed used in the IMSL random number generators. If the seed is not initialized prior to invocation of any of the routines for random number generation by calling RNSET, the seed is initialized via the system clock. The seed can be reinitialized to a
clock-dependent value by calling RNSET with ISEED set to 0.

The effect of RNSET is to set some values in a FORTRAN COMMON block that is used by the random number generators.

A common use of RNSET is in conjunction with RNGET to restart a simulation.

Example

The following FORTRAN statements illustrate the use of RNSET:

```
      INTEGER ISEED
!                             Call RNSET to initialize the seed via the
!                             system clock.
```

```
          CALL RNSET(0)
 !                          Do some simulations.
              ...
              ...
 !                          Obtain the current value of the seed.
          CALL RNGET(ISEED)
 !                          If the simulation is to be continued in a
 !                          different program, ISEED should be output,
 !                          possibly to a file.
               ...
               ...
 !                          When the simulations begun above are to be
 !                          restarted, restore ISEED to the value
 !                          obtained above, and use as input to RNSET.
          CALL RNSET(ISEED)
 !                          Now continue the simulations.
               ...
               ...
```

RNOPT

Selects the uniform (0, 1) multiplicative congruential pseudorandom number generator.

Required Arguments

IOPT — Indicator of the generator. (Input)
The random number generator is either a multiplicative congruential generator with modulus $2^{31} - 1$ or a GFSR generator. `IOPT` is used to choose the multiplier and whether or not shuffling is done, or is used to choose the GFSR method, or is used to choose the Mersenne Twister generator.

IOPT	Generator
1	The multiplier 16807 is used.
2	The multiplier 16807 is used with shuffling.
3	The multiplier 397204094 is used.
4	The multiplier 397204094 is used with shuffling.
5	The multiplier 950706376 is used.
6	The multiplier 950706376 is used with shuffling.
7	GFSR, with the recursion $X_t = X_{t-1563} \oplus X_{t-96}$ is used.
8	A 32-bit Mersenne Twister generator is used. The real and double random numbers are generated from 32-bit integers.
9	A 64-bit Mersenne Twister generator is used. The real and double random numbers are generated from 64-bit integers. This ensures that all bits of both float and double are random.

FORTRAN 90 Interface

Generic: `CALL RNOPT (IOPT)`

Specific: The specific interface name is `RNOPT`.

FORTRAN 77 Interface

Single: `CALL RNOPT (IOPT)`

Description

The uniform pseudorandom number generators use a multiplicative congruential method, with or without shuffling or a GFSR method, or the Mersenne Twister method. Routine RNOPT determines which method is used; and in the case of a multiplicative congruential method, it determines the value of the multiplier and whether or not to use shuffling. The description of RNUN may provide some guidance in the choice of the form of the generator. If no selection is made explicitly, the generators use the multiplier 16807 without shuffling. This form of the generator has been in use for some time (see Lewis, Goodman, and Miller, 1969). This is the generator formerly known as GGUBS in the IMSL Library. It is the "minimal standard generator" discussed by Park and Miller (1988).

Both of the Mersenne Twister generators have a period of 2^{19937} -1 and a 624-dimensional equi-distribution property. See Matsumoto et al. 1998 for details.

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The IMSL 32-bit Mersenne Twister generator is based on the Matsumoto and Nishimura code 'mt19937ar' and the 64-bit code is based on 'mt19937-64'.

Example

The FORTRAN statement

```
CALL RNOPT(1)
```

would select the simple multiplicative congruential generator with multiplier 16807. Since this is the same as the default, this statement would have no effect unless RNOPT had previously been called in the same program to select a different generator.

RNIN32

Initializes the 32-bit Mersenne Twister generator using an array.

Required Arguments

KEY— Integer array of length `LEN` used to initialize the 32-bit Mersenne Twister generator. (Input)

Optional Arguments

LEN — Length of the array key. (Input)

FORTRAN 90 Interface

Generic: `CALL RNIN32 (KEY [, …])`

Specific: The specific interface name is `S_RNIN32`.

FORTRAN 77 Interface

Single: `CALL RNIN32 (KEY, LEN)`

Description

By default, the Mersenne Twister random number generator is initialized using the current seed value (see `RNGET`). The seed is limited to one integer for initialization. This function allows an arbitrary length array to be used for initialization. This subroutine completely replaces the use of the seed for initialization of the 32-bit Mersenne Twister generator.

Example

See routine `RNGE32`.

RNGE32

Retrieves the current table used in the 32-bit Mersenne Twister generator.

Required Arguments

MTABLE — Integer array of length 625 containing the table used in the 32-bit Mersenne Twister generator. (Output)

FORTRAN 90 Interface

Generic: `CALL RNGE32 (MTABLE)`

Specific: The specific interface name is `RNGE32`

FORTRAN 77 Interface

Single: `CALL RNGE32 (MTABLE)`

Description

The values in the table contain the state of the 32-bit Mersenne Twister random number generator. The table can be used by `RNSE32` to set the generator back to this state.

Example

In this example, four simulation streams are generated. The first series is generated with the seed used for initialization. The second series is generated using an array for initialization. The third series is obtained by resetting the generator back to the state it had at the beginning of the second stream. Therefore, the second and third streams are identical. The fourth stream is obtained by resetting the generator back to its original, uninitialized state, and having it reinitialize using the seed. The first and fourth streams are therefore the same.

```
      USE RNIN32_INT
      USE RNGE32_INT
      USE RNSET_INT
      USE UMACH_INT
      USE RNUN_INT
      IMPLICIT   NONE
      INTEGER    I, ISEED, NOUT
      INTEGER INIT(4)
      DATA INIT/291,564,837,1110/
      DATA ISEED/123457/
```

```
      INTEGER NR
      REAL R(5)
      INTEGER MTABLE(625)
      CHARACTER CLABEL(5)*5, FMT*8, RLABEL(3)*5
      RLABEL(1)='NONE'
      CLABEL(1)='NONE'
      DATA FMT/'(W10.4)'/
      NR=5
      CALL UMACH (2, NOUT)
      ISEED = 123457
      CALL RNOPT(8)
      CALL RNSET(ISEED)
      CALL RNUN(R)
      CALL WRRRL('FIRST STREAM OUTPUT',1,5,R,1,0, &
                 FMT, RLABEL, CLABEL)
!     REINITIALIZE MERSENNE TWISTER SERIES WITH AN ARRAY
      CALL RNIN32(INIT)
!     SAVE THE STATE OF THE SERIES
      CALL RNGE32(MTABLE)
      CALL RNUN(R)
      CALL WRRRL('SECOND STREAM OUTPUT',1,5,R,1,0, &
                  FMT, RLABEL, CLABEL)
!     RESTORE THE STATE OF THE TABLE
      CALL RNSE32(MTABLE)
      CALL RNUN(R)
      CALL WRRRL('THIRD STREAM OUTPUT',1,5,R,1,0, &
                  FMT, RLABEL, CLABEL)
!     RESET THE SERIES - IT WILL REINITIALIZE FROM THE SEED
      MTABLE(1)=1000
      CALL RNSE32(MTABLE)
      CALL RNUN(R)
      CALL WRRRL('FOURTH STREAM OUTPUT',1,5,R,1,0, &
                  FMT, RLABEL, CLABEL)
      END
```

Output

```
                First stream output
     0.4347      0.3522      0.0139      0.2091      0.4956
               Second stream output
     0.2486      0.2226      0.1111      0.9563      0.9846
                Third stream output
     0.2486      0.2226      0.1111      0.9563      0.9846
               Fourth stream output
     0.4347      0.3522      0.0139      0.2091      0.4956
```

RNSE32

Sets the current table used in the 32-bit Mersenne Twister generator.

Required Arguments

MTABLE — Integer array of length 625 containing the table used in the 32-bit Mersenne Twister generator. (Input)

FORTRAN 90 Interface

Generic: `CALL RNSE32 (MTABLE)`

Specific: The specific interface name is `RNSE32`

FORTRAN 77 Interface

Single: `CALL RNSE32 (MTABLE)`

Description

The values in `MTABLE` are the state of the 32-bit Mersenne Twister random number generator obtained by a call to `RNGE32`. The values in the table can be used to restore the state of the generator.

Alternatively, if `MTABLE` [1] > 625 then the generator is set to its original, uninitialized, state.

Example

See routine `RNGE32`.

RNIN64

Initializes the 64-bit Mersenne Twister generator using an array.

Required Arguments

KEY— Integer(kind=8) array of length `LEN` used to initialize the 64-bit Mersenne Twister generator. (Input)

Optional Arguments

LEN — Length of the array key. (Input)

FORTRAN 90 Interface

Generic: `CALL RNIN64 (KEY [, …])`

Specific: The specific interface name is `S_RNIN64`.

FORTRAN 77 Interface

Single: `CALL RNIN64 (KEY, LEN)`

Description

By default, the Mersenne Twister random number generator is initialized using the current seed value (see `RNGET`). The seed is limited to one integer for initialization. This function allows an arbitrary length array to be used for initialization. This subroutine completely replaces the use of the seed for initialization of the 64-bit Mersenne Twister generator.

RNGE64

Retrieves the current table used in the 64-bit Mersenne Twister generator.

Required Arguments

MTABLE — Integer(kind=8) array of length 313 containing the table used in the 64-bit Mersenne Twister generator. (Output)

FORTRAN 90 Interface

Generic: `CALL RNGE64 (MTABLE)`

Specific: The specific interface name is `RNGE64`

FORTRAN 77 Interface

Single: `CALL RNGE64 (MTABLE)`

Description

The values in the table contain the state of the 64-bit Mersenne Twister random number generator. The table can be used by `RNSE64` to set the generator back to this state.

Example

In this example, four simulation streams are generated. The first series is generated with the seed used for initialization. The second series is generated using an array for initialization. The third series is obtained by resetting the generator back to the state it had at the beginning of the second stream. Therefore, the second and third streams are identical. The fourth stream is obtained by resetting the generator back to its original, uninitialized state, and having it reinitialize using the seed. The first and fourth streams are therefore the same.

```
      USE RNIN64_INT
      USE RNGE64_INT
      USE RNSET_INT
      USE UMACH_INT
      USE RNUN_INT
      IMPLICIT   NONE
      INTEGER    I, ISEED, NOUT
      INTEGER(KIND=8) INIT(4)
      DATA INIT/291,564,837,1110/
      DATA ISEED/123457/
```

```
      INTEGER NR
      REAL R(5)
      INTEGER(KIND=8) MTABLE(313)
      CHARACTER CLABEL(5)*5, FMT*8, RLABEL(3)*5
      RLABEL(1)='NONE'
      CLABEL(1)='NONE'
      DATA FMT/'(W10.4)'/
      NR=5
      CALL UMACH (2, NOUT)
      ISEED = 123457
      CALL RNOPT(9)
      CALL RNSET(ISEED)
      CALL RNUN(R)
      CALL WRRRL('FIRST STREAM OUTPUT',1,5,R,1,0, &
                  FMT, RLABEL, CLABEL)
!     REINITIALIZE MERSENNE TWISTER SERIES WITH AN ARRAY
      CALL RNIN64(INIT)
!     SAVE THE STATE OF THE SERIES
      CALL RNGE64(MTABLE)
      CALL RNUN(R)
      CALL WRRRL('SECOND STREAM OUTPUT',1,5,R,1,0, &
                   FMT, RLABEL, CLABEL)
!     RESTORE THE STATE OF THE TABLE
      CALL RNSE64(MTABLE)
      CALL RNUN(R)
      CALL WRRRL('THIRD STREAM OUTPUT',1,5,R,1,0, &
                   FMT, RLABEL, CLABEL)
!     RESET THE SERIES - IT WILL REINITIALIZE FROM THE SEED
      MTABLE(1)=1000
      CALL RNSE64(MTABLE)
      CALL RNUN(R)
      CALL WRRRL('FOURTH STREAM OUTPUT',1,5,R,1,0, &
                   FMT, RLABEL, CLABEL)
      END
```

Output

```
                First stream output
     0.5799      0.9401      0.7102      0.1640      0.5457
               Second stream output
     0.4894      0.7397      0.5725      0.0863      0.7588
                Third stream output
     0.4894      0.7397      0.5725      0.0863      0.7588
               Fourth stream output
     0.5799      0.9401      0.7102      0.1640      0.5457
```

RNSE64

Sets the current table used in the 64-bit Mersenne Twister generator.

Required Arguments

MTABLE — Integer (kind=8) array of length 313 containing the table used in the 64-bit Mersenne Twister generator. (Input)

FORTRAN 90 Interface

Generic: `CALL RNSE64 (MTABLE)`

Specific: The specific interface name is `RNSE64`

FORTRAN 77 Interface

Single: `CALL RNSE64 (MTABLE)`

Description

The values in `MTABLE` are the state of the 64-bit Mersenne Twister random number generator obtained by a call to `RNGE64`. The values in the table can be used to restore the state of the generator. Alternatively, if `MTABLE` [1] > 313 then the generator is set to its original, uninitialized, state.

Example

See function `RNGE64`.

RNUNF

This function generates a pseudorandom number from a uniform (0, 1) distribution.

Function Return Value

RNUNF — Function value, a random uniform (0, 1) deviate. (Output)
See Comment 1.

Required Arguments

None

FORTRAN 90 Interface

Generic: `RNUNF ()`

Specific: The specific interface names are `S_RNUNF` and `D_RNUNF`.

FORTRAN 77 Interface

Single: `RNUNF ()`

Double: The double precision name is `DRNUNF`.

Description

Routine `RNUNF` is the function form of `RNUN`. The routine `RNUNF` generates pseudorandom numbers from a uniform (0, 1) distribution. The algorithm used is determined by `RNOPT`. The values returned by `RNUNF` are positive and less than 1.0.

If several uniform deviates are needed, it may be more efficient to obtain them all at once by a call to `RNUN` rather than by several references to `RNUNF`.

Comments

1. If the generic version of this function is used, the immediate result must be stored in a variable before use in an expression. For example:

```
X = RNUNF(6)
Y = SQRT(X)
```

must be used rather than

```
Y = SQRT(RNUNF(6))
```

If this is too much of a restriction on the programmer, then the specific name can be used without this restriction.

2. Routine RNSET can be used to initialize the seed of the random number generator. The routine RNOPT can be used to select the form of the generator.

3. This function has a side effect: it changes the value of the seed, which is passed through a common block.

Example

In this example, RNUNF is used to generate five pseudorandom uniform numbers. Since RNOPT is not called, the generator used is a simple multiplicative congruential one with a multiplier of 16807.

```
      USE RNUNF_INT
      USE RNSET_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    I, ISEED, NOUT
      REAL       R(5)
!
      CALL UMACH (2, NOUT)
      ISEED = 123457
      CALL RNSET (ISEED)
      DO 10  I=1, 5
         R(I) = RNUNF()
   10 CONTINUE
      WRITE (NOUT,99999) R
99999 FORMAT ('      Uniform random deviates: ', 5F8.4)
      END
```

Output

```
Uniform random deviates:   0.9662  0.2607  0.7663  0.5693  0.8448
```

RNUN

Generates pseudorandom numbers from a uniform (0, 1) distribution.

Required Arguments

R — Vector of length NR containing the random uniform (0, 1) deviates. (Output)

Optional Arguments

NR — Number of random numbers to generate. (Input)
Default: NR = size (R,1).

FORTRAN 90 Interface

Generic: CALL RNUN (R [, …])

Specific: The specific interface names are S_RNUN and D_RNUN.

FORTRAN 77 Interface

Single: CALL RNUN (NR, R)

Double: The double precision name is DRNUN.

Description

Routine RNUN generates pseudorandom numbers from a uniform (0,1) distribution using either a multiplicative congruential method or a generalized feedback shift register (GFSR) method, or the Mersenne Twister generator. The form of the multiplicative congruential generator is

$$x_i \equiv cx_{i-1}\mathrm{mod}(2^{31} - 1)$$

Each x_i is then scaled into the unit interval (0,1). The possible values for c in the IMSL generators are 16807, 397204094, and 950706376. The selection is made by the routine RNOPT. The choice of 16807 will result in the fastest execution time. If no selection is made explicitly, the routines use the multiplier 16807.

The user can also select a shuffled version of the multiplicative congruential generators. In this scheme, a table is filled with the first 128 uniform (0,1) numbers resulting from the simple multiplicative congruential generator. Then, for each x_i from the simple generator, the low-order bits of x_i are used to select a random integer, j, from 1 to 128. The j-th entry in the table is then delivered as the random number; and x_i, after being scaled into the unit interval, is inserted into the j-th position in the table.

The GFSR method is based on the recursion $X_t = X_{t-1563} \oplus X_{t-96}$. This generator, which is different from earlier GFSR generators, was proposed by Fushimi (1990), who discusses the theory behind the generator and reports on several empirical tests of it.

Mersenne Twister(MT) is a pseudorandom number generating algorithm developed by Makoto Matsumoto and Takuji Nishimura in 1996-1997. MT has far longer period and far higher order of equidistribution than any other implemented generators. The values returned in `R` by `RNUN` are positive and less than 1.0. Values in `R` may be smaller than the smallest relative spacing, however. Hence, it may be the case that some value `R`(i) is such that 1.0 − `R`(i) = 1.0.

Deviates from the distribution with uniform density over the interval (`A`, `B`) can be obtained by scaling the output from `RNUN`. The following statements (in single precision) would yield random deviates from a uniform (`A`, `B`) distribution:

CALL RNUN (NR, R)
CALL SSCAL (NR, B-A, R, 1)
CALL SADD (NR, A, R, 1)

Comments

1. The routine `RNSET` can be used to initialize the seed of the random number generator. The routine `RNOPT` can be used to select the form of the generator.

Example

In this example, `RNUN` is used to generate five pseudorandom uniform numbers. Since `RNOPT` is not called, the generator used is a simple multiplicative congruential one with a multiplier of 16807.

```
      USE RNUN_INT
      USE RNSET_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    ISEED, NOUT, NR
      REAL       R(5)
!
      CALL UMACH (2, NOUT)
      NR    = 5
```

```
      ISEED = 123457
      CALL RNSET (ISEED)
      CALL RNUN (R)
      WRITE (NOUT,99999) R
99999 FORMAT ('      Uniform random deviates: ', 5F8.4)
      END
```

Output

```
      Uniform random deviates:   0.9662  0.2607  0.7663  0.5693  0.8448
```

FAURE_INIT

Shuffled Faure sequence initialization.

Required Arguments

NDIM — The dimension of the hyper-rectangle. (Input)

STATE — An `IMSL_FAURE` pointer for the derived type created by the call to `FAURE_INIT`. The output contains information about the sequence. Use `?_IMSL_FAURE` as the type, where `?_` is `S_` or `D_` depending on precision. (Output)

Optional Arguments

NBASE — The base of the Faure sequence. (Input)

Default: The smallest prime number greater than or equal to `NDIM`.

NSKIP — The number of points to be skipped at the beginning of the Faure sequence. (Input)

Default: $\lfloor base^{m/2-1} \rfloor$, where $m = \lfloor \log B / \log \text{base} \rfloor$ and *B* is the largest machine representable integer.

FORTRAN 90 Interface

Generic: `CALL FAURE_INIT (NDIM, STATE [, …])`

Specific: The specific interface names are `S_FAURE_INIT` and `D_FAURE_INIT`.

FAURE_FREE

Frees the structure containing information about the Faure sequence.

Required Arguments

STATE — An `IMSL_FAURE` pointer containing the structure created by the call to `FAURE_INIT`. (Input/Output)

FORTRAN 90 Interface

Generic:`CALL FAURE_FREE (STATE)`

Specific:The specific interface names are `S_FAURE_FREE` and `D_FAURE_FREE`.

FAURE_NEXT

Computes a shuffled Faure sequence.

Required Arguments

STATE — An IMSL_FAURE pointer containing the structure created by the call to FAURE_INIT. The structure contains information about the sequence. The structure should be freed using FAURE_FREE after it is no longer needed. (Input/Output)

NEXT_PT — Vector of length NDIM containing the next point in the shuffled Faure sequence, where NDIM is the dimension of the hyper-rectangle specified in FAURE_INIT. (Output)

Optional Arguments

IMSL_RETURN_SKIP — Returns the current point in the sequence. The sequence can be restarted by calling FAURE_INIT using this value for NSKIP, and using the same value for NDIM. (Input)

FORTRAN 90 Interface

Generic: CALL FAURE_NEXT (STATE, NEXT_PT [, …])

Specific: The specific interface names are S_FAURE_NEXT and D_FAURE_NEXT.

Description

The routines FAURE_INIT and FAURE_NEXT are used to generate shuffled Faure sequence of low discrepancy *n*-dimensional points. Low discrepancy series fill an *n*-dimensional cube more uniformly than pseudo-random sequences, and are used in multivariate quadrature, simulation, and global optimization. Because of this uniformity, use of low discrepancy series is generally more efficient than pseudo-random series for multivariate Monte Carlo methods. See the IMSL routine QMC (in *Chapter 4, "Integration and Differentiation"*) for a discussion of quasi-Monte Carlo quadrature based on low discrepancy series.

Discrepancy measures the deviation from uniformity of a point set.

The discrepancy of the point set $x_1, \dots\ x_n \in \left[\,0,1\,\right]^d$, $d \geq 1$, is defined

$$D_n^{(d)} = \sup_E \left| \frac{A(E;n)}{n} - \lambda(E) \right|,$$

where the supremum is over all subsets of [0, 1]^d of the form

$$E = [0,t_1) \times \ \ldots \ \times [0,t_d), \ 0 \le t_j \le 1, \ 1 \le j \le d,$$

λ is the Lebesque measure, and $A(E;n)$ is the number of the x_j contained in E.

The sequence x_1, x_2, … of points $[0,1]^d$ is a low-discrepancy sequence if there exists a constant $c(d)$, depending only on d, such that

$$D_n^{(d)} \le c(d) \frac{(\log n)^d}{n}$$

for all n>1.

Generalized Faure sequences can be defined for any prime base $b \ge d$. The lowest bound for the discrepancy is obtained for the smallest prime $b \ge d$, so the optional argument `NBASE` defaults to the smallest prime greater than or equal to the dimension.

The generalized Faure sequence x_1, x_2, …, is computed as follows:

Write the positive integer n in its b-ary expansion,

$$n = \sum_{i=0}^{\infty} a_i(n) b^i$$

where $a_i(n)$ are integers, $0 \le a_i(n) < b$.

The j-th coordinate of x_n is

$$x_n^{(j)} = \sum_{k=0}^{\infty} \sum_{d=0}^{\infty} c_{kd}^{(j)} a_d(n) b^{-k-1}, 1 \le j \le d$$

The generator matrix for the series, $c_{kd}^{(j)}$, is defined to be

$$c_{kd}^{(j)} = j^{d-k} c_{kd}$$

and c_{kd} is an element of the Pascal matrix,

$$c_{kd} = \begin{cases} \dfrac{d!}{c!(d-c)!} & k \le d \\ 0 & k > d \end{cases}$$

It is faster to compute a shuffled Faure sequence than to compute the Faure sequence itself. It can be shown that this shuffling preserves the low-discrepancy property.

The shuffling used is the b-ary Gray code. The function $G(n)$ maps the positive integer n into the integer given by its b-ary expansion.

The sequence computed by this function is $x(G(n))$, where x is the generalized Faure sequence.

Example

In this example, five points in the Faure sequence are computed. The points are in the three-dimensional unit cube.

Note that `FAURE_INIT` is used to create a structure that holds the state of the sequence. Each call to `FAURE_NEXT` returns the next point in the sequence and updates the `IMSL_FAURE` structure. The final call to `FAURE_FREE` frees data items, stored in the structure, that were allocated by `FAURE_INIT`.

```
      use faure_int
      implicit none
      type (s_imsl_faure), pointer  :: state
      real(kind(1e0))          :: x(3)
      integer,parameter :: ndim=3
      integer           :: k
!                              CREATE THE STRUCTURE THAT HOLDS
!                              THE STATE OF THE SEQUENCE.
      call faure_init(ndim, state)
!                              GET THE NEXT POINT IN THE SEQUENCE
      do k=1,5
         call faure_next(state, x)
         write(*,'(3F15.3)') x(1), x(2) , x(3)
      enddo
!                               FREE DATA ITEMS STORED IN
!                               state STRUCTURE
      call faure_free(state)
             end
```

Output

```
    0.334          0.493          0.064
    0.667          0.826          0.397
    0.778          0.270          0.175
    0.111          0.604          0.509
    0.445          0.937          0.842
```

IUMAG

This routine handles MATH/LIBRARY and STAT/LIBRARY type INTEGER options.

Required Arguments

PRODNM — Product name. Use either "MATH" or "STAT." (Input)

ICHP — Chapter number of the routine that uses the options. (Input)

IACT — 1 if user desires to "get" or read options, or 2 if user desires to "put" or write options. (Input)

NUMOPT — Size of IOPTS. (Input)

IOPTS — Integer array of size NUMOPT containing the option numbers to "get" or "put." (Input)

IVALS — Integer array containing the option values. These values are arrays corresponding to the individual options in IOPTS in sequential order. The size of IVALS is the sum of the sizes of the individual options. (Input/Output)

FORTRAN 90 Interface

Generic: CALL IUMAG (PRODNM, ICHP, IACT, NUMOPT, IOPTS, IVALS)

Specific: The specific interface name is IUMAG.

FORTRAN 77 Interface

Single: CALL IUMAG (PRODNM, ICHP, IACT, NUMOPT, IOPTS, IVALS)

Description

The Options Manager routine IUMAG reads or writes INTEGER data for some MATH/LIBRARY and STAT/LIBRARY codes. See Atchison and Hanson (1991) for more complete details.

There are MATH/LIBRARY routines in Chapters 1, 2, and 5 that now use IUMAG to communicate optional data from the user.

Comments

1. Users can normally avoid reading about options when first using a routine that calls `IUMAG`.

2. Let `I` be any value between 1 and `NUMOPT`. A negative value of `IOPTS(I)` refers to option number `–IOPTS(I)` but with a different effect: For a "get" operation, the default values are returned in `IVALS`. For a "put" operation, the default values replace the current values. In the case of a "put," entries of `IVALS` are not allocated by the user and are not used by `IUMAG`.

3. Both positive and negative values of `IOPTS` can be used.

4. `INTEGER` Options

   1 If the value is positive, print the next activity for any library routine that uses the Options Manager codes `IUMAG`, `SUMAG`, or `DUMAG`. Each printing step decrements the value if it is positive. Default value is 0.

   2 If the value is 2, perform error checking in `IUMAG`, `SUMAG` , and `DUMAG` such as the verifying of valid option numbers and the validity of input data. If the value is 1, do not perform error checking. Default value is 2.

   3 This value is used for testing the installation of `IUMAG` by other IMSL software. Default value is 3.

Example

The number of iterations allowed for the constrained least squares solver `LCLSQ` that calls `L2LSQ` is changed from the default value of max(*nra*, *nca*) to the value 6. The default value is restored after the call to `LCLSQ`. This change has no effect on the solution. It is used only for illustration. The first two arguments required for the call to `IUMAG` are defined by the product name, "MATH," and chapter number, 1, where `LCLSQ` is documented. The argument `IACT` denotes a write or "put" operation. There is one option to change so `NUMOPT` has the value 1. The arguments for the option number, 14, and the new value, 6, are defined by reading the documentation for `LCLSQ`.

```
      USE IUMAG_INT
      USE LCLSQ_INT
      USE UMACH_INT
      USE SNRM2_INT

      IMPLICIT     NONE
!
!     Solve the following in the least squares sense:
!           3x1 + 2x2 +  x3 = 3.3
!           4x1 + 2x2 +  x3 = 2.3
!           2x1 + 2x2 +  x3 = 1.3
!            x1 +  x2 +  x3 = 1.0
!
!     Subject to:  x1 + x2 + x3 <= 1
!                  0 <= x1 <= .5
```

```
!                   0 <= x2 <= .5
!                   0 <= x3 <= .5
!
! ----------------------------------------------------------------------
!                                 Declaration of variables
!
      INTEGER    ICHP, IPUT, LDA, LDC, MCON, NCA, NEWMAX, NRA, NUMOPT
      PARAMETER  (ICHP=1, IPUT=2, MCON=1, NCA=3, NEWMAX=14, NRA=4, &
                NUMOPT=1, LDA=NRA, LDC=MCON)
!
      INTEGER    IOPT(1), IRTYPE(MCON), IVAL(1), NOUT
      REAL       A(LDA,NCA), B(NRA), BC(MCON), C(LDC,NCA), RES(NRA), &
                RESNRM, XLB(NCA), XSOL(NCA), XUB(NCA)
!                                 Data initialization
!
      DATA A/3.0E0, 4.0E0, 2.0E0, 1.0E0, 2.0E0, 2.0E0, 2.0E0, 1.0E0, &
          1.0E0, 1.0E0, 1.0E0, 1.0E0/, B/3.3E0, 2.3E0, 1.3E0, 1.0E0/, &
          C/3*1.0E0/, BC/1.0E0/, IRTYPE/1/, XLB/3*0.0E0/, XUB/3*.5E0/
! ----------------------------------------------------------------------
!
!                                 Reset the maximum number of

!                                 iterations to use in the solver.
!                                 The value 14 is the option number.
!                                 The value 6 is the new maximum.
      IOPT(1) = NEWMAX
      IVAL(1) = 6
      CALL IUMAG ('math', ICHP, IPUT, NUMOPT, IOPT, IVAL)
!                                 -------------------------------------
!                                 ---------------------------------
!
!                                 Solve the bounded, constrained
!                                 least squares problem.
!
      CALL LCLSQ (A, B, C, BC, B, IRTYPE, XLB, XUB, XSOL, RES=RES)

!                                 Compute the 2-norm of the residuals.
      RESNRM = SNRM2(NRA,RES,1)
!                                 Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) XSOL, RES, RESNRM
!                                 -------------------------------------
!                                 ---------------------------------
!                                 Reset the maximum number of
!                                 iterations to its default value.
!                                 This is not required but is
!                                 recommended programming practice.
      IOPT(1) = -IOPT(1)
      CALL IUMAG ('math', ICHP, IPUT, NUMOPT, IOPT, IVAL)
!                                 -------------------------------------
!                                 ---------------------------------
!
99999 FORMAT ('  The solution is ', 3F9.4, //, '  The residuals ', &
             'evaluated at the solution are ', /, 18X, 4F9.4, //, &
             '  The norm of the residual vector is ', F8.4)
!
      END
```

Output

```
 The solution is    0.5000   0.3000   0.2000

 The residuals evaluated at the solution are
                  -1.0000   0.5000   0.5000   0.0000
```

```
    The norm of the residual vector is   1.2247
```

UMAG

This routine handles MATH/LIBRARY and STAT/LIBRARY type REAL and double precision options.

Required Arguments

PRODNM — Product name. Use either "MATH" or "STAT." (Input)

ICHP — Chapter number of the routine that uses the options. (Input)

IACT — 1 if user desires to "get" or read options, or 2 if user desires to "put" or write options. (Input)

IOPTS — Integer array of size NUMOPT containing the option numbers to "get" or "put." (Input)

SVALS — Array containing the option values. These values are arrays corresponding to the individual options in IOPTS in sequential order. The size of SVALS is the sum of the sizes of the individual options. (Input/Output)

Optional Arguments

NUMOPT — Size of IOPTS. (Input)
Default: NUMOPT = size (IOPTS,1).

FORTRAN 90 Interface

Generic: CALL UMAG (PRODNM, ICHP, IACT, IOPTS, SVALS [, …])

Specific: The specific interface names are S_UMAG and D_UMAG.

FORTRAN 77 Interface

Single: CALL SUMAG (PRODNM, ICHP, IACT, NUMOPT, IOPTS, SVALS)

Double: The double precision name is DUMAG.

Description

The Options Manager routine SUMAG reads or writes REAL data for some MATH/LIBRARY and STAT/LIBRARY codes. See Atchison and Hanson (1991) for more complete details. There are MATH/LIBRARY routines in Chapters 1 and 5 that now use SUMAG to communicate optional data from the user.

Comments

1. Users can normally avoid reading about options when first using a routine that calls SUMAG.
2. Let I be any value between 1 and NUMOPT. A negative value of IOPTS(I) refers to option number –IOPTS(I) but with a different effect: For a "get" operation, the default values are returned in SVALS. For a "put" operation, the default values replace the current values. In the case of a "put," entries of SVALS are not allocated by the user and are not used by SUMAG.
3. Both positive and negative values of IOPTS can be used.
4. Floating Point Options

   1 This value is used for testing the installation of SUMAG by other IMSL software. Default value is 3.0E0.

Example

The rank determination tolerance for the constrained least squares solver LCLSQ that calls L2LSQ is changed from the default value of SQRT(AMACH(4)) to the value 0.01. The default value is restored after the call to LCLSQ. This change has no effect on the solution. It is used only for illustration. The first two arguments required for the call to SUMAG are defined by the product name, "MATH," and chapter number, 1, where LCLSQ is documented. The argument IACT denotes a write or "put" operation. There is one option to change so NUMOPT has the value 1. The arguments for the option number, 2, and the new value, 0.01E+0, are defined by reading the documentation for LCLSQ.

```
      USE UMAG_INT
      USE LCLSQ_INT
      USE UMACH_INT
      USE SNRM2_INT

      IMPLICIT     NONE
!
!     Solve the following in the least squares sense:
!           3x1 + 2x2 +  x3 = 3.3
!           4x1 + 2x2 +  x3 = 2.3
!           2x1 + 2x2 +  x3 = 1.3
!            x1 +  x2 +  x3 = 1.0
!
!     Subject to:  x1 + x2 + x3 <= 1
!                  0 <= x1 <= .5
!                  0 <= x2 <= .5
!                  0 <= x3 <= .5
!
! ----------------------------------------------------------------------
!                                Declaration of variables
!
      INTEGER    ICHP, IPUT, LDA, LDC, MCON, NCA, NEWTOL, NRA, NUMOPT
      PARAMETER  (ICHP=1, IPUT=2, MCON=1, NCA=3, NEWTOL=2, NRA=4, &
                 NUMOPT=1, LDA=NRA, LDC=MCON)
!
      INTEGER    IOPT(1), IRTYPE(MCON), NOUT
```

```
      REAL       A(LDA,NCA), B(NRA), BC(MCON), C(LDC,NCA), RES(NRA), &
                RESNRM, SVAL(1), XLB(NCA), XSOL(NCA), XUB(NCA)
!                                 Data initialization
!
      DATA A/3.0E0, 4.0E0, 2.0E0, 1.0E0, 2.0E0, 2.0E0, 2.0E0, 1.0E0, &
          1.0E0, 1.0E0, 1.0E0, 1.0E0/, B/3.3E0, 2.3E0, 1.3E0, 1.0E0/, &
          C/3*1.0E0/, BC/1.0E0/, IRTYPE/1/, XLB/3*0.0E0/, XUB/3*.5E0/
! ----------------------------------------------------------------------
!
!                                 Reset the rank determination
!                                 tolerance used in the solver.
!                                 The value 2 is the option number.
!                                 The value 0.01 is the new tolerance.
!
      IOPT(1) = NEWTOL
      SVAL(1) = 0.01E+0
      CALL UMAG ('math', ICHP, IPUT, IOPT, SVAL)
!                                 -------------------------------------
!                                 ---------------------------------
!
!                                 Solve the bounded, constrained
!                                 least squares problem.
!
      CALL LCLSQ (A, B, C, BC, BC, IRTYPE, XLB, XUB, XSOL, RES=RES)
!                                 Compute the 2-norm of the residuals.
      RESNRM = SNRM2(NRA,RES,1)
!                                 Print results
      CALL UMACH (2, NOUT)
      WRITE (NOUT,99999) XSOL, RES, RESNRM
!                                 -------------------------------------
!                                 ---------------------------------

!                                 Reset the rank determination
!                                 tolerance to its default value.
!                                 This is not required but is
!                                 recommended programming practice.
      IOPT(1) = -IOPT(1)
      CALL UMAG ('math', ICHP, IPUT, IOPT, SVAL)
!                                 -------------------------------------
!                                 ---------------------------------
!
99999 FORMAT ('  The solution is ', 3F9.4, //, '  The residuals ', &
            'evaluated at the solution are ', /, 18X, 4F9.4, //, &
            '  The norm of the residual vector is ', F8.4)
!
      END
```

Output

```
  The solution is    0.5000   0.3000   0.2000

  The residuals evaluated at the solution are
                  -1.0000   0.5000   0.5000   0.0000

  The norm of the residual vector is   1.2247
```

DUMAG

See `UMAG`.

PLOTP

Prints a plot of up to 10 sets of points.

Required Arguments

X — Vector of length NDATA containing the values of the independent variable. (Input)

A — Matrix of dimension NDATA by NFUN containing the NFUN sets of dependent variable values. (Input)

SYMBOL — CHARACTER string of length NFUN. (Input)
SYMBOL(I : I) is the symbol used to plot function I.

XTITLE — CHARACTER string used to label the *x*-axis. (Input)

YTITLE — CHARACTER string used to label the *y*-axis. (Input)

TITLE — CHARACTER string used to label the plot. (Input)

Optional Arguments

NDATA — Number of independent variable data points. (Input)
Default: NDATA = size (X,1).

NFUN — Number of sets of points. (Input)
NFUN must be less than or equal to 10.
Default: NFUN = size (A,2).

LDA — Leading dimension of A exactly as specified in the dimension statement of the calling program. (Input)
Default: LDA = size (A,1).

INC — Increment between elements of the data to be used. (Input)
PLOTP plots X(1 + (I − 1) * INC) for I = 1, 2, …, NDATA.
Default: INC = 1.

RANGE — Vector of length four specifying minimum *x*, maximum *x*, minimum *y* and maximum *y*. (Input)
PLOTP will calculate the range of the axis if the minimum and maximum of that range are equal.
Default: RANGE = 1.e0.

FORTRAN 90 Interface

Generic: CALL PLOTP (X, A, SYMBOL, XTITLE, YTITLE, TITLE [, …])

Specific: The specific interface names are S_PLOTP and D_PLOTP.

FORTRAN 77 Interface

Single: CALL PLOTP (NDATA, NFUN, X, A, LDA, INC, RANGE, SYMBOL, XTITLE, YTITLE, TITLE)

Double: The double precision name is DPLOTP.

Description

Routine PLOTP produces a line printer plot of up to ten sets of points superimposed upon the same plot. A character "M" is printed to indicate multiple points. The user may specify the *x* and *y*-axis plot ranges and plotting symbols. Plot width and length may be reset in advance by calling PGOPT.

Comments

1. Informational errors

Type	Code	Description
3	7	NFUN is greater than 10. Only the first 10 functions are plotted.
3	8	TITLE is too long. TITLE is truncated from the right side.
3	9	YTITLE is too long. YTITLE is truncated from the right side.
3	10	XTITLE is too long. XTITLE is truncated from the right side. The maximum number of characters allowed depends on the page width and the page length. See Comment 5 below for more information.

2. YTITLE and TITLE are automatically centered.

3. For multiple plots, the character M is used if the same print position is shared by two or more data sets.

4. Output is written to the unit specified by UMACH (see *Reference Material*).

5. Default page width is 78 and default page length is 60. They may be changed by calling PGOPT in advance.

Example

This example plots the sine and cosine functions from − 3.5 to + 3.5 and sets page width and length to 78 and 40, respectively, by calling PGOPT in advance.

```
      USE PLOTP_INT
      USE CONST_INT
      USE PGOPT_INT

      IMPLICIT   NONE
      INTEGER    I, IPAGE
      REAL       A(200,2), DELX, PI, RANGE(4), X(200)
      CHARACTER  SYMBOL*2
      INTRINSIC  COS, SIN
!
      DATA SYMBOL/'SC'/
      DATA RANGE/-3.5, 3.5, -1.2, 1.2/
!
      PI     = 3.14159
      DELX   = 2.*PI/199.
      DO 10  I= 1, 200
         X(I)   = -PI + FLOAT(I-1) * DELX
         A(I,1) = SIN(X(I))
         A(I,2) = COS(X(I))
   10 CONTINUE
!                                 Set page width and length
      IPAGE = 78
      CALL PGOPT (-1, IPAGE)
      IPAGE = 40
      CALL PGOPT (-2, IPAGE)
      CALL PLOTP (X, A, SYMBOL, 'X AXIS', 'Y AXIS', ' C = COS,   S = SIN', &
      RANGE=RANGE)
!
      END
```

Output

```
                          C = COS,   S = SIN

          1.2 ::::+:::::::::::::::+:::::::::::::::+:::::::::::::::+::::
              .                           I                           .
              .                           I                           .
              .                        CCCCCCC     SSSSSSSS           .
              .                       CC  I  CC   SS      SS          .
         0.8 +                      C    I    C SS        SS         +
              .                     C     I     MS          SS        .
              .                    C      I    SSC           SS       .
              .                   CC      I   SS CC           SS      .
              .                  CC       I   S   CC           S      .
         0.4 +                  C        I  S     C            S     +
              .                 C         I SS      C           SS    .
 Y            .                CC         I S       CC           S    .
              .                C          IS         C            S   .
 A            .               C           SS          C           SS  .
 X        0.0 +--S-----------CC-----------S-----------CC-----------S--+
 I            .  SS         CC           SS            CC             .
 S            .   S         C            SI             C             .
              .    S       CC           S I             CC            .
              .    SS      C           SS I              C            .
         -0.4 +     S     C            S  I               C           +
              .      S   CC           S   I               CC          .
              .      SS CC           SS   I                CC         .
```

```
          .       SSC            SS     I                 C         .
          .        MS           SS      I                  C        .
     -0.8 +       C SS         SS       I                   C       +
          .     CC   SS       SS        I                    CC     .
          .  CCCC     SSSSSSSS          I                     CCCC  .
          .  C                          I                        C  .
          .                             I                           .
     -1.2 ::::+:::::::::::::::+:::::::::::::::+:::::::::::::::+::::
             -3              -1               1               3
                                     X AXIS
```

PRIME

Decomposes an integer into its prime factors.

Required Arguments

N — Integer to be decomposed. (Input)

NPF — Number of different prime factors of ABS(N). (Output)
If N is equal to −1, 0, or 1, NPF is set to 0.

IPF — Integer vector of length 13. (Output)
IPF(I) contains the prime factors of the absolute value of N, for I = 1, …, NPF. The remaining 13 − NPF locations are not used.

IEXP — Integer vector of length 13. (Output)
IEXP(I) is the exponent of IPF(I), for I = 1, …, NPF. The remaining 13 − NPF locations are not used.

IPW — Integer vector of length 13. (Output)
IPW(I) contains the quantity IPF(I)**IEXP(I), for I = 1, …, NPF. The remaining 13 − NPF locations are not used.

FORTRAN 90 Interface

Generic: CALL PRIME (N, NPF, IPF, IPW)

Specific: The specific interface name is PRIME.

FORTRAN 77 Interface

Single: CALL PRIME (N, NPF, IPF, IEXP, IPW)

Description

Routine PRIME decomposes an integer into its prime factors. The number to be factored, *N*, may not have more than 13 distinct factors. The smallest number with more than 13 factors is about 1.3×10^{16}. Most computers do not allow integers of this size.

The routine PRIME is based on a routine by Brenner (1973).

Comments

1. The output from PRIME should be interpreted in the following way:
   ABS(N) = IPF(1)**IEXP(1) * … * IPF(NPF)**IEXP(NPF).

Example

This example factors the integer 144 = $2^4 3^2$.

```
      USE PRIME_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    N
      PARAMETER  (N=144)
!
      INTEGER    IEXP(13), IPF(13), IPW(13), NOUT, NPF
!                                 Get prime factors of 144
      CALL PRIME (N, NPF, IPF, IEXP, IPW)
!                                 Get output unit number
      CALL UMACH (2, NOUT)
!                                 Print results
      WRITE (NOUT,99999) N, IPF(1), IPF(2), IEXP(1), IEXP(2), IPW(1), &
                       IPW(2), NPF
!
99999 FORMAT ('  The prime factors for', I5, ' are: ', /, 10X, 2I6, // &
             '  IEXP =', 2I6, /, '  IPW  =', 2I6, /, '  NPF  =', I6, /)
      END
```

Output

```
  The prime factors for  144 are:
               2     3

  IEXP =     4     2
  IPW  =    16     9
  NPF  =     2
```

CONST

This function returns the value of various mathematical and physical constants.

Function Return Value

CONST — Value of the constant. (Output)
See Comment 1.

Required Arguments

NAME — Character string containing the name of the desired constant. (Input)
See Comment 3 for a list of valid constants.

FORTRAN 90 Interface

Generic: `CONST (NAME)`

Specific: The specific interface names are `S_CONST` and `D_CONST`.

FORTRAN 77 Interface

Single: `CONST (NAME)`

Double: The double precision name is `DCONST`.

Description

Routine `CONST` returns the value of various mathematical and physical quantities. For all of the physical values, the Systeme International d'Unites (SI) are used.

The reference for constants are indicated by the code in [ ] Comment above.

[1]Cohen and Taylor (1986)

[2]Liepman (1964)

[3]Precomputed mathematical constants

The constants marked with an `E` before the [ ] are exact (to machine precision).

To change the units of the values returned by `CONST`, see `CUNIT`.

Comments

1. If the generic version of this function is used, the immediate result must be stored in a variable before use in an expression. For example:

   ```
   X = CONST('PI')
   Y = COS(x)
   ```

   must be used rather than

   `Y = COS(CONST('PI'))`.

   If this is too much of a restriction on the programmer, then the specific name can be used without this restriction.

2. The case of the character string in `NAME` does not matter. The names "`PI`", "`Pi`", "`Pi`", and "`pi`" are equivalent.

3. The units of the physical constants are in `SI` units (meter kilogram-second).

4. The names allowed are as follows:

Name	Description	Value	Ref.
`AMU`	Atomic mass unit	1.6605402E – 27 kg	[1]
`ATM`	Standard atm pressure	1.01325E + 5N/m^2E	[2]
`AU`	Astronomical unit	1.496E + 11m	[ ]
Avogadro	Avogadro's number	6.0221367E + 231/mole	[1]
Boltzman	Boltzman's constant	1.380658E – 23J/K	[1]
C	Speed of light	2.997924580E + 8m/sE	[1]
Catalan	Catalan's constant	0.915965 ... E	[3]
E	Base of natural logs	2.718...E	[3]
ElectronCharge	Electron change	1.60217733E –19C	[1]
ElectronMass	Electron mass	9.1093897E – 31 kg	[1]
ElectronVolt	Electron volt	1.60217733E – 19J	[1]
Euler	Euler's constant gamma	0.577 ... E	[3]
Faraday	Faraday constant	9.6485309E + 4C/mole	[1]
FineStructure	fine structure	7.29735308E – 3	[1]
Gamma	Euler's constant	0.577 ... E	[3]

Name	Description	Value	Ref.
Gas	Gas constant	8.314510J/mole/k	[1]
Gravity	Gravitational constant	$6.67259E - 11N * m^2/kg^2$	[1]
Hbar	Planck constant / 2 pi	$1.05457266E - 34J * s$	[1]
PerfectGasVolume	Std vol ideal gas	$2.241383E - 2m^3$/mole	[*]
Pi	Pi	3.141 ... E	[3]
Planck	Planck's constant *h*	$6.6260755E - 34J * s$	[1]
ProtonMass	Proton mass	1.6726231E – 27 kg	[1]
Rydberg	Rydberg's constant	$1.0973731534E + 7/m$	[1]
SpeedLight	Speed of light	$2.997924580E + 8m/s$ E	[1]
StandardGravity	Standard *g*	$9.80665m/s^2$E	[2]
StandardPressure	Standard atm pressure	$1.01325E + 5N/m^2$E	[2]
StefanBoltzmann	Stefan-Boltzman	$5.67051E - 8W/K^4/m^2$	[1]
WaterTriple	Triple point of water	2.7316E + 2K E	[2]

Example

In this example, Euler's constant γ is obtained and printed. Euler's constant is defined to be

$$\gamma = \lim_{n\to\infty}\left[\sum_{k=1}^{n-1}\frac{1}{k} - \ln\ n\right]$$

```
      USE CONST_INT
      USE UMACH_INT

      IMPLICIT   NONE
      INTEGER    NOUT
      REAL       GAMA
!                                 Get output unit number
      CALL UMACH (2, NOUT)
!                                 Get gamma
      GAMA = CONST('GAMMA')
!                                 Print gamma
      WRITE (NOUT,*) 'GAMMA = ', GAMA
      END
```

Output

```
GAMMA =  0.5772157
```

For another example, see `CUNIT`.

CUNIT

Converts X in units XUNITS to Y in units YUNITS.

Required Arguments

X — Value to be converted. (Input)

XUNITS — Character string containing the name of the units for X. (Input)
See Comments for a description of units allowed.

Y — Value in YUNITS corresponding to X in XUNITS. (Output)

YUNITS — Character string containing the name of the units for Y. (Input)
See Comments for a description of units allowed.

FORTRAN 90 Interface

Generic: CALL CUNIT (X, XUNITS, Y, YUNITS [, …])

Specific: The specific interface names are S_CUNIT and D_CUNIT.

FORTRAN 77 Interface

Single: CALL CUNIT (X, XUNITS, Y, YUNITS)

Double The double precision name is DCUNIT.

Description

Routine CUNIT converts a value expressed in one set of units to a value expressed in another set of units.

The input and output units are checked for consistency unless the input unit is "SI". SI means the Systeme International d'Unites. This is the meter−kilogram−second form of the metric system. If the input units are "SI", then the input is assumed to be expressed in the SI units consistent with the output units.

Comments

1. Strings XUNITS and YUNITS have the form $U_1 * U_2 * \ldots * U_m/V_1 \ldots V_n$, where U_i and V_i are the names of basic units or are the names of basic units raised to a power. Examples are, "METER * KILOGRAM/SECOND", "M * KG/S", "METER", or "M/KG^2".

2. The case of the character string in XUNITS and YUNITS does not matter. The names "METER", "Meter" and "meter" are equivalent.

3. If XUNITS is "SI", then X is assumed to be in the standard international units corresponding to YUNITS. Similarly, if YUNITS is "SI", then Y is assumed to be in the standard international units corresponding to XUNITS.

4. The basic unit names allowed are as follows:

   Units of time
      day, hour = hr, min = minute, s = sec = second, year
   Units of frequency
      Hertz = Hz
   Units of mass
      AMU, g = gram, lb = pound, ounce = oz, slug
   Units of distance
      Angstrom, AU, feet = foot = ft, in = inch, m = meter = metre, micron, mile, mill, parsec, yard
   Units of area
      acre
   Units of volume
      l = liter = litre
   Units of force
      dyne, N = Newton, poundal
   Units of energy
      BTU(thermochemical), Erg, J = Joule
   Units of work
      W = watt
   Units of pressure
      ATM = atomosphere, bar, Pascal
   Units of temperature
      degC = Celsius, degF = Fahrenheit, degK = Kelvin
   Units of viscosity
      poise, stoke
   Units of charge
      Abcoulomb, C = Coulomb, statcoulomb
   Units of current
      A = ampere, abampere, statampere,
   Units of voltage
      Abvolt, V = volt

Units of magnetic induction
T = Tesla, Wb = Weber

Other units
1, farad, mole, Gauss, Henry, Maxwell, Ohm

The following metric prefixes may be used with the above units. Note that the one or two letter prefixes may only be used with one letter unit abbreviations.

A	Atto	1.E – 18
F	Femto	1.E – 15
P	Pico	1.E – 12
N	Nano	1.E – 9
U	Micro	1.E – 6
M	Milli	1.E – 3
C	Centi	1.E – 2
D	Deci	1.E – 1
DK	Deca	1.E + 2
K	Kilo	1.E + 3
	Myriad	1.E + 4 (no single letter prefix; M means milli
	Mega	1.E + 6 (no single letter prefix; M means milli
G	Giga	1.E + 9
T	Tera	1.E + 12

5. Informational error

Type	Code	Description
3	8	A conversion of units of mass to units of force was required for consistency.

Example

The routine CONST is used to obtain the speed on light, *c*, in SI units. CUNIT is then used to convert *c* to mile/second and to parsec/year. An example involving substitution of force for mass is required in conversion of Newtons/Meter^2 to Pound/Inch^2.

```
      USE CONST_INT
      USE CUNIT_INT
      USE UMACH_INT

      IMPLICIT    NONE
      INTEGER    NOUT
```

```
      REAL       CMH, CMS, CPY, CPSI
!                                 Get output unit number
      CALL UMACH (2, NOUT)
!                                 Get speed of light in SI (m/s)
      CMS = CONST('SpeedLight')
      WRITE (NOUT,*) 'Speed of Light = ', CMS, ' meter/second'
!                                 Get speed of light in mile/second
      CALL CUNIT (CMS, 'SI', CMH, 'Mile/Second')
      WRITE (NOUT,*) 'Speed of Light = ', CMH, ' mile/second'
!                                 Get speed of light in parsec/year
      CALL CUNIT (CMS, 'SI', CPY, 'Parsec/Year')
      WRITE (NOUT,*) 'Speed of Light = ', CPY, ' Parsec/Year'
!                                 Convert Newton/Meter**2 to
!                                 Pound/Inch**2.
      CALL CUNIT(1.E0, 'Newton/Meter**2', CPSI, &
                'Pound/Inch**2')
      WRITE(NOUT,*)' Atmospheres, in Pound/Inch**2 = ',CPSI
      END
```

Output

```
Speed of Light =  299792440.0  meter/second
Speed of Light =  186282.39  mile/second
Speed of Light =  0.3063872  Parsec/Year

*** WARNING  ERROR 8 from CUNIT.  A conversion of units of mass to units of
***          force was required for consistency.
Atmospheres, in Pound/Inch**2 =  1.4503773E-4
```

HYPOT

This functions computes SQRT(A**2 + B**2) without underflow or overflow.

Function Return Value

HYPOT — SQRT(A**2 + B**2). (Output)

Required Arguments

A — First parameter. (Input)

B — Second parameter. (Input)

FORTRAN 90 Interface

Generic: HYPOT (A, B)

Specific: The specific interface names are S_HYPOT and D_HYPOT.

FORTRAN 77 Interface

Single: HYPOT (A, B)

Double: The double precision name is DHYPOT.

Description

Routine HYPOT is based on the routine PYTHAG, used in EISPACK 3. This is an update of the work documented in Garbow et al. (1972).

Example

Computes

$$c = \sqrt{a^2 + b^2}$$

where $a = 10^{20}$ and $b = 2 \times 10^{20}$ without overflow.

```
      USE HYPOT_INT
      USE UMACH_INT

      IMPLICIT    NONE
!                                  Declare variables
      INTEGER    NOUT
      REAL       A, B, C
!
      A = 1.0E+20
      B = 2.0E+20
      C = HYPOT(A,B)
!                                  Get output unit number
      CALL UMACH (2, NOUT)
!                                  Print the results
      WRITE (NOUT,'(A,1PE10.4)') ' C = ', C
      END
```

Output

```
C = 2.2361E+20
```

MP_SETUP

more...

Initializes or finalizes MPI.

Function Return Value

Number of nodes, MP_NPROCS, in the communicator, MP_LIBRARY_WORLD. (Output)
Returned when MP_SETUP is called with no arguments:
MP_NPROCS = MP_SETUP ().

Required Argument

None.

Optional Arguments

NOTE — Character string 'Final'. (Input)
With 'Final' all pending error messages are sent from the nodes to the root and printed. If any node should STOP after printing messages, then MPI_Finalize() and a STOP are executed. Otherwise, only MPI_Finalize() is called. The character string 'Final' is the only valid string for this argument.

N — Size of array to be allocated for timing. (Input)
When this argument is supplied, the array MPI_NODE_PRIORITY is allocated with MP_PROCS components. The matrix products A .x. B are timed individually at each node of the machine. The elapsed time is noted and sorted to determine the node priority order. A and B are allocated to size N by N, and initialized with random data. The priority order is finally broadcast to the other nodes.

FORTRAN 90 Interface

MP_SETUP ([,…])

Description

Following a call to the function `MP_SETUP()`, the module `MPI_node_int` will contain information about the number of processors, the rank of a processor, the communicator for IMSL Fortran Numerical Library, and the usage priority order of the node machines:

```
MODULE MPI_NODE_INT

 INTEGER, ALLOCATABLE :: MPI_NODE_PRIORITY(:)

 INTEGER, SAVE :: MP_LIBRARY_WORLD = huge(1)

 LOGICAL, SAVE :: MPI_ROOT_WORKS = .TRUE.

 INTEGER, SAVE :: MP_RANK = 0, MP_NPROCS = 1

END MODULE
```

When the function `MP_SETUP()` is called with no arguments, the following events occur:

- If MPI has not been initialized, it is first initialized. This step uses the routines MPI_Initialized() and possibly `MPI_Init()`. Users who choose not to call `MP_SETUP()` must make the required initialization call before using any IMSL Fortran Numerical Library code that relies on MPI for its execution. If the user's code calls an IMSL Fortran Numerical Library function utilizing the box data type and MPI has not been initialized, then the computations are performed on the root node. The only MPI routine always called in this context is `MPI_Initialized()`. The name `MP_SETUP` is pushed onto the subprogram or call stack.
- If `MP_LIBRARY_WORLD` equals its initial value (=`huge(1)`) then `MPI_COMM_WORLD`, the default MPI communicator, is duplicated and becomes its handle. This uses the routine `MPI_Comm_dup()`. Users can change the handle of `MP_LIBRARY_WORLD` as required by their application code. Often this issue can be ignored.
- The integers `MP_RANK` and `MP_NPROCS` are respectively the node's rank and the number of nodes in the communicator, `MP_LIBRARY_WORLD`. Their values require the routines `MPI_Comm_size()` and `MPI_Comm_rank()`. The default values are important when MPI is not initialized and a box data type is computed. In this case the root node is the only node and it will do all the work. No calls to MPI communication routines are made when `MP_NPROCS = 1` when computing the box data type functions. A program can temporarily assign this value to force box data type computation entirely at the root node. This is desirable for problems where using many nodes would be less efficient than using the root node exclusively.
- `The array MPI_NODE_PRIORITY(:)` is not allocated unless the user allocates it. The IMSL Fortran Numerical Library codes use this array for assigning tasks to processors, if it is allocated. If it is not allocated, the default priority of the nodes is

(`0,1,...,MP_NPROCS-1`). Use of the function call `MP_SETUP(N)` allocates the array, as explained below. Once the array is allocated its size is `MP_NPROCS`. The contents of the array is a permutation of the integers `0,...,MP_NPROCS-1`. Nodes appearing at the start of the list are used first for parallel computing. A node other than the root can avoid any computing, except receiving the schedule, by setting the value `MPI_NODE_PRIORITY(I)` < 0. This means that node `|MPI_NODE_PRIORITY(I)|` will be sent the task schedule but will not perform any significant work as part of box data type function evaluations.

- The `LOGICAL` flag `MPI_ROOT_WORKS` designates whether or not the root node participates in the major computation of the tasks. The root node communicates with the other nodes to complete the tasks but can be designated to do no other work. Since there may be only one processor, this flag has the default value `.TRUE.`, assuring that one node exists to do work. When more than one processor is available users can consider assigning `MPI_ROOT_WORKS=.FALSE.`. This is desirable when the alternate nodes have equal or greater computational resources compared with the root node. Parallel Example 4 illustrates this usage. A single problem is given a box data type, with one rack. The computing is done at the node, other than the root, with highest priority. This example requires more than one processor since the root does no work.

When the generic function `MP_SETUP(N)` is called, where `N` is a positive integer, a call to `MP_SETUP()` is first made, using no argument. Use just one of these calls to `MP_SETUP()`. This initializes the MPI system and the other parameters described above. The array `MPI_NODE_PRIORITY(:)` is allocated with size `MP_NPROCS`. Then `DOUBLE PRECISION` matrix products $C = AB$, where A and B are N by N matrices, are computed at each node and the elapsed time is recorded. These elapsed times are sorted and the contents of `MPI_NODE_PRIORITY(:)` are permuted in accordance with the shortest times yielding the highest priority. All the nodes in the communicator `MP_LIBRARY_WORLD` are timed. The array `MPI_NODE_PRIORITY(:)` is then broadcast from the root to the remaining nodes of `MP_LIBRARY_WORLD` using the routine `MPI_Bcast()`. Timing matrix products to define the node priority is relevant because the effort to compute C is comparable to that of many linear algebra computations of similar size. Users are free to define their own node priority and broadcast the array `MPI_NODE_PRIORITY(:)` to the alternate nodes in the communicator.

To print any IMSL Fortran Numerical Library error messages that have occurred at any node, and to finalize MPI, use the function call `MP_SETUP('Final')`. The case of the string '`Final`' is not important. Any error messages pending will be discarded after printing on the root node. This is triggered by popping the name '`MP_SETUP`' from the subprogram stack or returning to Level 1 in the stack. Users can obtain error messages by popping the stack to Level 1 and still continuing with MPI calls. This requires executing `call e1pop ('MP_SETUP')`. To continue on after summarizing errors execute `call e1psh ('MP_SETUP')`. More details about the error processor are found in Reference Material chapter of this manual.

Messages are printed by nodes from largest rank to smallest, which is the root node. Use of the routine `MPI_Finalize()` is made within `MP_SETUP('Final')`, which shuts down MPI. After `MPI_Finalize()` is called, the value of `MP_NPROCS = 0`. This flags that MPI has been initialized and terminated. It cannot be initialized again in the same program unit execution. No MPI routine is defined when `MP_NPROCS` has this value.

Examples

Parallel Example (parallel_ex01.f90)

```
      use linear_operators
      use mpi_setup_int

      implicit none

! This is the equivalent of Parallel Example 1 for .ix., with box data types
! and functions.

      integer, parameter :: n=32, nr=4
      real(kind(1e0)) :: one=1e0
      real(kind(1e0)), dimension(n,n,nr) :: A, b, x, err(nr)

! Setup for MPI.
      MP_NPROCS=MP_SETUP()

! Generate random matrices for A and b:
      A = rand(A); b=rand(b)

! Compute the box solution matrix of Ax = b.
      x = A .ix. b

! Check the results.
      err = norm(b - (A .x. x))/(norm(A)*norm(x)+norm(b))
      if (ALL(err <= sqrt(epsilon(one))) .and. MP_RANK == 0) &
        write (*,*) 'Parallel Example 1 is correct.'

! See to any error messages and quit MPI.
      MP_NPROCS=MP_SETUP('Final')

      end
```

Parallel Example (parallel_ex04.f90)

Here an alternate node is used to compute the majority of a single application, and the user does not need to make any explicit calls to MPI routines. The time-consuming parts are the evaluation of the eigenvalue-eigenvector expansion, the solving step, and the residuals. To do this, the rank-2 arrays are changed to a box data type with a unit third dimension. This uses parallel computing. The node priority order is established by the initial function call, `MP_SETUP(n)`. The root is restricted from working on the box data type by assigning `MPI_ROOT_WORKS=.false.`. This example anticipates that the most efficient node, other than the root, will perform the heavy computing. Two nodes are required to execute.

```
      use linear_operators
      use mpi_setup_int

      implicit none
```

```
! This is the equivalent of Parallel Example 4 for matrix exponential.
! The box dimension has a single rack.
      integer, parameter :: n=32, k=128, nr=1
      integer i
      real(kind(1e0)), parameter :: one=1e0, t_max=one, delta_t=t_max/(k-1)
      real(kind(1e0)) err(nr), sizes(nr), A(n,n,nr)
      real(kind(1e0)) t(k), y(n,k,nr), y_prime(n,k,nr)
      complex(kind(1e0)), dimension(n,nr) :: x(n,n,nr), z_0, &
        Z_1(n,nr,nr), y_0, d

! Setup for MPI.  Establish a node priority order.
! Restrict the root from significant computing.
! Illustrates using the 'best' performing node that
! is not the root for a single task.
      MP_NPROCS=MP_SETUP(n)

      MPI_ROOT_WORKS=.false.

! Generate a random coefficient matrix.
      A = rand(A)

! Compute the eigenvalue-eigenvector decomposition
! of the system coefficient matrix on an alternate node.
      D = EIG(A, W=X)

! Generate a random initial value for the ODE system.
      y_0 = rand(y_0)

! Solve complex data system that transforms the initial
! values, X z_0=y_0.

      z_1= X .ix. y_0 ; z_0(:,nr) = z_1(:,nr,nr)

! The grid of points where a solution is computed:
      t = (/(i*delta_t,i=0,k-1)/)


! Compute y and y' at the values t(1:k).
! With the eigenvalue-eigenvector decomposition AX = XD, this
! is an evaluation of EXP(A t)y_0 = y(t).
      y = X .x.exp(spread(d(:,nr),2,k)*spread(t,1,n))*spread(z_0(:,nr),2,k)

! This is y', derived by differentiating y(t).
      y_prime  = X .x. &
spread(d(:,nr),2,k)*exp(spread(d(:,nr),2,k)*spread(t,1,n))* &
                spread(z_0(:,nr),2,k)

! Check results. Is  y' - Ay = 0?
      err = norm(y_prime-(A .x. y))
      sizes=norm(y_prime)+norm(A)*norm(y)
      if (ALL(err <= sqrt(epsilon(one))*sizes) .and. MP_RANK == 0) &
        write (*,*) 'Parallel Example 4 is correct.'

! See to any error messages and quit MPI.
      MP_NPROCS=MP_SETUP('Final')

      end
```

Reference Material

Contents

User Errors

IMSL routines attempt to detect user errors and handle them in a way that provides as much information to the user as possible. To do this, we recognize various levels of severity of errors, and we also consider the extent of the error in the context of the purpose of the routine; a trivial error in one situation may be serious in another. IMSL routines attempt to report as many errors as they can reasonably detect. Multiple errors present a difficult problem in error detection because input is interpreted in an uncertain context after the first error is detected.

What Determines Error Severity

In some cases, the user's input may be mathematically correct, but because of limitations of the computer arithmetic and of the algorithm used, it is not possible to compute an answer accurately. In this case, the assessed degree of accuracy determines the severity of the error. In cases where the routine computes several output quantities, if some are not computable but most are, an error condition exists. The severity depends on an assessment of the overall impact of the error.

Terminal errors

If the user's input is regarded as meaningless, such as N = −1 when "N" is the number of equations, the routine prints a message giving the value of the erroneous input argument(s) and the reason for the erroneous input. The routine will then cause the user's program to stop. An error in which the user's input is meaningless is the most severe error and is called a *terminal error*. Multiple terminal error messages may be printed from a single routine.

Informational errors

In many cases, the best way to respond to an error condition is simply to correct the input and rerun the program. In other cases, the user may want to take actions in the program itself based on errors that occur. An error that may be used as the basis for corrective action within the program is called an *informational error*. If an informational error occurs, a user-retrievable code is set. A routine can return at most one informational error for a single reference to the routine. The codes for the informational error codes are printed in the error messages.

Other errors

In addition to informational errors, IMSL routines issue error messages for which no user- retrievable code is set. Multiple error messages for this kind of error may be printed. These errors, which generally are not described in the documentation, include terminal errors as well as less serious errors. Corrective action within the calling program is not possible for these errors.

Kinds of Errors and Default Actions

Five levels of severity of errors are defined in the MATH/LIBRARY. Each level has an associated PRINT attribute and a STOP attribute. These attributes have default settings (YES or NO), but they may also be set by the user. The purpose of having multiple error severity levels is to provide independent control of actions to be taken for errors of different severity. Upon return from an IMSL routine, exactly one error state exists. (A code 0 "error" is no informational error.) Even if more than one informational error occurs, only one message is printed (if the PRINT attribute is YES). Multiple errors for which no corrective action within the calling program is reasonable or necessary result in the printing of multiple messages (if the PRINT attribute for their severity level is YES). Errors of any of the severity levels except level 5 may be informational errors.

Level 1: Note. A *note* is issued to indicate the possibility of a trivial error or simply to provide information about the computations. Default attributes: PRINT=NO, STOP=NO

Level 2: Alert. An *alert* indicates that the user should be advised about events occurring in the software. Default attributes: PRINT=NO, STOP=NO

Level 3: Warning. A *warning* indicates the existence of a condition that may require corrective action by the user or calling routine. A warning error may be issued because the results are accurate to only a few decimal places, because some of the output may be erroneous but most of the output is correct, or because some assumptions underlying the analysis technique are violated. Often no corrective action is necessary and the condition can be ignored. Default attributes: PRINT=YES, STOP=NO

Level 4: Fatal. A *fatal* error indicates the existence of a condition that may be serious. In most cases, the user or calling routine must take corrective action to recover. Default attributes: PRINT=YES, STOP=YES

Level 5: Terminal. A *terminal* error is serious. It usually is the result of an incorrect specification, such as specifying a negative number as the number of equations. These errors may also be caused by various programming errors impossible to diagnose correctly in FORTRAN. The resulting error message may be perplexing to the user. In such cases, the user is advised to compare carefully the actual arguments passed to the routine with the dummy argument descriptions given in the documentation. Special attention should be given to checking argument order and data types.

A terminal error is not an informational error because corrective action within the program is generally not reasonable. In normal usage, execution is terminated immediately when a terminal error occurs. Messages relating to more than one terminal error are printed if they occur. Default attributes: PRINT=YES, STOP=YES

The user can set PRINT and STOP attributes by calling `ERSET` as described in "Routines for Error Handling."

Errors in Lower-Level Routines

It is possible that a user's program may call an IMSL routine that in turn calls a nested sequence of lower-level IMSL routines. If an error occurs at a lower level in such a nest of routines and if the lower-level routine cannot pass the information up to the original user-called routine, then a traceback of the routines is produced. The only common situation in which this can occur is when an IMSL routine calls a user-supplied routine that in turn calls another IMSL routine.

Routines for Error Handling

There are three ways in which the user may interact with the IMSL error handling system: (1) to change the default actions, (2) to retrieve the integer code of an informational error so as to take corrective action, and (3) to determine the severity level of an error. The routines to use are `ERSET`, `IERCD`, and `N1RTY`, respectively.

ERSET

Change the default printing or stopping actions when errors of a particular error severity level occur.

Required Arguments

IERSVR — Error severity level indicator. (Input)
If `IERSVR` = 0, actions are set for levels 1 to 5. If `IERSVR` is 1 to 5, actions are set for errors of the specified severity level.

IPACT — Printing action. (Input)

IPACT	Action
−1	Do not change current setting(s).
0	Do not print.
1	Print.
2	Restore the default setting(s).

ISACT — Stopping action. (Input)

ISACT	Action
−1	Do not change current setting(s).
0	Do not stop.
1	Stop.
2	Restore the default setting(s).

FORTRAN 90 Interface

Generic: `CALL ERSET (IERSVR, IPACT, ISACT)`

Specific: The specific interface name is `ERSET`.

FORTRAN 77 Interface

Single: `CALL ERSET (IERSVR, IPACT, ISACT)`

IERCD and N1RTY

The last two routines for interacting with the error handling system, `IERCD` and `N1RTY`, are `INTEGER` functions and are described in the following material.

`IERCD` retrieves the integer code for an informational error. Since it has no arguments, it may be used in the following way:

```
ICODE = IERCD()
```

The function retrieves the code set by the most recently called IMSL routine.

`N1RTY` retrieves the error type set by the most recently called IMSL routine. It is used in the following way:

```
ITYPE = N1RTY(1)
```

`ITYPE` = 1, 2, 4, and 5 correspond to error severity levels 1, 2, 4, and 5, respectively. `ITYPE` = 3 and `ITYPE` = 6 are both warning errors, error severity level 3. While `ITYPE` = 3 errors are informational errors (`IERCD`( ) ≠ 0), `ITYPE` = 6 errors are not informational errors (`IERCD`( ) = 0).

For software developers requiring additional interaction with the IMSL error handling system, see Aird and Howell (1991).

Examples

Changes to default actions

Some possible changes to the default actions are illustrated below. The default actions remain in effect for the kinds of errors not included in the call to `ERSET`.

To turn off printing of warning error messages:

```
CALL ERSET (3, 0, −1)
```

To stop if warning errors occur:

```
CALL ERSET (3, −1, 1)
```

To print all error messages:

```
CALL ERSET (0, 1, −1)
```

To restore all default settings:

```
CALL ERSET (0, 2, 2)
```

Use of informational error to determine program action

In the program segment below, the Cholesky factorization of a matrix is to be performed. If it is determined that the matrix is not nonnegative definite (and often this is not immediately obvious), the program is to take a different branch.

```
                     .
                     .
                     .
      CALL LFTDS (A, FACT)
      IF (IERCD() .EQ. 2) THEN
!                     Handle matrix that is not nonnegative definite
                     .
                     .
                     .
      END IF
```

Examples of errors

The program below illustrates each of the different types of errors detected by the MATH/LIBRARY routines.

The error messages refer to the argument names that are used in the documentation for the routine, rather than the user's name of the variable used for the argument. In the message generated by IMSL routine `LINRG` in this example, reference is made to `N`, whereas in the program a literal was used for this argument.

```
      USE_IMSL_LIBRARIES
      INTEGER    N
      PARAMETER  (N=2)
!
      REAL       A(N,N), AINV(N,N), B(N), X(N)
!
      DATA A/2.0, -3.0, 2.0, -3.0/
      DATA B/1.0, 2.0/
!                                 Turn on printing and turn off
!                                 stopping for all error types.
      CALL ERSET (0, 1, 0)
!                                 Generate level 4 informational error.
      CALL LSARG (A, B, X)
!                                 Generate level 5 terminal error.
      CALL LINRG (A, AINV, N = -1)
      END
```

Output

```
 *** FATAL    ERROR 2 from LSARG.  The input matrix is singular.  Some of
 ***          the diagonal elements of the upper triangular matrix U of the
 ***          LU factorization are close to zero.

 *** TERMINAL ERROR 1 from LINRG.  The order of the matrix must be positive
 ***          while N = -1 is given.
```

Example of traceback

The next program illustrates a situation in which a traceback is produced. The program uses the IMSL quadrature routines QDAG and QDAGS to evaluate the double integral

$$\int_0^1 \int_0^1 (x+y)\,dxdy = \int_0^1 g(y)\,dy$$

where

$$g(y) = \int_0^1 (x+y)\,dx = \int_0^1 f(x)\,dx, \text{ with } f(x) = x+y$$

Since both QDAG and QDAGS need 2500 numeric storage units of workspace, and since the workspace allocator uses some space to keep track of the allocations, 6000 numeric storage units of space are explicitly allocated for workspace. Although the traceback shows an error code associated with a terminal error, this code has no meaning to the user; the printed message contains all relevant information. It is not assumed that the user would take corrective action based on knowledge of the code.

```
      USE QDAGS_INT
!                                 Specifications for local variables
      REAL       A, B, ERRABS, ERREST, ERRREL, G, RESULT
      EXTERNAL   G
!                                 Set quadrature parameters
      A      = 0.0
      B      = 1.0
      ERRABS = 0.0
      ERRREL = 0.001
!                                 Do the outer integral
      CALL QDAGS (G, A, B, RESULT, ERRABS, ERRREL, ERREST)
!
      WRITE (*,*) RESULT, ERREST
      END
!
      REAL FUNCTION G (ARGY)
      USE QDAG_INT
      REAL       ARGY
!
      INTEGER    IRULE
      REAL       C, D, ERRABS, ERREST, ERRREL, F, Y
      COMMON     /COMY/ Y
      EXTERNAL   F
!
      Y      = ARGY
      C      = 0.0
      D      = 1.0
      ERRABS = 0.0
      ERRREL = -0.001
      IRULE  = 1
!
      CALL QDAG (F, C, D, G, ERRABS, ERRREL, IRULE, ERREST)
      RETURN
      END
!
      REAL FUNCTION F (X)
      REAL       X
!
```

```
      REAL        Y
      COMMON      /COMY/ Y
!
      F = X + Y
      RETURN
      END
```

Output

```
*** TERMINAL ERROR 4 from Q2AG.  The relative error desired ERRREL =
***          -1.000000E-03.  It must be at least zero.
Here is a traceback of subprogram calls in reverse order:
Routine name                    Error type  Error code
------------                    ----------  ----------
Q2AG                                5           4    (Called internally)
QDAG                                0           0
Q2AGS                               0           0    (Called internally)
QDAGS                               0           0
USER                                0           0
```

Machine-Dependent Constants

The function subprograms in this section return machine-dependent information and can be used to enhance portability of programs between different computers. The routines `IMACH`, and `AMACH` describe the computer's arithmetic. The routine `UMACH` describes the input, ouput, and error output unit numbers.

IMACH

This function retrieves machine integer constants that define the arithmetic used by the computer.

Function Return Value

`IMACH`(1) = Number of bits per integer storage unit.

`IMACH`(2) = Number of characters per integer storage unit:

Integers are represented in M-digit, base A form as

$$\sigma \sum_{k=0}^{M} x_k A^k$$

where σ is the sign and $0 \le x_k < A$, $k = 0, \ldots, M$.

Then,

`IMACH`(3) = A, the base.

`IMACH`(4) = M, the number of base-A digits.

`IMACH`(5) = $A^M - 1$, the largest integer.

The machine model assumes that floating-point numbers are represented in normalized N-digit, base B form as

$$\sigma B^E \sum_{k=1}^{N} x_k B^{-k}$$

where σ is the sign, $0 < x_1 < B$, $0 \le x_k < B$, k = 2, …, N and $E_{min} \le E \le E_{max}$. Then,

`IMACH`(6) = B, the base.

`IMACH`(7) = N_s, the number base-B-digits in single precision.

`IMACH`(8) = $E_{\min_s}$, the smallest single precision exponent.

`IMACH`(9) = $E_{\max_s}$, the largest single precision exponent.

`IMACH`(10) = N_d, the number base-B-digits in double precision.

`IMACH`(11) = $E_{\min_d}$, the smallest double precision exponent.

`IMACH`(12) = $E_{\max_d}$, largest double precision exponent.

Required Arguments

I — Index of the desired constant. (Input)

FORTRAN 90 Interface

Generic: `IMACH (I)`

Specific: The specific interface name is `IMACH`.

FORTRAN 77 Interface

Single: `IMACH (I)`

AMACH

The function subprogram `AMACH` retrieves machine constants that define the computer's single-precision or double precision arithmetic. Such floating-point numbers are represented in normalized *N*-digit, base *B* form as

$$\sigma B^E \sum_{k=1}^{N} x_k B^{-k}$$

where **σ** is the sign, $0 < x_1 < B$, $0 \le x_k < B$, $k = 2, \ldots, N$ and

$$E_{\min} \le E \le E_{\max}$$

Function Return Value

`AMACH`(1) = $B^{E_{\min}-1}$, the smallest normalized positive number.

`AMACH`(2) = $B^{E_{\max}-1}\left(1 - B^{-N}\right)$, the largest number.

`AMACH`(3) = B^{-N}, the smallest relative spacing.

`AMACH`(4) = B^{1-N}, the largest relative spacing.

`AMACH`(5) = $\log_{10}(B)$.

`AMACH`(6) = NaN (non-signaling not a number).

`AMACH`(7) = positive machine infinity.

`AMACH`(8) = negative machine infinity.

See *Comment 1* for a description of the use of the generic version of this function.

See *Comment 2* for a description of *min*, *max*, and *N*.

Required Arguments

I — Index of the desired constant. (Input)

FORTRAN 90 Interface

Generic: `AMACH (I)`

Specific: The specific interface names are `S_AMACH` and `D_AMACH`.

FORTRAN 77 Interface

Single: AMACH(I)

Double: The double precision name is DMACH.

Comments

1. If the generic version of this function is used, the immediate result must be stored in a variable before use in an expression. For example:

```
X = AMACH(I)
Y = SQRT(X)
```

must be used rather than

```
Y = SQRT(AMACH(I)).
```

If this is too much of a restriction on the programmer, then the specific name can be used without this restriction.

2. Note that for single precision B = IMACH(6), N = IMACH(7).
E_{min} = IMACH(8), and E_{max} = IMACH(9).
For double precision B = IMACH(6), N = IMACH(10).
E_{min} = IMACH(11), and E_{max} = IMACH(12).

3. The IEEE standard for binary arithmetic (see IEEE 1985) specifies *quiet* NaN (not a number) as the result of various invalid or ambiguous operations, such as 0/0. The intent is that AMACH(6) return a *quiet* NaN. On IEEE format computers that do not support a quiet NaN, a special value near AMACH(2) is returned for AMACH(6). On computers that do not have a special representation for infinity, AMACH(7) returns the same value as AMACH(2).

DMACH

See AMACH.

IFNAN(X)

This logical function checks if the argument X is NaN (not a number).

Function Return Value

IFNAN - Logical function value. True is returned if the input argument is a NAN. Otherwise, False is returned. (Output)

Required Arguments

X – Argument for which the test for NAN is desired. (Input)

FORTRAN 90 Interface

Generic: IFNAN(X)

Specific: The specific interface names are S_IFNAN and D_IFNAN.

FORTRAN 77 Interface

Single: IFNAN (X)

Double: The double precision name is DIFNAN.

Description

The logical function IFNAN checks if the single or double precision argument X is NaN (not a number). The function IFNAN is provided to facilitate the transfer of programs across computer systems. This is because the check for NaN can be tricky and not portable across computer systems that do not adhere to the IEEE standard. For example, on computers that support the IEEE standard for binary arithmetic (see IEEE 1985), NaN is specified as a bit format not equal to itself. Thus, the check is performed as

```
IFNAN = X .NE. X
```

On other computers that do not use IEEE floating-point format, the check can be performed as:

```
IFNAN = X .EQ. AMACH(6)
```

The function IFNAN is equivalent to the specification of the function Isnan listed in the Appendix, (IEEE 1985). The following example illustrates the use of IFNAN. If X is NaN, a message is printed instead of X. (Routine UMACH, which is described in the following section, is used to retrieve the output unit number for printing the message.)

Example

```
      USE IFNAN_INT
      USE AMACH_INT
      USE UMACH_INT
      INTEGER      NOUT
      REAL         X
!
      CALL UMACH (2, NOUT)
!
      X = AMACH(6)
      IF (IFNAN(X)) THEN
         WRITE (NOUT,*) ' X is NaN (not a number).'
      ELSE
         WRITE (NOUT,*) ' X = ', X
      END IF
!
      END
```

Output

```
X is NaN (not a number).
```

UMACH

Routine UMACH sets or retrieves the input, output, or error output device unit numbers.

Required Arguments

N — Integer value indicating the action desired. If the value of N is negative, the input, output, or error output unit number is reset to NUNIT. If the value of N is positive, the input, output, or error output unit number is returned in NUNIT. See the table in argument NUNIT for legal values of N. (Input)

NUNIT — The unit number that is either retrieved or set, depending on the value of input argument N. (Input/Output)

The arguments are summarized by the following table:

N	**Effect**
1	Retrieves input unit number in NUNIT.
2	Retrieves output unit number in NUNIT.
3	Retrieves error output unit number in NUNIT.
−1	Sets the input unit number to NUNIT.
−2	Sets the output unit number to NUNIT.
−3	Sets the error output unit number to NUNIT.

FORTRAN 90 Interface

Generic: CALL UMACH (N, NUNIT)

Specific: The specific interface name is UMACH.

FORTRAN 77 Interface

Single: CALL UMACH (N, NUNIT)

Description

Routine UMACH sets or retrieves the input, output, or error output device unit numbers. UMACH is set automatically so that the default FORTRAN unit numbers for standard input, standard output, and standard error are used. These unit numbers can be changed by inserting a call to UMACH at the beginning of the main program that calls MATH/LIBRARY routines. If these unit numbers are changed from the standard values, the user should insert an appropriate OPEN statement in the calling program.

Example

In the following example, a terminal error is issued from the MATH/LIBRARY AMACH function since the argument is invalid. With a call to UMACH, the error message will be written to a local file named “CHECKERR”.

```
      USE AMACH_INT
      USE UMACH_INT
      INTEGER     N, NUNIT
      REAL        X
!                                          Set Parameter
      N = 0
      NUNIT = 9
!
      CALL UMACH (-3, NUNIT)
      OPEN (UNIT=NUNIT,FILE='CHECKERR')
      X = AMACH(N)
      END
```

Output

```
The output from this example, written to “CHECKERR” is:
*** TERMINAL ERROR 5 from AMACH.  The argument must be between 1 and 8
***            inclusive. N = 0
```

Matrix Storage Modes

In this section, the word *matrix* will be used to refer to a mathematical object, and the word *array* will be used to refer to its representation as a FORTRAN data structure.

General Mode

A *general* matrix is an $N \times N$ matrix A. It is stored in a FORTRAN array that is declared by the following statement:

```
DIMENSION A(LDA,N)
```

The parameter `LDA` is called the *leading dimension* of `A`. It must be at least as large as `N`. IMSL general matrix subprograms only refer to values A_{ij} for $i = 1, \ldots, N$ and $j = 1, \ldots, N$. The data type of a general array can be one of `REAL`, `DOUBLE PRECISION`, or `COMPLEX`. If your FORTRAN compiler allows, the nonstandard data type `DOUBLE COMPLEX` can also be declared.

Rectangular Mode

A *rectangular* matrix is an $M \times N$ matrix A. It is stored in a FORTRAN array that is declared by the following statement:

```
DIMENSION A(LDA,N)
```

The parameter `LDA` is called the *leading dimension* of `A`. It must be at least as large as `M`. IMSL rectangular matrix subprograms only refer to values A_{ij} for $i = 1, \ldots, M$ and $j = 1, \ldots, N$. The data type of a rectangular array can be `REAL`, `DOUBLE PRECISION`, or `COMPLEX`. If your FORTRAN compiler allows, you can declare the nonstandard data type `DOUBLE COMPLEX`.

Symmetric Mode

A symmetric matrix is a square $N \times N$ matrix A, such that $A^T = A$. (A^T is the transpose of A.) It is stored in a FORTRAN array that is declared by the following statement:

```
DIMENSION A(LDA,N)
```

The parameter `LDA` is called the *leading dimension* of `A`. It must be at least as large as `N`. IMSL symmetric matrix subprograms only refer to the upper or to the lower half of `A` (i.e., to values A_{ij} for $i = 1, \ldots, N$ and $j = i, \ldots, N$, or A_{ij} for $j = 1, \ldots, N$ and $i = j, \ldots, N$). The data type of a symmetric array can be one of `REAL` or `DOUBLE PRECISION`.

Use of the upper half of the array is denoted in the BLAS that compute with symmetric matrices, see Chapter 9, *"Basic Matrix/Vector Operations"*, using the `CHARACTER*1` flag `UPLO = 'U'`. Otherwise, `UPLO = 'L'` denotes that the lower half of the array is used.

Hermitian Mode

A *Hermitian* matrix is a square $N \times N$ matrix A, such that

$$\overline{A}^T = A$$

The matrix

$$\overline{A}$$

is the complex conjugate of A and

$$A^H \equiv \overline{A}^T$$

is the conjugate transpose of A. For Hermitian matrices, $A^H = A$. The matrix is stored in a FORTRAN array that is declared by the following statement:

```
DIMENSION A(LDA,N)
```

The parameter `LDA` is called the *leading dimension* of `A`. It must be at least as large as N. IMSL Hermitian matrix subprograms only refer to the upper or to the lower half of `A` (i.e., to values A_{ij} for $i = 1, \ldots, N$ and $j = i, \ldots, N$, or A_{ij} for $j = 1, \ldots, N$ and $i = j, \ldots, N$). Use of the upper half of the array is denoted in the BLAS that compute with Hermitian matrices, see Chapter 9, *"Basic Matrix/Vector Operations"*, using the `CHARACTER*1` flag `UPLO = 'U'`. Otherwise, `UPLO = 'L'` denotes that the lower half of the array is used. The data type of a Hermitian array can be `COMPLEX` or, if your FORTRAN compiler allows, the nonstandard data type `DOUBLE COMPLEX`.

Triangular Mode

A *triangular* matrix is a square $N \times N$ matrix A such that values $A_{ij} = 0$ for $i < j$ or $A_{ij} = 0$ for $i > j$. The first condition defines a *lower* triangular matrix while the second condition defines an *upper* triangular matrix. A lower triangular matrix A is stored in the lower triangular part of a FORTRAN array `A`. An upper triangular matrix is stored in the upper triangular part of a FORTRAN array. Triangular matrices are called *unit* triangular whenever $A_{jj} = 1$, $j = 1, \ldots, N$. For unit triangular matrices, only the strictly lower or upper parts of the array are referenced. This is denoted in the BLAS that compute with triangular matrices, see Chapter 9, *"Basic Matrix/Vector Operations"*, using the `CHARACTER*1` flag `DIAGNL = 'U'`. Otherwise, `DIAGNL = 'N'` denotes that the diagonal array terms should be used. For unit triangular matrices, the diagonal terms are each used with the mathematical value 1. The array diagonal term does not need to be 1.0 in this usage. Use of the upper half of the array is denoted in the

BLAS that compute with triangular matrices, see *Chapter 9, "Basic Matrix/Vector Operations"*, using the `CHARACTER*1` flag `UPLO = 'U'`. Otherwise, `UPLO = 'L'` denotes that the lower half of the array is used. The data type of an array that contains a triangular matrix can be one of `REAL`, `DOUBLE PRECISION`, or `COMPLEX`. If your FORTRAN compiler allows, the nonstandard data type `DOUBLE COMPLEX` can also be declared.

Band Storage Mode

A *band matrix* is an $M \times N$ matrix A with all of its nonzero elements "close" to the main diagonal. Specifically, values $A_{ij} = 0$ if $i - j >$ `NLCA` or $j - i >$ `NUCA`. The integers `NLCA` and `NUCA` are the *lower* and *upper* band widths. The integer m = `NLCA` + `NUCA` + 1 is the total band width. The diagonals, other than the main diagonal, are called *codiagonals*. While any $M \times N$ matrix is a band matrix, the band matrix mode is most useful only when the number of nonzero codiagonals is much less than m.

In the band storage mode, the `NLCA` lower codiagonals and `NUCA` upper codiagonals are stored in the rows of a FORTRAN array of dimension $m \times N$. The elements are stored in the same column of the array as they are in the matrix. The values A_{ij} inside the band width are stored in array positions ($i - j$ + `NUCA` + 1, j). This array is declared by the following statement:

```
DIMENSION A(LDA,N)
```

The parameter `LDA` is called the *leading dimension* of A. It must be at least as large as m. The data type of a band matrix array can be one of `REAL`, `DOUBLE PRECISION`, `COMPLEX` or, if your FORTRAN compiler allows, the nonstandard data type `DOUBLE COMPLEX` . Use of the `CHARACTER*1` flag `TRANS='N'` in the BLAS, see *Chapter 9, "Basic Matrix/Vector Operations"*, specifies that the matrix A is used. The flag value

$$\text{TRANS} = \text{'T' uses } A^T$$

while

$$\text{TRANS} = \text{'C' uses } \overline{A}^T$$

For example, consider a real 5×5 band matrix with 1 lower and 2 upper codiagonals, stored in the FORTRAN array declared by the following statements:

```
PARAMETER (N=5, NLCA=1, NUCA=2)
REAL A(NLCA+NUCA+1,N)
```

The matrix A has the form

$$A = \begin{bmatrix} A_{11} & A_{12} & A_{13} & 0 & 0 \\ A_{21} & A_{22} & A_{23} & A_{24} & 0 \\ 0 & A_{32} & A_{33} & A_{34} & A_{35} \\ 0 & 0 & A_{43} & A_{44} & A_{45} \\ 0 & 0 & 0 & A_{54} & A_{55} \end{bmatrix}$$

As a FORTRAN array, it is

$$A = \begin{bmatrix} \times & \times & A_{13} & A_{24} & A_{35} \\ \times & A_{12} & A_{23} & A_{34} & A_{45} \\ A_{11} & A_{22} & A_{33} & A_{44} & A_{55} \\ A_{21} & A_{32} & A_{43} & A_{54} & \times \end{bmatrix}$$

The entries marked with an `x` in the above array are not referenced by the IMSL band subprograms.

Band Symmetric Storage Mode

A *band symmetric* matrix is a band matrix that is also symmetric. The band symmetric storage mode is similar to the band mode except only the lower or upper codiagonals are stored.

In the band symmetric storage mode, the `NCODA` upper codiagonals are stored in the rows of a FORTRAN array of dimension (`NCODA` + `1`) × *N*. The elements are stored in the same column of the array as they are in the matrix. Specifically, values A_{ij}, $j \le i$ inside the band are stored in array positions ($i - j +$ `NCODA` $+ 1, j$). This is the storage mode designated by using the `CHARACTER*1` flag `UPLO = 'U'` in Level 2 BLAS that compute with band symmetric matrices (see *Chapter 9, "Basic Matrix/Vector Operations"*). Alternatively, A_{ij}, $j \le i$, inside the band, are stored in array positions ($i - j + 1, j$). This is the storage mode designated by using the `CHARACTER*1` flag `UPLO = 'L'` in these Level 2 BLAS (see *Chapter 9, "Basic Matrix/Vector Operations"*). The array is declared by the following statement:

```
DIMENSION A(LDA,N)
```

The parameter `LDA` is called the *leading dimension* of *A*. It must be at least as large as `NCODA` + 1. The data type of a band symmetric array can be `REAL` or `DOUBLE PRECISION`.

For example, consider a real 5 × 5 band matrix with 2 codiagonals. Its FORTRAN declaration is

```
PARAMETER (N=5, NCODA=2)
REAL A(NCODA+1, N)
```

The matrix *A* has the form

$$A = \begin{bmatrix} A_{11} & A_{12} & A_{13} & 0 & 0 \\ A_{12} & A_{22} & A_{23} & A_{24} & 0 \\ A_{13} & A_{23} & A_{33} & A_{34} & A_{35} \\ 0 & A_{24} & A_{34} & A_{44} & A_{45} \\ 0 & 0 & A_{35} & A_{45} & A_{55} \end{bmatrix}$$

Since A is symmetric, the values $A_{ij} = A_{ji}$. In the FORTRAN array, it is

$$A = \begin{bmatrix} \times & \times & A_{13} & A_{24} & A_{35} \\ \times & A_{12} & A_{23} & A_{34} & A_{45} \\ A_{11} & A_{22} & A_{33} & A_{44} & A_{55} \end{bmatrix}$$

The entries marked with an $\times$ in the above array are not referenced by the IMSL band symmetric subprograms.

An alternate storage mode for band symmetric matrices is designated using the `CHARACTER*1` flag `UPLO = 'L'` in Level 2 BLAS that compute with band symmetric matrices (see *Chapter 9, "Basic Matrix/Vector Operations"*). In that case, the example matrix is represented as

$$A = \begin{bmatrix} A_{11} & A_{22} & A_{33} & A_{44} & A_{55} \\ A_{12} & A_{23} & A_{34} & A_{45} & \times \\ A_{13} & A_{24} & A_{35} & \times & \times \end{bmatrix}$$

Band Hermitian Storage Mode

A *band Hermitian* matrix is a band matrix that is also Hermitian. The band Hermitian mode is a complex analogue of the band symmetric mode.

In the band Hermitian storage mode, the `NCODA` upper codiagonals are stored in the rows of a FORTRAN array of dimension (`NCODA` + 1) $\times$ N. The elements are stored in the same column of the array as they are in the matrix. In the Level 2 BLAS (see *Chapter 9, "Basic Matrix/Vector Operations"*) this is denoted by using the `CHARACTER*1` flag `UPLO ='U'`. The array is declared by the following statement:

```
DIMENSION A(LDA,N)
```

The parameter `LDA` is called the *leading dimension* of *A*. It must be at least as large as `(NCODA + 1)`. The data type of a band Hermitian array can be `COMPLEX` or, if your FORTRAN compiler allows, the nonstandard data type `DOUBLE COMPLEX`.

For example, consider a complex 5 $\times$ 5 band matrix with 2 codiagonals. Its FORTRAN declaration is

```
PARAMETER (N=5, NCODA = 2)
COMPLEX A(NCODA + 1, N)
```

The matrix A has the form

$$A = \begin{bmatrix} A_{11} & A_{12} & A_{13} & 0 & 0 \\ \overline{A}_{12} & A_{22} & A_{23} & A_{24} & 0 \\ \overline{A}_{13} & \overline{A}_{23} & A_{33} & A_{34} & A_{35} \\ 0 & \overline{A}_{24} & \overline{A}_{34} & A_{44} & A_{45} \\ 0 & 0 & \overline{A}_{35} & \overline{A}_{45} & A_{55} \end{bmatrix}$$

where the value

$$\overline{A}_{ij}$$

is the complex conjugate of A_{ij}. This matrix represented as a FORTRAN array is

$$A = \begin{bmatrix} \times & \times & A_{13} & A_{24} & A_{35} \\ \times & A_{12} & A_{23} & A_{34} & A_{45} \\ A_{11} & A_{22} & A_{33} & A_{44} & A_{55} \end{bmatrix}$$

The entries marked with an × in the above array are not referenced by the IMSL band Hermitian subprograms.

An alternate storage mode for band Hermitian matrices is designated using the `CHARACTER*1` flag `UPLO = 'L'` in Level 2 BLAS that compute with band Hermitian matrices (see *Chapter 9, "Basic Matrix/Vector Operations"*). In that case, the example matrix is represented as

$$A = \begin{bmatrix} A_{11} & A_{22} & A_{33} & A_{44} & A_{55} \\ \overline{A}_{12} & \overline{A}_{23} & \overline{A}_{34} & \overline{A}_{45} & \times \\ \overline{A}_{13} & \overline{A}_{24} & \overline{A}_{35} & \times & \times \end{bmatrix}$$

Band Triangular Storage Mode

A *band triangular* matrix is a band matrix that is also triangular. In the band triangular storage mode, the `NCODA` codiagonals are stored in the rows of a FORTRAN array of dimension `(NCODA + 1)` × *N*. The elements are stored in the same column of the array as they are in the matrix. For usage in the Level 2 BLAS (see *Chapter 9*, section *Programming Notes for Level 2 and Level 3 BLAS*) the `CHARACTER*1` flag `DIAGNL` has the same meaning as used in section "Triangular Storage Mode". The flag `UPLO` has the meaning analogous with its usage in the section "Banded Symmetric Storage Mode". This array is declared by the following statement:

```
DIMENSION A(LDA,N)
```

The parameter `LDA` is called the *leading dimension* of *A*. It must be at least as large as `(NCODA + 1)`.

For example, consider a 5 × 5 band upper triangular matrix with 2 codiagonals. Its FORTRAN declaration is

```
PARAMETER (N = 5, NCODA = 2)
COMPLEX A(NCODA + 1, N)
```

The matrix *A* has the form

$$A = \begin{bmatrix} A_{11} & A_{12} & A_{13} & 0 & 0 \\ 0 & A_{22} & A_{23} & A_{24} & 0 \\ 0 & 0 & A_{33} & A_{34} & A_{35} \\ 0 & 0 & 0 & A_{44} & A_{45} \\ 0 & 0 & 0 & 0 & A_{55} \end{bmatrix}$$

This matrix represented as a FORTRAN array is

$$A = \begin{bmatrix} \times & \times & A_{13} & A_{24} & A_{35} \\ \times & A_{12} & A_{23} & A_{34} & A_{45} \\ A_{11} & A_{22} & A_{33} & A_{44} & A_{55} \end{bmatrix}$$

This corresponds to the CHARACTER*1 flags DIAGNL = 'N' and UPLO = 'U'. The matrix A^T is represented as the FORTRAN array

$$A = \begin{bmatrix} A_{11} & A_{22} & A_{33} & A_{44} & A_{55} \\ A_{12} & A_{23} & A_{34} & A_{45} & \times \\ A_{13} & A_{24} & A_{35} & \times & \times \end{bmatrix}$$

This corresponds to the CHARACTER*1 flags DIAGNL = 'N' and UPLO = 'L'. In both examples, the entries indicated with an × are not referenced by IMSL subprograms.

Codiagonal Band Symmetric Storage Mode

This is an alternate storage mode for band symmetric matrices. It is not used by any of the BLAS, see *Chapter 9, "Basic Matrix/Vector Operations"*. Storing data in a form transposed from the **Band Symmetric Storage Mode** maintains unit spacing between consecutive referenced array elements. This data structure is used to get good performance in the Cholesky decomposition algorithm that solves positive definite symmetric systems of linear equations *Ax* = *b*. The data type can be REAL or DOUBLE PRECISION. In the codiagonal band symmetric storage mode, the NCODA upper codiagonals and right-hand-side are stored in columns of this FORTRAN array. This array is declared by the following statement:

```
DIMENSION A(LDA, NCODA + 2)
```

The parameter LDA is the *leading positive dimension* of *A*. It must be at least as large as N + NCODA.

Consider a real symmetric 5 × 5 matrix with 2 codiagonals

$$A = \begin{bmatrix} A_{11} & A_{12} & A_{13} & 0 & 0 \\ A_{12} & A_{22} & A_{23} & A_{24} & 0 \\ A_{13} & A_{23} & A_{33} & A_{34} & A_{35} \\ 0 & A_{24} & A_{34} & A_{44} & A_{45} \\ 0 & 0 & A_{35} & A_{45} & A_{55} \end{bmatrix}$$

and a right-hand-side vector

$$b = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \end{bmatrix}$$

A FORTRAN declaration for the array to hold this matrix and right-hand-side vector is

```
PARAMETER (N = 5, NCODA = 2, LDA = N + NCODA)
REAL A(LDA, NCODA + 2)
```

The matrix and right-hand-side entries are placed in the FORTRAN array *A* as follows:

$$A = \begin{bmatrix} \times & \times & \times & \times \\ \times & \times & \times & \times \\ A_{11} & \times & \times & b_1 \\ A_{22} & A_{12} & \times & b_2 \\ A_{33} & A_{23} & A_{13} & b_3 \\ A_{44} & A_{34} & A_{24} & b_4 \\ A_{55} & A_{45} & A_{35} & b_5 \end{bmatrix}$$

Entries marked with an × do not need to be defined. Certain of the IMSL band symmetric subprograms will initialize and use these values during the solution process. When a solution is computed, the b_i, i = 1, …, 5, are replaced by x_i, i = 1, …, 5.

The nonzero A_{ij}, $j \ge i$, are stored in array locations $A(j$ + `NCODA`, $(j - i) + 1)$. The right-hand-side entries b_j are stored in locations $A(j$ + `NCODA`, `NCODA` + 2). The solution entries x_j are returned in $A(j$ + `NCODA`, `NCODA` + 2).

Codiagonal Band Hermitian Storage Mode

This is an alternate storage mode for band Hermitian matrices. It is not used by any of the BLAS (see *Chapter 9, "Basic Matrix/Vector Operations"*). In the codiagonal band Hermitian storage mode, the real and imaginary parts of the 2 * NCODA + 1 upper codiagonals and right-hand-side are stored in columns of a FORTRAN array. Note that there is no explicit use of the COMPLEX or the nonstandard data type DOUBLE COMPLEX data type in this storage mode.

For *Hermitian* complex matrices,

$$A = U + \sqrt{-1}\,V$$

where U and V are real matrices. They satisfy the conditions $U = U^T$ and $V = -V^T$. The right-hand-side is

$$b = c + \sqrt{-1}\,d$$

where c and d are real vectors. The solution vector is denoted as

$$x = u + \sqrt{-1}\,v$$

where u and v are real. The storage is declared with the following statement

```
DIMENSION A(LDA, 2*NCODA + 3)
```

The parameter LDA is the *leading positive dimension* of A. It must be at least as large as N + NCODA.

The diagonal terms U_{jj} are stored in array locations $A(j$ + NCODA, 1). The diagonal V_{jj} are zero and are not stored. The nonzero U_{ij}, $j > i$, are stored in locations $A(j$ + NCODA, 2 * $(j - i))$.

The nonzero V_{ij} are stored in locations $A(j$ + NCODA, 2*$(j - i) + 1)$. The right side vector b is stored with c_j and d_j in locations $A(j$ + NCODA, 2*NCODA + 2) and $A(j$ + NCODA, 2*NCODA + 3) respectively. The real and imaginary parts of the solution, u_j and v_j, respectively overwrite c_j and d_j.

Consider a complex hermitian 5 × 5 matrix with 2 codiagonals

$$A = \begin{bmatrix} U_{11} & U_{12} & U_{13} & 0 & 0 \\ U_{12} & U_{22} & U_{23} & U_{24} & 0 \\ U_{13} & U_{23} & U_{33} & U_{34} & U_{35} \\ 0 & U_{24} & U_{34} & U_{44} & U_{45} \\ 0 & 0 & U_{35} & U_{45} & U_{55} \end{bmatrix} + \sqrt{-1}\begin{bmatrix} 0 & V_{12} & V_{13} & 0 & 0 \\ -V_{12} & 0 & V_{23} & V_{24} & 0 \\ -V_{13} & -V_{23} & 0 & V_{34} & V_{35} \\ 0 & -V_{24} & -V_{34} & 0 & V_{45} \\ 0 & 0 & -V_{35} & -V_{45} & 0 \end{bmatrix}$$

and a right-hand-side vector

$$b = \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \\ c_5 \end{bmatrix} + \sqrt{-1} \begin{bmatrix} d_1 \\ d_2 \\ d_3 \\ d_4 \\ d_5 \end{bmatrix}$$

A FORTRAN declaration for the array to hold this matrix and right-hand-side vector is

```
PARAMETER (N = 5, NCODA = 2, LDA = N + NCODA)
REAL A(LDA,2*NCODA + 3)
```

The matrix and right-hand-side entries are placed in the FORTRAN array *A* as follows:

$$A = \begin{bmatrix} \times & \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times & \times \\ U_{11} & \times & \times & \times & \times & c_1 & d_1 \\ U_{22} & U_{12} & V_{12} & \times & \times & c_2 & d_2 \\ U_{33} & U_{23} & V_{23} & U_{13} & V_{13} & c_3 & d_3 \\ U_{44} & U_{34} & V_{34} & U_{24} & V_{24} & c_4 & d_4 \\ U_{55} & U_{45} & V_{45} & U_{35} & V_{35} & c_5 & d_5 \end{bmatrix}$$

Entries marked with an × do not need to be defined.

Sparse Matrix Storage Mode

The sparse linear algebraic equation solvers in Chapter 1 accept the input matrix in *sparse storage mode*. This structure consists of `INTEGER` values `N` and `NZ`, the matrix dimension and the total number of non-zero entries in the matrix. In addition, there are two `INTEGER` arrays `IROW(*)` and `JCOL(*)` that contain unique matrix row and column coordinates where values are given. There is also an array *A*(`*`) of values. All other entries of the matrix are zero. Each of the arrays `IROW(*)`, `JCOL(*)`, *A*(`*`) must be of size `NZ`. The correspondence between matrix and array entries is given by

$$A_{\mathrm{IROW}(i),\mathrm{ICOL}(i)} = A(i),\ I = 1,\ \ldots,\ NZ$$

The data type for *A*(`*`) can be one of `REAL`, `DOUBLE PRECISION`, or `COMPLEX`. If your FORTRAN compiler allows, the nonstandard data type `DOUBLE COMPLEX` can also be declared.

For example, consider a real 5 × 5 sparse matrix with 11 nonzero entries. The matrix *A* has the form

$$A = \begin{bmatrix} A_{11} & 0 & A_{13} & A_{14} & 0 \\ A_{21} & A_{22} & 0 & 0 & 0 \\ 0 & A_{32} & A_{33} & A_{34} & 0 \\ 0 & 0 & A_{43} & 0 & 0 \\ 0 & 0 & 0 & A_{54} & A_{55} \end{bmatrix}$$

Declarations of arrays and definitions of the values for this sparse matrix are

```
PARAMETER (NZ = 11, N = 5)
DIMENSION IROW(NZ), JCOL(NZ), A(NZ)
DATA IROW /1,1,1,2,2,3,3,3,4,5,5/
DATA JCOL /1,3,4,1,2,2,3,4,3,4,5/
DATA A    /A11,A13,A14,A21,A22,A32,A33,A34,A43,A54,A55/
```

Packed Symmetric Matrix Storage Mode

This structure contains either the upper or lower triangular portion of the symmetric data and is stored in an array of length *ncol*(*ncol* + 1)/2. For a matrix *A* and representative array `a`, the data is arranged sequentially column by column such that, for the upper triangular case, `a`(1) contains A_{11}, `a`(2) contains A_{12}, `a`(3) contains A_{22}, etc.

For example, consider the following real 5 × 5 symmetric matrix *A*

$$A = \begin{bmatrix} A_{11} & A_{12} & A_{13} & A_{14} & A_{15} \\ A_{12} & A_{22} & A_{23} & A_{24} & A_{25} \\ A_{13} & A_{23} & A_{33} & A_{34} & A_{35} \\ A_{14} & A_{24} & A_{34} & A_{44} & A_{45} \\ A_{15} & A_{25} & A_{35} & A_{45} & A_{55} \end{bmatrix}$$

The array declaration for the upper triangle of *A* would be

```
DATA a /A11,A12,A22,A13,A23,A33,A14,A24,A34,A44,A15,A25,A35,A45,A55/
```

Packed Triangular Matrix Storage Mode

This structure contains either the upper or lower triangular portion of a triangular matrix and is stored in an array of length *ncol*(*ncol* + 1)/2. For a matrix *A* and representative array `a`, the data is arranged sequentially column by column such that, for the upper triangular case, `a(1)` contains A_{11}, `a(2)` contains A_{12}, `a(3)` contains A_{22}, etc.

For example, consider the following real 5 × 5 upper triangular matrix *A*

$$A = \begin{bmatrix} A_{11} & A_{12} & A_{13} & A_{14} & A_{15} \\ 0 & A_{22} & A_{23} & A_{24} & A_{25} \\ 0 & 0 & A_{33} & A_{34} & A_{35} \\ 0 & 0 & 0 & A_{44} & A_{45} \\ 0 & 0 & 0 & 0 & A_{55} \end{bmatrix}$$

The array declaration for the upper triangle of *A* would be

```
DATA a /A11,A12,A22,A13,A23,A33,A14,A24,A34,A44,A15,A25,A35,A45,A55/
```

Packed Hermitian Matrix Storage Mode

This structure contains either the upper or lower triangular portion of a Hermitian matrix and is stored in an array of length *ncol*(*ncol* + 1)/2. For a matrix *A* and representative array `a`, the data is arranged sequentially column by column such that, for the upper triangular case, `a(1)` contains A_{11}, `a(2)` contains A_{12}, `a(3)` contains A_{22}, etc.

For example, consider the following 5 × 5 Hermitian matrix *A*

$$A = \begin{bmatrix} A_{11} & A_{12} & A_{13} & A_{14} & A_{15} \\ A_{21} & A_{22} & A_{23} & A_{24} & A_{25} \\ A_{31} & A_{32} & A_{33} & A_{34} & A_{35} \\ A_{41} & A_{42} & A_{43} & A_{44} & A_{45} \\ A_{51} & A_{52} & A_{53} & A_{54} & A_{55} \end{bmatrix}$$

The array declaration for the upper triangle of *A* would be

```
DATA a /A11,A12,A22,A13,A23,A33,A14,A24,A34,A44,A15,A25,A35,A45,A55/
```

Reserved Names

When writing programs accessing the MATH/LIBRARY, the user should choose FORTRAN names that do not conflict with names of IMSL subroutines, functions, or named common blocks, such as the workspace common block WORKSP (see *Automatic Workspace Allocation*). The user needs to be aware of two types of name conflicts that can arise. The first type of name conflict occurs when a name (technically a *symbolic name*) is not uniquely defined within a program unit (either a main program or a subprogram). For example, such a name conflict exists when the name RCURV is used to refer both to a type REAL variable and to the IMSL subroutine RCURV in a single program unit. Such errors are detected during compilation and are easy to correct. The second type of name conflict, which can be more serious, occurs when names of program units and named common blocks are not unique. For example, such a name conflict would be caused by the user defining a subroutine named WORKSP and also referencing an MATH/LIBRARY subroutine that uses the named common block WORKSP. Likewise, the user must not define a subprogram with the same name as a subprogram in the MATH/LIBRARY, that is referenced directly by the user's program or is referenced indirectly by other MATH/LIBRARY subprograms.

The MATH/LIBRARY consists of many routines, some that are described in the *User's Manual* and others that are not intended to be called by the user and, hence, that are not documented. If the choice of names were completely random over the set of valid FORTRAN names, and if a program uses only a small subset of the MATH/LIBRARY, the probability of name conflicts is very small. Since names are usually chosen to be mnemonic, however, the user may wish to take some precautions in choosing FORTRAN names.

Many IMSL names consist of a root name that may have a prefix to indicate the type of the routine. For example, the IMSL single precision subroutine for fitting a polynomial by least squares has the name RCURV, which is the root name, and the corresponding IMSL double precision routine has the name DRCURV. Associated with these two routines are R2URV and DR2URV. RCURV is listed in the Alphabetical Index of Routines, but DRCURV, R2URV, and DR2URV are not. The user of RCURV must consider both names RCURV and R2URV to be reserved; likewise, the user of DRCURV must consider both names DRCURV and DR2URV to be reserved. The root names of *all* routines and named common blocks that are used by the MATH/LIBRARY and that do not have a numeral in the second position of the root name are listed in the Alphabetical Index of Routines. Some of the routines in this Index (such as the "Level 2 BLAS") are not intended to be called by the user and so are not documented.

The careful user can avoid any conflicts with IMSL names if the following rules are observed:

- Do not choose a name that appears in the Alphabetical Summary of Routines in the *User's Manual*, nor one of these names preceded by a D, S_, D_, C_, or Z_.
- Do not choose a name of three or more characters with a numeral in the second or third position.

These simplified rules include many combinations that are, in fact, allowable. However, if the user selects names that conform to these rules, no conflict will be encountered.

Deprecated Features and Renamed Routines

Automatic Workspace Allocation

FORTRAN subroutines that work with arrays as input and output often require extra arrays for use as workspace while doing computations or moving around data. IMSL routines generally do not require the user explicitly to allocate such arrays for use as workspace. On most systems the workspace allocation is handled transparently. The only limitation is the actual amount of memory available on the system.

On some systems the workspace is allocated out of a stack that is passed as a FORTRAN array in a named common block `WORKSP`. A very similar use of a workspace stack is described by Fox et al. (1978, pages 116−121). (For compatiblity with older versions of the IMSL Libraries, space is allocated from the `COMMON` block, if possible.)

The arrays for workspace appear as arguments in lower-level routines. For example, the IMSL routine `LSARG` (in *Chapter 1, "Linear Systems"*), which solves systems of linear equations, needs arrays for workspace. `LSARG` allocates arrays from the common area, and passes them to the lower-level routine `L2ARG` which does the computations. In the "Comments" section of the documentation for `LSARG`, the amount of workspace is noted and the call to `L2ARG` is described. This scheme for using lower-level routines is followed throughout the IMSL Libraries. The names of these routines have a "2" in the second position (or in the third position in double precision routines having a "D" prefix). The user can provide workspace explicitly and call directly the "2-level" routine, which is documented along with the main routine. In a very few cases, the 2-level routine allows additional options that the main routine does not allow.

Prior to returning to the calling program, a routine that allocates workspace generally deallocates that space so that it becomes available for use in other routines.

Changing the Amount of Space Allocated

This section is relevant only to those systems on which the transparent workspace allocator is not available.

By default, the total amount of space allocated in the common area for storage of numeric data is 5000 numeric storage units. (A numeric storage unit is the amount of space required to store an integer or a real number. By comparison, a double precision unit is twice this amount. Therefore the total amount of space allocated in the common area for storage of numeric data is 2500 double precision units.) This space is allocated as needed for `INTEGER`, `REAL`, or other numeric data. For larger problems in which the default amount of workspace is insufficient, the user can change the allocation by supplying the FORTRAN statements to define the array in the named common block and by informing the IMSL workspace allocation system of the new size of the common array. To request 7000 units, the statements are

```
      COMMON /WORKSP/ RWKSP
      REAL RWKSP(7000)
      CALL IWKIN(7000)
```

If an IMSL routine attempts to allocate workspace in excess of the amount available in the common stack, the routine issues a fatal error message that indicates how much space is needed and prints statements like those above to guide the user in allocating the necessary amount. The program below uses IMSL routine `PERMA` to permute rows or columns of a matrix. This routine requires workspace equal to the number of columns, which in this example is too large. (Note that the work vector `RWKSP` must also provide extra space for bookkeeping.)

```
      USE_PERMA_INT
!                                 Specifications for local variables
      INTEGER    NRA, NCA, LDA, IPERMU(6000), IPATH
      REAL       A(2,6000)
!                                 Specifications for subroutines
!
      NRA = 2
      NCA = 6000
      LDA = 2
!                                 Initialize permutation index
      DO 10 I = 1, NCA
         IPERMU(I) = NCA + 1 - I
   10 CONTINUE
      IPATH = 2
      CALL PERMA (A, IPERMU, A, IPATH=IPATH)
      END
```

Output

```
 *** TERMINAL ERROR 10 from PERMA.  Insufficient workspace for current
 ***          allocation(s). Correct by calling IWKIN from main program with
 ***          the three following statements:  (REGARDLESS OF PRECISION)
 ***                COMMON /WORKSP/  RWKSP
 ***                REAL RWKSP(6018)
 ***                CALL IWKIN(6018)

 *** TERMINAL ERROR 10 from PERMA.  Workspace allocation was based on NCA =
 ***          6000.
```

In most cases, the amount of workspace is dependent on the parameters of the problem so the amount needed is known exactly. In a few cases, however, the amount of workspace is dependent on the data (for example, if it is necessary to count all of the unique values in a vector), so the IMSL routine cannot tell in advance exactly how much workspace is needed. In such cases the error message printed is an estimate of the amount of space required.

Character Workspace

Since character arrays cannot be equivalenced with numeric arrays, a separate named common block `WKSPCH` is provided for character workspace. In most respects this stack is managed in the same way as the numeric stack. The default size of the character workspace is 2000 character units. (A character unit is the amount of space required to store one character.) The routine analogous to `IWKIN` used to change the default allocation is `IWKCIN`.

The routines in the following list have been deprecated. A deprecated routine is one that is no longer used by anything in the library but is being included in the product for those users who may be currently referencing it in their application. However, any future versions of MATH/LIBRARY may not include these routines. If any of these routines are being called within an application, it is recommended that you change your code or retain the deprecated routine before replacing this library with the next version. Most of these routines were called by users only when they needed to set up their own workspace. Thus, the impact of these changes should be limited.

CZADD	DE2LRH	DNCONF	E3CRG
CZINI	DE2LSB	DNCONG	E4CRG
CZMUL	DE3CRG	E2ASF	E4ESF
CZSTO	DE3CRH	E2AHF	E5CRG
DE2AHF	DE3LSF	E2BHF	E7CRG
DE2ASF	DE4CRG	E2BSB	G2CCG
DE2BHF	DE4ESF	E2BSF	G2CRG
DE2BSB	DE5CRG	E2CCG	G2LCG
DE2BSF	DE7CRG	E2CCH	G2LRG
DE2CCG	DG2CCG	E2CHF	G3CCG
DE2CCH	DG2CRG	E2CRG	G4CCG
DE2CHF	DG2DF	E2CRH	G5CCG
DE2CRG	DG2IND	E2CSB	G7CRG
DE2CRH	DG2LCG	E2EHF	N0ONF
DE2CSB	DG2LRG	E2ESB	NCONF
DE2EHF	DG3CCG	E2FHF	NCONG
DE2ESB	DG3DF	E2FSB	SDADD
DE2FHF	DG4CCG	E2FSF	SDINI
DE2FSB	DG5CCG	E2LCG	SDMUL
DE2FSF	DG7CRG	E2LCH	SDSTO

DE2LCG	DHOUAP	E2LHF	SHOUAP
DE2LCH	DHOUTR	E2LRG	SHOUTR
DE2LHF	DIVPBS	E2LRH	
DE2LRG	DN0ONF	E2LSB	

The following routines have been renamed due to naming conflicts with other software manufacturers.

`CTIME` – replaced with `CPSEC`
`DTIME` – replaced with `TIMDY`
`PAGE` – replaced with `PGOPT`

Appendix A, Alphabetical Summary of Routines

A to Z

A | B | C | D | E | F | G | H | I | J | K | L | M | N | O | P | Q | R | S | T | U | V | W | Y | Z

A

Function	Purpose Statement
ACBCB	Adds two complex band matrices, both in band storage mode.
ACHAR	Returns a character given its ASCII value.
AMACH	Retrieves single-precision machine constants.
ARBRB	Adds two band matrices, both in band storage mode.
ARPACK_COMPLEX	Compute some eigenvalues and eigenvectors of the generalized eigenvalue problem $Ax = Bx$.
ARPACK_NONSYMMETRIC	Compute some eigenvalues and eigenvectors of the generalized eigenvalue problem $Ax = Bx$.
ARPACK_SYMMETRIC	Computes some eigenvalues and eigenvectors of the generalized real symmetric eigenvalue problem $Ax = Bx$.
ARPACK_SVD	Computes some singular values and left and right singular vectors of a real rectangular $A_{M \times N} = USV^T$.

B

Function	Purpose Statement
BCLSF	Solves a nonlinear least squares problem subject to bounds on the variables using a modified Levenberg-Marquardt algorithm and a finite-difference Jacobian.
BCLSJ	Solves a nonlinear least squares problem subject to bounds on the variables using a modified Levenberg-Marquardt algorithm and a user-supplied Jacobian.
BCNLS	Solves a nonlinear least-squares problem subject to bounds on the variables and general linear constraints.
BCOAH	Minimizes a function of N variables subject to bounds the variables using a modified Newton method and a user-supplied Hessian.
BCODH	Minimizes a function of N variables subject to bounds the variables using a modified Newton method and a finite-difference Hessian.
BCONF	Minimizes a function of N variables subject to bounds the variables using a quasi-Newton method and a finite-difference gradient.
BCONG	Minimizes a function of N variables subject to bounds the variables using a quasi-Newton method and a user-supplied gradient.
BCPOL	Minimizes a function of N variables subject to bounds the variables using a direct search complex algorithm.
BLINF	Computes the bilinear form x^TAy.
BS1GD	Evaluates the derivative of a spline on a grid, given its B-spline representation.
BS2DR	Evaluates the derivative of a two-dimensional tensor-product spline, given its tensor-product B-spline representation.
BS2GD	Evaluates the derivative of a two-dimensional tensor-product spline, given its tensor-product B-spline representation on a grid.
BS2IG	Evaluates the integral of a tensor-product spline on a rectangular domain, given its tensor-product B-spline representation.
BS2IN	Computes a two-dimensional tensor-product spline interpolant, returning the tensor-product B-spline coefficients.
BS2VL	Evaluates a two-dimensional tensor-product spline, given its tensor-product B-spline representation.
BS3DR	Evaluates the derivative of a three-dimensional tensor-product spline, given its tensor-product B-spline representation.

Function	Purpose Statement
BS3GD	Evaluates the derivative of a three-dimensional tensor-product spline, given its tensor-product B-spline representation on a grid.
BS3IG	Evaluates the integral of a tensor-product spline in three dimensions over a three-dimensional rectangle, given its tensorproduct B-spline representation.
BS3IN	Computes a three-dimensional tensor-product spline interpolant, returning the tensor-product B-spline coefficients.
BS3VL	Evaluates a three-dimensional tensor-product spline, given its tensor-product B-spline representation
BSCPP	Converts a spline in B-spline representation to piecewise polynomial representation.
BSDER	Evaluates the derivative of a spline, given its B-spline representation.
BSINT	Computes the spline interpolant, returning the B-spline coefficients.
BSITG	Evaluates the integral of a spline, given its B-spline representation.
BSLS2	Computes a two-dimensional tensor-product spline approximant using least squares, returning the tensor-product B-spline coefficients.
BSLS3	Computes a three-dimensional tensor-product spline approximant using least squares, returning the tensor-product B-spline coefficients.
BSLSQ	Computes the least-squares spline approximation, and return the B-spline coefficients.
BSNAK	Computes the 'not-a-knot' spline knot sequence.
BSOPK	Computes the 'optimal' spline knot sequence.
BSVAL	Evaluates a spline, given its B-spline representation.
BSVLS	Computes the variable knot B-spline least squares approximation to given data.
BVPFD	Solves a (parameterized) system of differential equations with boundary conditions at two points, using a variable order, variable step size finite-difference method with deferred corrections.
BVPMS	Solves a (parameterized) system of differential equations with boundary conditions at two points, using a multiple-shooting method.

C

Function	Purpose Statement
CADD	Adds a scalar to each component of a vector, $x \leftarrow x + a$, all complex.
CAXPY	Computes the scalar times a vector plus a vector, $y \leftarrow ax + y$, all complex.
CCBCB	Copies a complex band matrix stored in complex band storage mode.
CCBCG	Converts a complex matrix in band storage mode to a complex matrix in full storage mode.
CCGCB	Converts a complex general matrix to a matrix in complex band storage mode.
CCGCG	Copies a complex general matrix.
CCONV	Computes the convolution of two complex vectors.
CCOPY	Copies a vector x to a vector y, both complex.
CCORL	Computes the correlation of two complex vectors.
CDGRD	Approximates the gradient using central differences.
CDOTC	Computes the complex conjugate dot product, $\overline{x}^T y$.
CDOTU	Computes the complex dot product $x^T y$.
CGBMV	Computes one of the matrix-vector operations: $y \leftarrow \alpha Ax + \beta y,\ y \leftarrow \alpha A^T x + \beta y,\ \text{or}\ y \leftarrow \alpha \overline{A}^T + \beta y$, where A is a matrix stored in band storage mode.
CGEMM	Computes one of the matrix-matrix operations: $C \leftarrow \alpha AB + \beta C,\ C \leftarrow \alpha A^T B + \beta C,\ C \leftarrow \alpha AB^T + \beta C,$ $C \leftarrow \alpha A^T B^T + \beta C,\ C \leftarrow \alpha A\overline{B}^T + \beta C,$ $\text{or}\ C \leftarrow \alpha \overline{A}^T B + \beta C,\ C \leftarrow \alpha A^T \overline{B}^T + \beta C,\ C \leftarrow \alpha \overline{A}^T B^T + \beta C,$ $\text{or}\ C \leftarrow \alpha \overline{A}^T \overline{B}^T + \beta C$
CGEMV	Computes one of the matrix-vector operations: $y \leftarrow \alpha Ax + \beta y,\ y \leftarrow \alpha A^T x + \beta y,\ \text{or}\ y \leftarrow \alpha \overline{A}^T + \beta y$
CGERC	Computes the rank-one update of a complex general matrix: $A \leftarrow A + \alpha x \overline{y}^T$.
CGERU	Computes the rank-one update of a complex general matrix: $A \leftarrow A + \alpha x y^T$.

Function	Purpose Statement
CHBCB	Copies a complex Hermitian band matrix stored in band Hermitian storage mode to a complex band matrix stored in band storage mode.
CHBMV	Computes the matrix-vector operation $y \leftarrow \alpha Ax + \beta y$, where *A* is an Hermitian band matrix in band Hermitian storage.
CHEMM	Computes one of the matrix-matrix operations: $C \leftarrow \alpha AB + \beta C \text{ or } C \leftarrow \alpha BA + \beta C$, where *A* is an Hermitian matrix and *B* and *C* are *m* by *n* matrices.
CHEMV	Computes the matrix-vector operation $y \leftarrow \alpha Ax + \beta y$, where *A* is an Hermitian matrix.
CHER	Computes the rank-one update of an Hermitian matrix: $A \leftarrow A + \alpha x\overline{x}^T$ with *x* complex and α real.
CHER2	Computes a rank-two update of an Hermitian matrix: $A \leftarrow A + \alpha x\overline{y}^T + \overline{\alpha} y\overline{x}^T$.
CHER2K	Computes one of the Hermitian rank 2*k* operations: $C \leftarrow \alpha A\overline{B}^T + \overline{\alpha}B\overline{A}^T + \beta C \text{ or } C \leftarrow \alpha\overline{A}^T B + \overline{\alpha}\overline{B}^T A + \beta C$, where *C* is an *n* by *n* Hermitian matrix and *A* and *B* are *n* by *k* matrices in the first case and *k* by *n* matrices in the second case.
CHERK	Computes one of the Hermitian rank *k* operations: $C \leftarrow \alpha A\overline{A}^T + \beta C \text{ or } C \leftarrow \alpha\overline{A}^T A + \beta C$, where *C* is an *n* by *n* Hermitian matrix and *A* is an *n* by *k* matrix in the first case and a *k* by *n* matrix in the second case.
CHFCG	Extends a complex Hermitian matrix defined in its upper triangle to its lower triangle.
CHGRD	Checks a user-supplied gradient of a function.
CHHES	Checks a user-supplied Hessian of an analytic function.
CHJAC	Checks a user-supplied Hessian of an analytic function.
CHOL	Checks a user-supplied Jacobian of a system of equations with `M` functions in `N` unknowns.
CHPMV	Computes the matrix-vector operation $y \leftarrow \alpha Ax + \beta y$ where *A* is an Hermitian matrix.
CHPR	Performs the matrix-vector operation: $A \leftarrow A + \alpha x\overline{x}^T$, where *A* is a triangular packed Hermitian.
COND	Computes the condition number of a matrix.
CONFT	Computes the least-squares constrained spline approximation, returning the B-spline coefficients.
CONST	Returns the value of various mathematical and physical constants.
CPSEC	Returns CPU time used in seconds.

Function	Purpose Statement
CRBCB	Converts a real matrix in band storage mode to a complex matrix in band storage mode.
CRBRB	Copies a real band matrix stored in band storage mode.
CRBRG	Converts a real matrix in band storage mode to a real general matrix.
CRGCG	Copies a real general matrix to a complex general matrix.
CRGRB	Converts a real general matrix to a matrix in band storage mode.
CRGRG	Copies a real general matrix.
CRRCR	Copies a real rectangular matrix to a complex rectangular matrix.
CS1GD	Evaluates the derivative of a cubic spline on a grid.
CSAKM	Computes the Akima cubic spline interpolant.
CSBRB	Copies a real symmetric band matrix stored in band symmetric storage mode to a real band matrix stored in band storage mode.
CSCAL	Multiplies a vector by a scalar, $y \leftarrow ay$, both complex.
CSCON	Computes a cubic spline interpolant that is consistent with the concavity of the data.
CSDEC	Computes the cubic spline interpolant with specified derivative endpoint conditions.
CSDER	Evaluates the derivative of a cubic spline.
CSET	Sets the components of a vector to a scalar, all complex.
CSFRG	Extends a real symmetric matrix defined in its upper triangle to its lower triangle.
CSHER	Computes the Hermite cubic spline interpolant.
CSIEZ	Computes the cubic spline interpolant with the 'not-a-knot' condition and return values of the interpolant at specified points.
CSINT	Computes the cubic spline interpolant with the 'not-a-knot' condition.
CSITG	Evaluates the integral of a cubic spline.
CSPER	Computes the cubic spline interpolant with periodic boundary conditions.
CSROT	Applies a complex Givens plane rotation.
CSROTM	Applies a complex modified Givens plane rotation.
CSSCAL	Multiplies a complex vector by a single-precision scalar, $y \leftarrow ay$.
CSSCV	Computes a smooth cubic spline approximation to noisy data using cross-validation to estimate the smoothing parameter.
CSSED	Smooths one-dimensional data by error detection.
CSSMH	Computes a smooth cubic spline approximation to noisy data.

Function	Purpose Statement
CSUB	Subtracts each component of a vector from a scalar, $x \leftarrow a - x$, all complex.
CSVAL	Evaluates a cubic spline.
CSVCAL	Multiplies a complex vector by a single-precision scalar and store the result in another complex vector, $y \leftarrow ax$.
CSWAP	Interchanges vectors *x* and *y*, both complex.
CSYMM	Computes one of the matrix-matrix operations: $C \leftarrow \alpha AB + \beta C$ or $C \leftarrow \alpha BA + \beta C$, where *A* is a symmetric matrix and *B* and *C* are *m* by *n* matrices.
CSYR2K	Computes one of the symmetric rank 2*k* operations: $C \leftarrow \alpha AB^T + \alpha BA^T + \beta C$ or $C \leftarrow \alpha A^T B + \alpha B^T A + \beta C$, where *C* is an *n* by *n* symmetric matrix and *A* and *B* are *n* by *k* matrices in the first case and *k* by *n* matrices in the second case.
CSYRK	Computes one of the symmetric rank *k* operations: $C \leftarrow \alpha AA^T + \beta C$ or $C \leftarrow \alpha A^T A + \beta C$, where *C* is an *n* by *n* symmetric matrix and *A* is an *n* by *k* matrix in the first case and a *k* by *n* matrix in the second case.
CTBMV	Computes one of the matrix-vector operations: $x \leftarrow Ax$, $x \leftarrow A^T x$, or $x \leftarrow \overline{A}^T x$, where *A* is a triangular matrix in band storage mode.
CTBSV	Solves one of the complex triangular systems: $x \leftarrow A^{-1}x$, $x \leftarrow \left(A^{-1}\right)^T x$, or $x \leftarrow \left(\overline{A}^T\right)^{-1} x$, where *A* is a triangular matrix in band storage mode.
CTPSV	Solves one of the system of equations: $x \leftarrow \left(\overline{A}^T\right)^{-1} x \equiv \left(A^H\right)^{-1} x$ where A is a packed upper or lower triangular matrix.
CTPMV	Performes the matrix-vector operation, $x \leftarrow \overline{A}^T x$, where *A* is a packed triangular matrix.
CTRMM	Computes one of the matrix-matrix operations: $B \leftarrow \alpha AB,\ B \leftarrow \alpha A^T B,\ B \leftarrow \alpha BA,\ B \leftarrow \alpha BA^T,$ $B \leftarrow \alpha \overline{A}^T B,\ or\ B \leftarrow \alpha B\overline{A}^T$ where *B* is an m by n matrix and *A* is a triangular matrix.
CTRMV	Computes one of the matrix-vector operations: $x \leftarrow Ax$, $x \leftarrow A^T x$, or $x \leftarrow \overline{A}^T x$, where *A* is a triangular matrix.

Function	Purpose Statement
CTRSM	Solves one of the complex matrix equations: $B \leftarrow \alpha A^{-1}B,\ B \leftarrow \alpha BA^{-1},\ B \leftarrow \alpha\left(A^{-1}\right)^{T}B,\ B \leftarrow \alpha B\left(A^{-1}\right)^{T},$ $B \leftarrow \alpha\left(\overline{A}^{T}\right)^{-1}B$, or $B \leftarrow \alpha B\left(\overline{A}^{T}\right)^{-1}$ where A is a traiangular matrix
CTRSV	Solves one of the complex triangular systems: $x \leftarrow A^{-1}x,\ x \leftarrow \left(A^{-1}\right)^{T}x$, or $x \leftarrow \left(\overline{A}^{T}\right)^{-1}x,$ where A is a triangular matrix.
CUNIT	Converts X in units XUNITS to Y in units YUNITS.
CVCAL	Multiplies a vector by a scalar and store the result in another vector, $y \leftarrow ax$, all complex.
CVTSI	Converts a character string containing an integer number into the corresponding integer form.
CZCDOT	Computes the sum of a complex scalar plus a complex conjugate dot product, $a + \overline{x}^{T}y$, using a double-precision accumulator.
CZDOTA	Computes the sum of a complex scalar, a complex dot product and the double-complex accumulator, which is set to the result ACC $\leftarrow$ ACC $+ a + x^{T}y$.
CZDOTC	Computes the complex conjugate dot product, $\overline{x}^{T}y$, using a double-precision accumulator.
CZDOTI	Computes the sum of a complex scalar plus a complex dot product using a double-complex accumulator, which is set to the result ACC $\leftarrow a + x^{T}y$.
CZDOTU	Computes the complex dot product $x^{T}y$ using a double-precision accumulator.
CZUDOT	Computes the sum of a complex scalar plus a complex dot product, $a + x^{T}y$, using a double-precision accumulator.

D

Function	Purpose Statement
DAESL	Solves a first order differential-algebraic system of equations, $g(t, y, y') = 0$, possibly with additional constraints.
DDJAC	Approximates the Jacobian of m functions in n unknowns using divided differences
DENSE_LP	Solves a linear programming problem.
DERIV	Computes the first, second or third derivative of a user-supplied function.
DET	Computes the determinant of a rectangular matrix, A.
DIAG	Constructs a square diagonal matrix from a rank-1 array or several diagonal matrices from a rank-2 array.
DIAGONALS	Extracts a rank-1 array whose values are the diagonal terms of a rank-2 array argument.
DISL1	Computes the 1-norm distance between two points.
DISL2	Computes the Euclidean (2-norm) distance between two points.
DISLI	Computes the infinity norm distance between two points.
DLPRS	Solves a linear programming problem via the revised simplex algorithm.
DMACH	See AMACH.
DQADD (See *Extended Precision Arithmetic*, *Chapter 9*)	Adds a double-precision scalar to the accumulator in extended precision.
DQINI (See *Extended Precision Arithmetic*, *Chapter 9*)	Initializes an extended-precision accumulator with a double-precision scalar.
DQMUL (See *Extended Precision Arithmetic*, *Chapter 9*)	Multiplies double-precision scalars in extended precision.
DQSTO (See Extended Precision Arithmetic *Chapter 9*)	Stores a double-precision approximation to an extended-precision scalar.
DSDOT (See *Chapter 9*)	Computes the single-precision dot product $x^T y$ using a double precision accumulator.
DUMAG	This routine handles MATH/LIBRARY and STAT/LIBRARY type DOUBLE PRECISION options.

E

Function	Purpose Statement
EIG	Computes the eigenvalue-eigenvector decomposition of an ordinary or generalized eigenvalue problem.
EPICG	Computes the performance index for a complex eigensystem.
EPIHF	Computes the performance index for a complex Hermitian eigensystem.
EPIRG	Computes the performance index for a real eigensystem.
EPISB	Computes the performance index for a real symmetric eigensystem in band symmetric storage mode.
EPISF	Computes the performance index for a real symmetric eigensystem.
ERROR_POST	Prints error messages that are generated by IMSL routines using EPACK.
ERSET	Sets error handler default print and stop actions.
EVAHF	Computes the largest or smallest eigenvalues of a complex Hermitian matrix.
EVASB	Computes the largest or smallest eigenvalues of a real symmetric matrix in band symmetric storage mode.
EVASF	Computes the largest or smallest eigenvalues of a real symmetric matrix.
EVBHF	Computes the eigenvalues in a given range of a complex Hermitian matrix.
EVBSB	Computes the eigenvalues in a given interval of a real symmetric matrix stored in band symmetric storage mode.
EVBSF	Computes selected eigenvalues of a real symmetric matrix.
EVCCG	Computes all of the eigenvalues and eigenvectors of a complex matrix.
EVCCH	Computes all of the eigenvalues and eigenvectors of a complex upper Hessenberg matrix.
EVCHF	Computes all of the eigenvalues and eigenvectors of a complex Hermitian matrix.
EVCRG	Computes all of the eigenvalues and eigenvectors of a real matrix.
EVCRH	Computes all of the eigenvalues and eigenvectors of a real upper Hessenberg matrix.
EVCSB	Computes all of the eigenvalues and eigenvectors of a real symmetric matrix in band symmetric storage mode.

Function	Purpose Statement
EVCSF	Computes all of the eigenvalues and eigenvectors of a real symmetric matrix.
EVEHF	Computes the largest or smallest eigenvalues and the corresponding eigenvectors of a complex Hermitian matrix.
EVESB	Computes the largest or smallest eigenvalues and the corresponding eigenvectors of a real symmetric matrix in band symmetric storage mode.
EVESF	Computes the largest or smallest eigenvalues and the corresponding eigenvectors of a real symmetric matrix.
EVFHF	Computes the eigenvalues in a given range and the corresponding eigenvectors of a complex Hermitian matrix.
EVFSB	Computes the eigenvalues in a given interval and the corresponding eigenvectors of a real symmetric matrix stored in band symmetric storage mode.
EVFSF	Computes selected eigenvalues and eigenvectors of a real symmetric matrix.
EVLCG	Computes all of the eigenvalues of a complex matrix.
EVLCH	Computes all of the eigenvalues of a complex upper Hessenberg matrix.
EVLHF	Computes all of the eigenvalues of a complex Hermitian matrix.
EVLRG	Computes all of the eigenvalues of a real matrix.
EVLRH	Computes all of the eigenvalues of a real upper Hessenberg matrix.
EVLSB	Computes all of the eigenvalues of a real symmetric matrix in band symmetric storage mode.
EVLSF	Computes all of the eigenvalues of a real symmetric matrix.
EYE	Creates a rank-2 square array whose diagonals are all the value one.

F

Function	Purpose Statement
FAURE_FREE	Frees the structure containing information about the Faure sequence.
FAURE_INIT	Shuffled Faure sequence initialization.

Function	Purpose Statement
FAURE_NEXT	Computes a shuffled Faure sequence.
FAST_DFT	Computes the Discrete Fourier Transform of a rank-1 complex array, *x*.
FAST_2DFT	Computes the Discrete Fourier Transform (2DFT) of a rank-2 complex array, *x*.
FAST_3DFT	Computes the Discrete Fourier Transform (2DFT) of a rank-3 complex array, *x*.
FCOSI	Computes parameters needed by FCOST.
FCOST	Computes the discrete Fourier cosine transformation of an even sequence.
FDGRD	Approximates the gradient using forward differences.
FDHES	Approximates the Hessian using forward differences and function values.
FDJAC	Approximates the Jacobian of M functions in N unknowns using forward differences.
FEYNMAN_KAC	Solves the generalized Feynman-Kac PDE on a rectangular grid using a finite element Galerkin method. Initial and boundary conditions are provided.
FFT	The Discrete Fourier Transform of a complex sequence and its inverse transform.
FFT_BOX	The Discrete Fourier Transform of several complex or real sequences.
FFT2B	Computes the inverse Fourier transform of a complex periodic two-dimensional array.
FFT2D	Computes Fourier coefficients of a complex periodic two-dimensional array.
FFT3B	Computes the inverse Fourier transform of a complex periodic three-dimensional array.
FFT3F	Computes Fourier coefficients of a complex periodic three-dimensional array.
FFTCB	Computes the complex periodic sequence from its Fourier coefficients.
FFTCF	Computes the Fourier coefficients of a complex periodic sequence.
FFTCI	Computes parameters needed by FFTCF and FFTCB.
FFTRB	Computes the real periodic sequence from its Fourier coefficients.
FFTRF	Computes the Fourier coefficients of a real periodic sequence.
FFTRI	Computes parameters needed by FFTRF and FFTRB.

Function	Purpose Statement
FNLSQ	Computes a least-squares approximation with user-supplied basis functions.
FPS2H	Solves Poisson's or Helmholtz's equation on a two-dimensional rectangle using a fast Poisson solver based on the HODIE finite-difference scheme on a uni mesh.
FPS3H	Solves Poisson's or Helmholtz's equation on a three-dimensional box using a fast Poisson solver based on the HODIE finite-difference scheme on a uniform mesh.
FQRUL	Computes a Fejér quadrature rule with various classical weight functions.
FSINI	Computes parameters needed by FSINT.
FSINT	Computes the discrete Fourier sine transformation of an odd sequence.

G

Function	Purpose Statement
GDHES	Approximates the Hessian using forward differences and a user-supplied gradient.
GGUES	Generates points in an N-dimensional space.
GMRES	Uses restarted GMRES with reverse communication to generate an approximate solution of $Ax = b$.
GPICG	Computes the performance index for a generalized complex eigensystem $Az = \lambda Bz$.
GPIRG	Computes the performance index for a generalized real eigensystem $Az = \lambda Bz$.
GPISP	Computes the performance index for a generalized real symmetric eigensystem problem.
GQRCF	Computes a Gauss, Gauss-Radau or Gauss-Lobatto quadrature rule given the recurrence coefficients for the monic polynomials orthogonal with respect to the weight function.
GQRUL	Computes a Gauss, Gauss-Radau, or Gauss-Lobatto quadrature rule with various classical weight functions.
GVCCG	Computes all of the eigenvalues and eigenvectors of a generalized complex eigensystem $Az = \lambda Bz$.

Function	Purpose Statement
GVCRG	Computes all of the eigenvalues and eigenvectors of a generalized real eigensystem $Az = \lambda Bz$.
GVCSP	Computes all of the eigenvalues and eigenvectors of the generalized real symmetric eigenvalue problem $Az = \lambda Bz$, with B symmetric positive definite.
GVLCG	Computes all of the eigenvalues of a generalized complex eigensystem $Az = \lambda Bz$.
GVLRG	Computes all of the eigenvalues of a generalized real eigensystem $Az = \lambda Bz$.
GVLSP	Computes all of the eigenvalues of the generalized real symmetric eigenvalue problem $Az = \lambda Bz$, with B symmetric positive definite.

H

Function	Purpose Statement
HRRRR	Computes the Hadamard product of two real rectangular matrices.
HYPOT	Computes $\sqrt{a^2 + b^2}$ without underflow or overflow.

I

Function	Purpose Statement
IACHAR	Returns the integer ASCII value of a character argument.
IADD	Adds a scalar to each component of a vector, $x \leftarrow x + a$, all integer..
ICAMAX	Finds the smallest index of the component of a complex vector having maximum magnitude.
ICAMIN	Finds the smallest index of the component of a complex vector having minimum magnitude.

Function	Purpose Statement
ICASE	Returns the ASCII value of a character converted to uppercase.
ICOPY	Copies a vector *x* to a vector *y*, both integer.
IDYWK	Computes the day of the week for a given date.
IERCD and N1RTY	Retrieves the code for an informational error.
IFFT	The inverse of the Discrete Fourier Transform of a complex sequence.
IFFT_BOX	The inverse Discrete Fourier Transform of several complex or real sequences.
IFNAN(X)	Checks if a value is NaN (not a number).
IICSR	Compares two character strings using the ASCII collating sequence but without regard to case.
IIDEX	Determines the position in a string at which a given character sequence begins without regard to case.
IIMAX	Finds the smallest index of the maximum component of a integer vector.
IIMIN	Finds the smallest index of the minimum of an integer vector.
IMACH	Retrieves integer machine constants.
INLAP	Computes the inverse Laplace transform of a complex function.
ISAMAX	Finds the smallest index of the component of a single-precision vector having maximum absolute value.
ISAMIN	Finds the smallest index of the component of a single-precision vector having minimum absolute value.
ISET	Sets the components of a vector to a scalar, all integer.
ISMAX	Finds the smallest index of the component of a single-precision vector having maximum value.
ISMIN	Finds the smallest index of the component of a single-precision vector having minimum value.
ISNAN	This is a generic logical function used to test scalars or arrays for occurrence of an IEEE 754 Standard format of floating point (ANSI/IEEE 1985) NaN, or not-a-number.
ISRCH	Searches a sorted integer vector for a given integer and return its index.
ISUB	Subtracts each component of a vector from a scalar, $x \leftarrow a - x$, all integer.
ISUM	Sums the values of an integer vector.
ISWAP	Interchanges vectors *x* and *y*, both integer.
IUMAG	Sets or retrieves MATH/LIBRARY integer options.

Function	Purpose Statement
IVMRK	Solves an initial-value problem $y' = f(t, y)$ for ordinary differential equations using Runge-Kutta pairs of various orders.
IVOAM	Solves an initial-value problem for a system of ordinary differential equations of order one or two using a variable order Adams method.
IVPAG	Solves an initial-value problem for ordinary differential equations using either Adams-Moulton's or Gear's BDF method.
IVPRK	Solves an initial-value problem for ordinary differential equations using the Runge-Kutta-Verner fifth-order and sixth-order method.

J

Function	Purpose Statement
JCGRC	Solves a real symmetric definite linear system using the Jacobi preconditioned conjugate gradient method with reverse communication.

L

Function	Purpose Statement
LCHRG	Computes the Cholesky decomposition of a symmetric positive semidefinite matrix with optional column pivoting.
LCLSQ	Solves a linear least-squares problem with linear constraints.
LCONF	Minimizes a general objective function subject to linear equality/inequality constraints.
LCONG	Minimizes a general objective function subject to linear equality/inequality constraints.
LDNCH	Downdates the $R^T R$ Cholesky factorization of a real symmetric positive definite matrix after a rank-one matrix is removed

Function	Purpose Statement
LFCCB	Computes the *LU* factorization of a complex matrix in band storage mode and estimate its L_1. condition number.
LFCCG	Computes the *LU* factorization of a complex general matrix and estimate its L_1 condition number.
LFCCT	Estimates the condition number of a complex triangular matrix.
LFCDH	Computes the $R^H R$ factorization of a complex Hermitian positive definite matrix and estimate its L_1 condition number.
LFCDS	Computes the $R^T R$ Cholesky factorization of a real symmetric positive definite matrix and estimate its L_1condition number.
LFCHF	Computes the $U DU^H$ factorization of a complex Hermitian matrix and estimate its L_1 condition number.
LFCQH	Computes the $R^H R$ factorization of a complex Hermitian positive definite matrix in band Hermitian storage mode and estimate its L_1 condition number.
LFCQS	Computes the $R^T R$ Cholesky factorization of a real symmetric positive definite matrix in band symmetric storage mode and estimate its L_1 condition number.
LFCRB	Computes the *LU* factorization of a real matrix in band storage mode and estimate its L_1 condition number.
LFCRG	Computes the *LU* factorization of a real general matrix and estimate its L_1 condition number.
LFCRT	Estimates the condition number of a real triangular matrix.
LFCSF	Computes the $U DU^T$ factorization of a real symmetric matrix and estimate its L_1 condition number.
LFDCB	Computes the determinant of a complex matrix given the *LU* factorization of the matrix in band storage mode.
LFDCG	Computes the determinant of a complex general matrix given the *LU* factorization of the matrix.
LFDCT	Computes the determinant of a complex triangular matrix.
LFDDH	Computes the determinant of a complex Hermitian positive definite matrix given the $R^H R$ Cholesky factorization of the matrix.
LFDDS	Computes the determinant of a real symmetric positive definite matrix given the $R^H R$ Cholesky factorization of the matrix.
LFDHF	Computes the determinant of a complex Hermitian matrix given the $U DU^H$ factorization of the matrix.

Function	Purpose Statement
LFDQH	Computes the determinant of a complex Hermitian positive definite matrix given the $R^H R$ Cholesky factorization in band Hermitian storage mode.
LFDQS	Computes the determinant of a real symmetric positive definite matrix given the $R^T R$ Cholesky factorization of the band symmetric storage mode.
LFDRB	Computes the determinant of a real matrix in band storage mode given the *LU* factorization of the matrix.
LFDRG	Computes the determinant of a real general matrix given the *LU* factorization of the matrix.
LFDRT	Computes the determinant of a real triangular matrix.
LFDSF	Computes the determinant of a real symmetric matrix given the $U D U^T$ factorization of the matrix.
LFICB	Uses iterative refinement to improve the solution of a complex system of linear equations in band storage mode.
LFICG	Uses iterative refinement to improve the solution of a complex general system of linear equations.
LFIDH	Uses iterative refinement to improve the solution of a complex Hermitian positive definite system of linear equations.
LFIDS	Uses iterative refinement to improve the solution of a real symmetric positive definite system of linear equations.
LFIHF	Uses iterative refinement to improve the solution of a complex Hermitian system of linear equations.
LFIQH	Uses iterative refinement to improve the solution of a complex Hermitian positive definite system of linear equations in band Hermitian storage mode.
LFIQS	Uses iterative refinement to improve the solution of a real symmetric positive definite system of linear equations in band symmetric storage mode.
LFIRB	Uses iterative refinement to improve the solution of a real system of linear equations in band storage mode.
LFIRG	Uses iterative refinement to improve the solution of a real general system of linear equations.
LFISF	Uses iterative refinement to improve the solution of a real symmetric system of linear equations.
LFSCB	Solves a complex system of linear equations given the *LU* factorization of the coefficient matrix in band storage mode.
LFSCG	Solves a complex general system of linear equations given the *LU* factorization of the coefficient matrix.
LFSDH	Solves a complex Hermitian positive definite system of linear equations given the $R^H R$ factorization of the coefficient matrix.

Function	Purpose Statement
LFSDS	Solves a real symmetric positive definite system of linear equations given the $R^T R$ Choleksy factorization of the coefficient matrix.
LFSHF	Solves a complex Hermitian system of linear equations given the $U DU^H$ factorization of the coefficient matrix.
LFSQH	Solves a complex Hermitian positive definite system of linear equations given the factorization of the coefficient matrix in band Hermitian storage mode.
LFSQS	Solves a real symmetric positive definite system of linear equations given the factorization of the coefficient matrix in band symmetric storage mode.
LFSRB	Solves a real system of linear equations given the *LU* factorization of the coefficient matrix in band storage mode.
LFSRG	Solves a real general system of linear equations given the *LU* factorization of the coefficient matrix.
LFSSF	Solves a real symmetric system of linear equations given the $U DU^T$ factorization of the coefficient matrix.
LFSXD	Solves a real sparse symmetric positive definite system of linear equations, given the Cholesky factorization of the coefficient matrix.
LFSXG	Solves a sparse system of linear equations given the *LU* factorization of the coefficient matrix.
LFSZD	Solves a complex sparse Hermitian positive definite system of linear equations, given the Cholesky factorization of the coefficient matrix.
LFSZG	Solves a complex sparse system of linear equations given the *LU* factorization of the coefficient matrix.
LFTCB	Computes the *LU* factorization of a complex matrix in band storage mode.
LFTCG	Computes the *LU* factorization of a complex general matrix.
LFTDH	Computes the $R^H R$ factorization of a complex Hermitian positive definite matrix.
LFTDS	Computes the $R^T R$ Cholesky factorization of a real symmetric positive definite matrix.
LFTHF	Computes the $U DU^H$ factorization of a complex Hermitian matrix.
LFTQH	Computes the $R^H R$ factorization of a complex Hermitian positive definite matrix in band Hermitian storage mode.
LFTQS	Computes the $R^T R$ Cholesky factorization of a real symmetric positive definite matrix in band symmetric storage mode.

Function	Purpose Statement
LFTRB	Computes the *LU* factorization of a real matrix in band storage mode.
LFTRG	Computes the *LU* factorization of a real general matrix.
LFTSF	Computes the $U\,DU^T$ factorization of a real symmetric matrix.
LFTXG	Computes the *LU* factorization of a real general sparse matrix.
LFTZG	Computes the *LU* factorization of a complex general sparse matrix.
LINCG	Computes the inverse of a complex general matrix.
LINCT	Computes the inverse of a complex triangular matrix.
LINDS	Computes the inverse of a real symmetric positive definite matrix.
LINRG	Computes the inverse of a real general matrix.
LINRT	Computes the inverse of a real triangular matrix.
LIN_EIG_GEN	Computes the eigenvalues of a self-adjoint matrix, *A*.
LIN_EIG_SELF	Computes the eigenvalues of a self-adjoint matrix, *A*.
LIN_GEIG_GEN	Computes the generalized eigenvalues of an $n \times n$ matrix pencil, $Av = \lambda Bv$.
LIN_SOL_GEN	Solves a general system of linear equations $Ax = b$.
LIN_SOL_LSQ	Solves a rectangular system of linear equations $Ax \cong b$, in a least-squares sense.
LIN_SOL_SELF	Solves a system of linear equations $Ax = b$, where *A* is a self-adjoint matrix.
LIN_SOL_SVD	Solves a rectangular least-squares system of linear equations $Ax \cong b$ using singular value decomposition.
LIN_SOL_TRI	Solves multiple systems of linear equations.
LIN_SVD	Computes the singular value decomposition (SVD) of a rectangular matrix, *A*.
LNFXD	Computes the numerical Cholesky factorization of a sparse symmetrical matrix *A*.
LNFZD	Computes the numerical Cholesky factorization of a sparse Hermitian matrix *A*.
LQERR	Accumulates the orthogonal matrix *Q* from its factored form given the *QR* factorization of a rectangular matrix *A*.
LQRRR	Computes the *QR* decomposition, $AP = QR$, using Householder transformations.
LQRRV	Computes the least-squares solution using Householder transformations applied in blocked form.

Function	Purpose Statement
LQRSL	Computes the coordinate transformation, projection, and complete the solution of the least-squares problem $Ax = b$.
LSACB	Solves a complex system of linear equations in band storage mode with iterative refinement.
LSACG	Solves a complex general system of linear equations with iterative refinement.
LSADH	Solves a Hermitian positive definite system of linear equations with iterative refinement.
LSADS	Solves a real symmetric positive definite system of linear equations with iterative refinement.
LSAHF	Solves a complex Hermitian system of linear equations with iterative refinement.
LSAQH	Solves a complex Hermitian positive definite system of linear equations in band Hermitian storage mode with iterative refinement.
LSAQS	Solves a real symmetric positive definite system of linear equations in band symmetric storage mode with iterative refinement.
LSARB	Solves a real system of linear equations in band storage mode with iterative refinement.
LSARG	Solves a real general system of linear equations with iterative refinement.
LSASF	Solves a real symmetric system of linear equations with iterative refinement.
LSBRR	Solves a linear least-squares problem with iterative refinement.
LSCXD	Performs the symbolic Cholesky factorization for a sparse symmetric matrix using a minimum degree ordering or a userspecified ordering, and set up the data structure for the numerical Cholesky factorization.
LSGRR	Computes the generalized inverse of a real matrix.
LSLCB	Solves a complex system of linear equations in band storage mode without iterative refinement.
LSLCC	Solves a complex circulant linear system.
LSLCG	Solves a complex general system of linear equations without iterative refinement.
LSLCQ	Computes the *LDU* factorization of a complex tridiagonal matrix *A* using a cyclic reduction algorithm.
LSLCR	Computes the *LDU* factorization of a real tridiagonal matrix *A* using a cyclic reduction algorithm.
LSLCT	Solves a complex triangular system of linear equations.

Function	Purpose Statement
LSLDH	Solves a complex Hermitian positive definite system of linear equations without iterative refinement.
LSLDS	Solves a real symmetric positive definite system of linear equations without iterative refinement.
LSLHF	Solves a complex Hermitian system of linear equations without iterative refinement.
LSLPB	Computes the $R^T DR$ Cholesky factorization of a real symmetric positive definite matrix *A* in codiagonal band symmetric storage mode. Solve a system $Ax = b$.
LSLQB	Computes the $R^H DR$ Cholesky factorization of a complex hermitian positive-definite matrix *A* in codiagonal band hermitian storage mode. Solve a system $Ax = b$.
LSLQH	Solves a complex Hermitian positive definite system of linearequations in band Hermitian storage mode without iterative refinement.
LSLQS	Solves a real symmetric positive definite system of linear equations in band symmetric storage mode without iterative refinement.
LSLRB	Solves a real system of linear equations in band storage mode without iterative refinement.
LSLRG	Solves a real general system of linear equations without iterative refinement.
LSLRT	Solves a real triangular system of linear equations.
LSLSF	Solves a real symmetric system of linear equations without iterative refinement.
LSLTC	Solves a complex Toeplitz linear system.
LSLTO	Solves a real Toeplitz linear system.
LSLTQ	Solves a complex tridiagonal system of linear equations.
LSLTR	Solves a real tridiagonal system of linear equations.
LSLXD	Solves a sparse system of symmetric positive definite linear algebraic equations by Gaussian elimination.
LSLXG	Solves a sparse system of linear algebraic equations by Gaussian elimination.
LSLZD	Solves a complex sparse Hermitian positive definite system of linear equations by Gaussian elimination.
LSLZG	Solves a complex sparse system of linear equations by Gaussian elimination.
LSQRR	Solves a linear least-squares problem without iterative refinement.

Function	Purpose Statement
LSVCR	Computes the singular value decomposition of a complex matrix.
LSVRR	Computes the singular value decomposition of a real matrix.
LUPCH	Updates the $R^T R$ Cholesky factorization of a real symmetric positive definite matrix after a rank-one matrix is added.
LUPQR	Computes an updated QR factorization after the rank-one matrix αxy^T is added.

M

Function	Purpose Statement
MCRCR	Multiplies two complex rectangular matrices, *AB*.
MMOLCH	Solves a system of partial differential equations of the form $u_t = f(x, t, u, u_x, u_{xx})$ using the method of lines. The solution is represented with cubic Hermite polynomials.
MP_SETUP	Initializes or finalizes MPI.
MPS_FREE	Deallocates the space allocated for the IMSL derived type `s_MPS`. This routine is usually used in conjunction with `READ_MPS`.
MRRRR	Multiplies two real rectangular matrices, *AB*.
MUCBV	Multiplies a complex band matrix in band storage mode by a complex vector.
MUCRV	Multiplies a complex rectangular matrix by a complex vector.
MURBV	Multiplies a real band matrix in band storage mode by a real vector.
MURRV	Multiplies a real rectangular matrix by a vector.
MXTXF	Computes the transpose product of a matrix, A^TA.
MXTYF	Multiplies the transpose of matrix *A* by matrix *B*, A^TB.
MXYTF	Multiplies a matrx *A* by the transpose of a matrix *B*, AB^T.

N

Function	Purpose Statement
NAN	Returns, as a scalar function, a value corresponding to the IEEE 754 Standard format of floating point (ANSI/IEEE 1985) for NaN.
IERCD and N1RTY	Retrieves an error type for the most recently called IMSL routine.
NDAYS	Computes the number of days from January 1, 1900, to the given date.
NDYIN	Gives the date corresponding to the number of days since January 1, 1900.
NEQBF	Solves a system of nonlinear equations using factored secant update with a finite-difference approximation to the Jacobian.
NEQBJ	Solves a system of nonlinear equations using factored secant update with a user-supplied Jacobian.
NEQNF	Solves a system of nonlinear equations using a modified Powell hybrid algorithm and a finite-difference approximation to the Jacobian.
NEQNJ	Solves a system of nonlinear equations using a modified Powell hybrid algorithm with a user-supplied Jacobian.
NNLPF	Uses a sequential equality constrained QP method.
NNLPG	Uses a sequential equality constrained QP method.
NORM	Computes the norm of a rank-1 or rank-2 array. For rank-3 arrays, the norms of each rank-2 array, in dimension 3, are computed.
NR1CB	Computes the 1-norm of a complex band matrix in band storage mode.
NR1RB	Computes the 1-norm of a real band matrix in band storage mode.
NR1RR	Computes the 1-norm of a real matrix.
NR2RR	Computes the Frobenius norm of a real rectangular matrix.
NRIRR	Computes the infinity norm of a real matrix.

O

Function	Purpose Statement
OPERATORS:	
.h.	Computes transpose and conjugate transpose of a matrix.
.hx.	Computes matrix-vector and matrix-matrix products.
.i.	Computes the inverse matrix, for square non-singular matrices.
.ix.	Computes the inverse matrix times a vector or matrix for square non-singular matrices.
.t.	Computes transpose and conjugate transpose of a matrix.
.tx.	Computes matrix-vector and matrix-matrix products.
.x.	Computes matrix-vector and matrix-matrix products.
.xh.	Computes matrix-vector and matrix-matrix products.
.xi.	Computes the inverse matrix times a vector or matrix for square non-singular matrices.
.xt.	Computes matrix-vector and matrix-matrix products.
ORTH	Orthogonalizes the columns of a rank-2 or rank-3 array.

P

Function	Purpose Statement
PCGRC	Solves a real symmetric definite linear system using a preconditioned conjugate gradient method with reverse communication.
PARALLEL_NONNEGATIVE_LSQ	Solves a linear, non-negative constrained least-squares system.
PARALLEL_BOUNDED_LSQ	Solves a linear least-squares system with bounds on the unknowns.
PDE_1D_MG	Method of lines with Variable Griddings.
PERMA	Permutes the rows or columns of a matrix.
PERMU	Rearranges the elements of an array as specified by a permutation.

Function	Purpose Statement
PGOPT	Prints a plot of up to 10 sets of points.
PLOTP	Prints a plot of up to 10 sets of points.
POLRG	Evaluates a real general matrix polynomial.
PP1GD	Evaluates the derivative of a piecewise polynomial on a grid.
PPDER	Evaluates the derivative of a piecewise polynomial.
PPITG	Evaluates the integral of a piecewise polynomial.
PPVAL	Evaluates a piecewise polynomial.
PRIME	Decomposes an integer into its prime factors.

Q

Function	Purpose Statement
QAND	Integrates a function on a hyper-rectangle.
QCOSB	Computes a sequence from its cosine Fourier coefficients with only odd wave numbers.
QCOSF	Computes the coefficients of the cosine Fourier transform with only odd wave numbers.
QCOSI	Computes parameters needed by QCOSF and QCOSB.
QD2DR	Evaluates the derivative of a function defined on a rectangular grid using quadratic interpolation.
QD2VL	Evaluates a function defined on a rectangular grid using quadratic interpolation.
QD3DR	Evaluates the derivative of a function defined on a rectangular three-dimensional grid using quadratic interpolation.
QD3VL	Evaluates a function defined on a rectangular three-dimensional grid using quadratic interpolation.
QDAG	Integrates a function using a globally adaptive scheme based on Gauss-Kronrod rules.
QDAGI	Integrates a function over an infinite or semi-infinite interval.
QDAGP	Integrates a function with singularity points given.
QDAG1D	Integrates a function with a possible internal or endpoint singularity.

Function	Purpose Statement
QDAG2D	Integrates a function of two variables with a possible internal or end point singularity.
QDAG3D	Integrates a function of three variables with a possible internal or endpoint singularity.
QDAGS	Integrates a function (which may have endpoint singularities).
QDAWC	Integrates a function F(X)/(X – C) in the Cauchy principal value sense.
QDAWF	Computes a Fourier integral.
QDAWO	Integrates a function containing a sine or a cosine.
QDAWS	Integrates a function with algebraic-logarithmic singularities.
QDDER	Evaluates the derivative of a function defined on a set of points using quadratic interpolation.
QDNG	Integrates a smooth function using a nonadaptive rule.
QDVAL	Evaluates a function defined on a set of points using quadratic interpolation.
QMC	Integrates a function over a hyperrectangle using a quasi-Monte Carlo method.
QPROG	Solves a quadratic programming problem subject to linear equality/inequality constraints.
QSINB	Computes a sequence from its sine Fourier coefficients with only odd wave numbers.
QSINF	Computes the coefficients of the sine Fourier transform with only odd wave numbers.
QSINI	Computes parameters needed by QSINF and QSINB.

R

Function	Purpose Statement
RAND	Computes a scalar, rank-1, rank-2 or rank-3 array of random numbers.
RAND_GEN	Generates a rank-1 array of random numbers.
RANK	Computes the mathematical rank of a rank-2 or rank-3 array.
RATCH	Computes a rational weighted Chebyshev approximation to a continuous function on an interval.

Function	Purpose Statement
RCONV	Computes the convolution of two real vectors.
RCORL	Computes the correlation of two real vectors.
RCURV	Fits a polynomial curve using least squares.
READ_MPS	Reads an MPS file containing a linear program problem or a quadratic programming problem.
RECCF	Computes recurrence coefficients for various monic polynomials.
RECQR	Computes recurrence coefficients for monic polynomials given a quadrature rule.
RLINE	Fits a line to a set of data points using least squares.
RNGET	Retrieves the current value of the seed used in the IMSL random number generators.
RNIN32	Initializes the 32-bit Merseene Twister generator using an array.
RNGE32	Retrieves the current table used in the 32-bit Mersenne Twister generator.
RNSE32	Sets the current table used in the 32-bit Mersenne Twister generator.
RNIN64	Initializes the 32-bit Merseene Twister generator using an array.
RNGE64	Retrieves the current table used in the 64-bit Mersenne Twister generator
RNSE64	Sets the current table used in the 64-bit Mersenne Twister generator.
RNOPT	Selects the uniform (0, 1) multiplicative congruential pseudorandom number generator.
RNSET	Initializes a random seed for use in the IMSL random number generators.
RNUN	Generates pseudorandom numbers from a uniform (0, 1) distribution.
RNUNF	Generates a pseudorandom number from a uniform (0, 1) distribution.

S

Function	Purpose Statement
SADD	Adds a scalar to each component of a vector, $x \leftarrow x + a$, all single precision.
SASUM	Sums the absolute values of the components of a single-precision vector.
SAXPY	Computes the scalar times a vector plus a vector, $y \leftarrow ax + y$, all single precision.
ScaLAPACK_EXIT	Exits ScaLAPACK mode for the IMSL Library routines.
ScaLAPACK_GETDIM	Calculates the row and column dimensions of a local distributed array based on the size of the array to be distributed and the row and column blocking factors to be used.
ScaLAPACK_MAP	Maps array data from a global array to local arrays in the two-dimensional block-cyclic form required by *ScaLAPACK* routines.
ScaLAPACK_READ	Reads matrix data from a file and transmits it into the two-dimensional block-cyclic form required by *ScaLAPACK* routines.
ScaLAPACK_SETUP	Sets up a processor grid and calculates default values for use in mapping arrays to the processor grid
ScaLAPACK_UNMAP	Unmaps array data from local distributed arrays to a global array.
ScaLAPACK_WRITE	Writes the matrix data to a file.
SCASUM	Sums the absolute values of the real part together with the absolute values of the imaginary part of the components of a complex vector.
SCNRM2	Computes the Euclidean norm of a complex vector.
SCOPY	Copies a vector x to a vector y, both single precision.
SDDOTA	Computes the sum of a single-precision scalar, a single-precision dot product and the double-precision accumulator, which is set to the result `ACC` `ACC` + $a + x^T y$.
SDDOTI	Computes the sum of a single-precision scalar plus a singleprecision dot product using a double-precision accumulator, which is set to the result `ACC` $a + x^T y$.
SDOT	Computes the single-precision dot product $x^T y$.
SDSDOT	Computes the sum of a single-precision scalar and a single precision dot product, $a + x^T y$, using a double-precision accumulator.

Function	Purpose Statement
SGBMV	Computes one of the matrix-vector operations: $y \leftarrow \alpha Ax + \beta y$, or $y \leftarrow \alpha A^T x + \beta y$, where *A* is a matrix stored in band storage mode.
SGEMM	Computes one of the matrix-matrix operations: $C \leftarrow \alpha AB + \beta C$, $C \leftarrow \alpha A^T B + \beta C$, $C \leftarrow \alpha AB^T + \beta C$, or $C \leftarrow \alpha A^T B^T + \beta C$
SGEMV	Computes one of the matrix-vector operations: $y \leftarrow \alpha Ax + \beta y$, or $y \leftarrow \alpha A^T x + \beta y$
SGER	Computes the rank-one update of a real general matrix: $A \leftarrow A + \alpha xy^T$
SHOW	Prints rank-1 or rank-2 arrays of numbers in a readable format.
SHPROD	Computes the Hadamard product of two single-precision vectors.
SINLP	Computes the inverse Laplace transform of a complex function.
SLCNT	Calculates the indices of eigenvalues of a Sturm-Liouville problem with boundary conditions (at regular points) in a specified subinterval of the real line, $[\alpha, \beta]$.
SLEIG	Determines eigenvalues, eigenfunctions and/or spectral density functions for Sturm-Liouville problems in the form with boundary conditions (at regular points).
SLPRS	Solves a sparse linear programming problem via the revised simplex algorithm.
SNRM2	Computes the Euclidean length or L_2 norm of a single-precision vector.
SORT_REAL	Sorts a rank-1 array of real numbers *x* so the *y* results are algebraically nondecreasing, $y_1 \le y_2 \le \ldots y_n$.
SPLEZ	Computes the values of a spline that either interpolates or fits user-supplied data.
SPLINE_CONSTRAINTS	Returns the derived type array result.
SPLINE_FITTING	Weighted least-squares fitting by B-splines to discrete One-Dimensional data is performed.
SPLINE_VALUES	Returns an array result, given an array of input
SPRDCT	Multiplies the components of a single-precision vector.
SRCH	Searches a sorted vector for a given scalar and return its index.
SROT	Applies a Givens plane rotation in single precision.
SROTG	Constructs a Givens plane rotation in single precision.

Function	Purpose Statement
SROTM	Applies a modified Givens plane rotation in single precision.
SROTMG	Constructs a modified Givens plane rotation in single precision.
SSBMV	Computes the matrix-vector operation $y \leftarrow \alpha Ax + \beta y$, where A is a symmetric matrix in band symmetric storage mode.
SSCAL	Multiplies a vector by a scalar, $y \leftarrow ay$, both single precision.
SSET	Sets the components of a vector to a scalar, all single precision.
SSPMV	Performs the matrix-vector operation $y := \alpha * A * x + \beta * y$.
SSPR	Performs the matrix-vector operation, $A \leftarrow A + \alpha xx^T$ where A is a packed symmetric matrix.
SSPR2	Performs the symmetric rank 2 operation,$A \leftarrow A + \alpha xy^T + \alpha yx^T$ where A is a packed symmetric matrix.
SSRCH	Searches a character vector, sorted in ascending ASCII order, for a given string and return its index.
SSUB	Subtracts each component of a vector from a scalar, $x \leftarrow a - x$, all single precision.
SSUM	Sums the values of a single-precision vector.
SSWAP	Interchanges vectors x and y, both single precision.
SSYMM	Computes one of the matrix-matrix operations: $C \leftarrow \alpha AB + \beta C$ or $C \leftarrow \alpha BA + \beta C$, where A is a symmetric matrix and B and C are m by n matrices.
SSYMV	Computes the matrix-vector operation $y \leftarrow \alpha Ax + \beta y$, where A is a symmetric matrix.
SSYR	Computes the rank-one update of a real symmetric matrix: $A \leftarrow A + \alpha xx^T$.
SSYR2	Computes the rank-two update of a real symmetric matrix: $A \leftarrow A + \alpha xy^T + \alpha yx^T$.
SSYR2K	Computes one of the symmetric rank 2k operations: $C \leftarrow \alpha AB^T + \alpha BA^T + \beta C$ or $C \leftarrow \alpha A^T B + \alpha B^T A + \beta C$ where C is an n by n symmetric matrix and A and B are n by k matrices in the first case and k by n matrices in the second case.
SSYRK	Computes one of the symmetric rank k operations: $C \leftarrow \alpha AA^T + \beta C$ or $C \leftarrow \alpha A^T A + \beta C$, where C is an n by n symmetric matrix and A is an n by k matrix in the first case and a k by n matrix in the second case.
STBMV	Computes one of the matrix-vector operations: $x \leftarrow Ax$ or $x \leftarrow A^T x$, where A is a triangular matrix in band storage mode.

Function	Purpose Statement
STBSV	Solves one of the triangular systems: $x \leftarrow A^{-1}x$ or $x \leftarrow \left(A^{-1}\right)^T x$, where *A* is a triangular matrix in band storage mode.
STPMV	Performs one of the matrix-vector operations, $x \leftarrow Ax$, $x \leftarrow A^T x$ where *A* is an $N \times N$ packed triangular matrix.
STPSV	Solves one of the systems of equations, $x \leftarrow A^{-1}x$, $x \leftarrow (A^{-1})^T x$ where *A* is an $N \times N$ packed triangular matrix.
STRMM	Computes one of the matrix-matrix operations: $B \leftarrow \alpha AB, B \leftarrow \alpha A^T B$, or $B \leftarrow \alpha BA, B \leftarrow \alpha BA^T$, where *B* is an *m* by *n* matrix and *A* is a triangular matrix.
STRMV	Computes one of the matrix-vector operations: $x \leftarrow Ax$ or $x \leftarrow A^T x$, where *A* is a triangular matrix.
STRSM	Solves one of the matrix equations: $B \leftarrow \alpha A^{-1}B$, $B \leftarrow \alpha BA^{-1}$, $B \leftarrow \alpha\left(A^{-1}\right)^T B$, or $B \leftarrow \alpha B\left(A^{-1}\right)^T$, where *B* is an *m* by *n* matrix and *A* is a triangular matrix.
STRSV	Solves one of the triangular linear systems: $x \leftarrow A^{-1}x$ or $x \leftarrow \left(A^{-1}\right)^T x$ where *A* is a triangular matrix.
SURF	Computes a smooth bivariate interpolant to scattered data that is locally a quintic polynomial in two variables.
SURFND	Multidimensional interpolation and differentiation.
SURFACE_CONSTRAINTS	Returns the derived type array result given optional input.
SURFACE_FITTING	Weighted least-squares fitting by tensor product B-splines to discrete two-dimensional data is performed.
SURFACE_VALUES	Returns a tensor product array result, given two arrays of independent variable values.
SVCAL	Multiplies a vector by a scalar and store the result in another vector, $y \leftarrow ax$, all single precision.
SVD	Computes the singular value decomposition of a rank-2 or rank-3 array, $A = USV^T$.
SVIBN	Sorts an integer array by nondecreasing absolute value.
SVIGN	Sorts an integer array by algebraically increasing value.
SVIGP	Sorts an integer array by algebraically increasing value and returns the permutation that rearranges the array.
SVRBN	Sorts a real array by nondecreasing absolute value.

Function	Purpose Statement
SVRBP	Sorts a real array by nondecreasing absolute value and returns the permutation that rearranges the array.
SVRGN	Sorts a real array by algebraically increasing value.
SVRGP	Sorts a real array by algebraically increasing value and returns the permutation that rearranges the array.
SXYZ	Computes a single-precision *xyz* product.

T

Function	Purpose Statement
TDATE	Gets today's date.
TIMDY	Gets time of day.
TRAN	Solves a transportation problem.
TRNRR	Transposes a rectangular matrix.
TWODQ	Computes a two-dimensional iterated integral.

U

Function	Purpose Statement
UMACH	Sets or retrieves input or output device unit numbers.
UMAG	Handles MATH/LIBRARY and STAT/LIBRARY type REAL and double precision options.
UMCGF	Minimizes a function of N variables using a conjugate gradient algorithm and a finite-difference gradient.
UMCGG	Minimizes a function of N variables using a conjugate gradient algorithm and a user-supplied gradient.
UMIAH	Minimizes a function of N variables using a modified Newton method and a user-supplied Hessian.

Function	Purpose Statement
UMIDH	Minimizes a function of N variables using a modified Newton method and a finite-difference Hessian.
UMINF	Minimizes a function of N variables using a modified Newton method and a finite-difference Hessian.
UMING	Minimizes a function of N variables using a quasi-Newton method and a finite-difference gradient.
UMPOL	Minimizes a function of N variables using a direct search polytope algorithm.
UNIT	Normalizes the columns of a rank-2 or rank-3 array so each has Euclidean length of value one.
UNLSF	Solves a nonlinear least squares problem using a modified Levenberg-Marquardt algorithm and a finite-difference Jacobian.
UNLSJ	Solves a nonlinear least squares problem using a modified Levenberg-Marquardt algorithm and a user-supplied Jacobian.
UVMGS	Finds the minimum point of a nonsmooth function of a single variable.
UVMID	Finds the minimum point of a smooth function of a single variable using both function evaluations and first derivative evaluations.
UVMIF	Finds the minimum point of a smooth function of a single variable using only function evaluations.

V

Function	Purpose Statement
VCONC	Computes the convolution of two complex vectors.
VCONR	Computes the convolution of two real vectors.
VERML	Obtains IMSL MATH/LIBRARY-related version and system information.

W

Function	Purpose Statement
WRCRL	Prints a complex rectangular matrix with a given format and labels.
WRCRN	Prints a complex rectangular matrix with integer row and column labels.
WRIRL	Prints an integer rectangular matrix with a given format and labels.
WRIRN	Prints an integer rectangular matrix with integer row and column labels.
WROPT	Sets or retrieves an option for printing a matrix.
WRRRL	Prints a real rectangular matrix with a given format and labels.
WRRRN	Prints a real rectangular matrix with integer row and column labels.

Z

Function	Purpose Statement
ZANLY	Finds the zeros of a univariate complex function using Müller's method.
ZBREN	Finds a zero of a real function that changes sign in a given interval.
ZPLRC	Finds the zeros of a polynomial with real coefficients using Laguerre's method.
ZPOCC	Finds the zeros of a polynomial with complex coefficients using the Jenkins-Traub three-stage algorithm.
ZPORC	Finds the zeros of a polynomial with real coefficients using the Jenkins-Traub three-stage algorithm.
ZQADD	Adds a double complex scalar to the accumulator in extended precision.
ZQINI	Initializes an extended-precision complex accumulator to a double complex scalar.
ZQMUL	Multiplies double complex scalars using extended precision.

Function	Purpose Statement
ZQSTO	Stores a double complex approximation to an extended-precision complex scalar.
ZREAL	Finds the real zeros of a real function using Müller's method.
ZUNI	Finds a zero of a real univariate function.

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Appendix C, Product Support

Contacting IMSL Support

Users within support warranty may contact IMSL regarding the use of the IMSL Fortran Numerical Library. IMSL Support can consult on the following topics:

- Clarity of documentation
- Possible IMSL-related programming problems
- Choice of IMSL Libraries functions or procedures for a particular problem

  Not included in these topics are mathematical/statistical consulting and debugging of your program.

  Refer to the following for IMSL Product Support contact information**:**

  https://www.imsl.com/support

The following describes the procedure for consultation with IMSL Support:

1. Include your IMSL license number.
2. Include the product name and version number.
3. Include compiler and operating system version numbers.
4. Include the name of the routine for which assistance is needed and a description of the problem.

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