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USER GUIDE FOR MINPACK-1

by

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and Kenneth E. Hillstom



ARGONNE NATIONAL LABORATORY, ARGONNE, ILLINOIS

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Jorge J. Moré, Burton S. Garbow, Kenneth E. Hillstom

Applied Mathematics Division

August 1980

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ABSTRACT

MINPACK-1 is a package of Fortran subprograms for the numerical solution of systems of nonlinear equations and nonlinear least squares problems. This report provides an overview of the algorithms and software in the package and includes the documentation and program listings.

Preface

The MINPACK Project is a research effort whose goal is the development of a systematized collection of quality optimization software. The first step towards this goal has been realized in MINPACK-1, a package of Fortran programs for the numerical solution of systems of nonlinear equations and nonlinear least squares problems.

The design of the algorithms and software in MINPACK-1 has several objectives; the main ones are reliability, ease of use, and transportability.

At the algorithmic level, reliability derives from the underlying algorithms having a sound theoretical basis. Entirely satisfactory global convergence results are available for the MINPACK-1 algorithms and, in addition, their properties allow scale invariant implementations.

At the software level, reliability derives from extensive testing. The heart of the testing aids is a large collection of test problems (More', Garbow, and Hillstom [1978]). These test problems have been used to measure the performance of the software on the following computing systems: IBM 360/370, CDC 6000-7000, Univac 1100, Cray-1, Burroughs 6700, DEC PDP-10, Honeywell 6000, Prime 400, Intel AS/6, and ICL 2980. At Argonne, software performance has been further measured with the help of WATFIV and BRNANL (Fosdick [1974]). WATFIV detects run-time errors such as undefined variables and out-of-range subscripts, while BRNANL provides execution counts for each block of a program and, in particular, has established that the MINPACK-1 test problems execute every non-trivial program block.

Reliability further implies efficient and robust implementations. For example, MINPACK-1 programs access matrices sequentially along columns (rather than rows), since this improves efficiency, especially on paged systems. Also, there are extensive checks on the input parameters, and computations are

formulated to avoid destructive underflows and overflows. Underflows can then be safely ignored; overflows due to the problem should of course be investigated.

Ease of use derives from the design of the user interface. Each algorithmic path in MINPACK-1 includes a core subroutine and a driver with a simplified calling sequence made possible by assuming default settings for certain parameters and by returning a limited amount of information; many applications do not require full flexibility and in these cases the drivers can be invoked. On the other hand, the core subroutines enable, for example, scaling of the variables and printing of intermediate results at specified iterations.

Ease of use is also facilitated by the documentation. Machine-readable documentation is provided for those programs normally called by the user. The documentation includes discussions of all calling sequence parameters and an actual example illustrating the use of the corresponding algorithm. In addition, each program includes detailed prologue comments on its purpose and the roles of its parameters; in-line comments introduce major blocks in the body of the program.

To further clarify the underlying structure of the algorithms, the programs have been formatted by the TAMPR system of Boyle and Dritz [1974]. TAMPR produces implementations in which the loops and logical structure of the programs are clearly delineated. In addition, TAMPR has been used to produce the single precision version of the programs from the master (double precision) version.

Transportability requires that a satisfactory transfer to a different computing system be possible with only a small number of changes to the software. In MINPACK-1, a change to a new computing system only requires changes to one program in each precision; all other programs are written in a portable subset of ANSI standard Fortran acceptable to the PFORT verifier (Ryder [1974]). This one machine-dependent program provides values of the machine precision, the smallest magnitude, and the largest magnitude. Most of the values for these parameters were obtained from the corresponding PORT library program (Fox, Hall, and Schryer [1978]); in particular, values are provided for all of the computing systems on which the programs were tested.

MINPACK-1 is fully supported. Comments, questions, and reports of poor or incorrect performance of the MINPACK-1 programs should be directed to

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Phone: (312) 972-7184

Of particular interest would be reports of performance of the MINPACK-1 package on machines not covered in the testing.

The MINPACK-1 package consists of the programs, their documentation, and the testing aids. The package comprises approximately 28,000 card images and is transmitted on magnetic tape. The tape is available from the following two sources.

National Energy Software Center
Argonne National Laboratory
9700 South Cass Avenue
Argonne, IL 60439
Phone: (312) 972-7250

IMSL
Sixth Floor-NBC Building
7500 Bellaire Blvd.
Houston, TX 77036
Phone: (713) 772-1927

The package includes both single and double precision versions of the programs, and for those programs normally called by the user machine-readable documentation is provided in both single and double precision forms. An implementation guide (Garbow, Hillstom, and Moré [1980]) is also included with the tape.

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CHAPTER 1

Introduction to MINPACK-1

The purpose of this chapter is to provide an overview of the algorithms and software in MINPACK-1. Most users need only be acquainted with the first six sections of this chapter; the remaining two sections describe lower-level software called from the main programs.

1.1 Systems of Nonlinear Equations

If n functions f_1, f_2, \dots, f_n of the n variables x_1, x_2, \dots, x_n are specified, then MINPACK-1 subroutines can be used to find values for x_1, x_2, \dots, x_n that solve the system of nonlinear equations

$$f_i(x_1, x_2, \dots, x_n) = 0, \quad 1 \leq i \leq n.$$

To solve this system we have implemented a modification of Powell's hybrid algorithm. There are two variants of this algorithm. The first variant only requires that the user calculate the functions f_i , while the second variant requires that the user calculate both the functions f_i and the n by n Jacobian matrix

$$\left(\frac{\partial f_i(x)}{\partial x_j} \right), \quad 1 \leq i \leq n, \quad 1 \leq j \leq n.$$

1.2 Nonlinear Least Squares Problems

If m functions f_1, f_2, \dots, f_m of the n variables x_1, x_2, \dots, x_n are specified with $m \geq n$, then MINPACK-1 subroutines can be used to find values for x_1, x_2, \dots, x_n that solve the nonlinear least squares problem

$$\min \left\{ \sum_{i=1}^m f_i(x)^2 : x \in R^n \right\}.$$

To solve this problem we have implemented a modification of the Levenberg-Marquardt algorithm. There are three variants of this algorithm. The first

variant only requires that the user calculate the functions f_i , while the second variant requires that the user calculate both the functions f_i and the m by n Jacobian matrix

$$\left(\frac{\partial f_i(x)}{\partial x_j} \right), \quad 1 \leq i \leq m, \quad 1 \leq j \leq n.$$

The third variant also requires that the user calculate the functions and the Jacobian matrix, but the latter only one row at a time. This organization only requires the storage of an n by n matrix (rather than m by n), and is thus attractive for nonlinear least squares problems with a large number of functions and a moderate number of variables.

1.3 Derivative Checking

The main advantage of providing the Jacobian matrix is increased reliability; for example, the algorithm is then much less sensitive to functions subject to errors. However, providing the Jacobian matrix is an error-prone task. To help identify errors, MINPACK-1 also contains a subroutine CHKDER that checks the Jacobian matrix for consistency with the function values.

1.4 Algorithmic Paths: Core Subroutines and Easy-to-Use Drivers

There are five general algorithmic paths in MINPACK-1. Each path includes a core subroutine and an easy-to-use driver with a simplified calling sequence made possible by assuming default settings for certain parameters and by returning a limited amount of information; many applications do not require full flexibility and in these cases easy-to-use drivers can be invoked. On the other hand, the core subroutines enable, for example, scaling of the variables and printing of intermediate results at specified iterations.

1.5 MINPACK-1 Subroutines: Systems of Nonlinear Equations

The MINPACK-1 subroutines for the numerical solution of systems of nonlinear equations are HYBRD1, HYBRD, HYBRJ1, and HYBRJ. These subroutines provide alternative ways to solve the system of nonlinear equations

$$f_i(x_1, x_2, \dots, x_n) = 0, \quad 1 \leq i \leq n$$

by a modification of Powell's hybrid algorithm. The principal requirements of the subroutines are as follows (see also Figure 1).

HYBRD1, HYBRD

The user must provide a subroutine to calculate the functions f_1, f_2, \dots, f_n . The Jacobian matrix is then calculated by a forward-difference approximation or by an update formula of Broyden. HYBRD1 is the easy-to-use driver for the core subroutine HYBRD.

HYBRJ1, HYBRJ

The user must provide a subroutine to calculate the functions f_1, f_2, \dots, f_n and the Jacobian matrix

$$\left(\frac{\partial f_i(x)}{\partial x_j} \right), \quad 1 \leq i \leq n, \quad 1 \leq j \leq n.$$

(Subroutine CHKDER can be used to check the Jacobian matrix for consistency with the function values.) HYBRJ1 is the easy-to-use driver for the core subroutine HYBRJ.

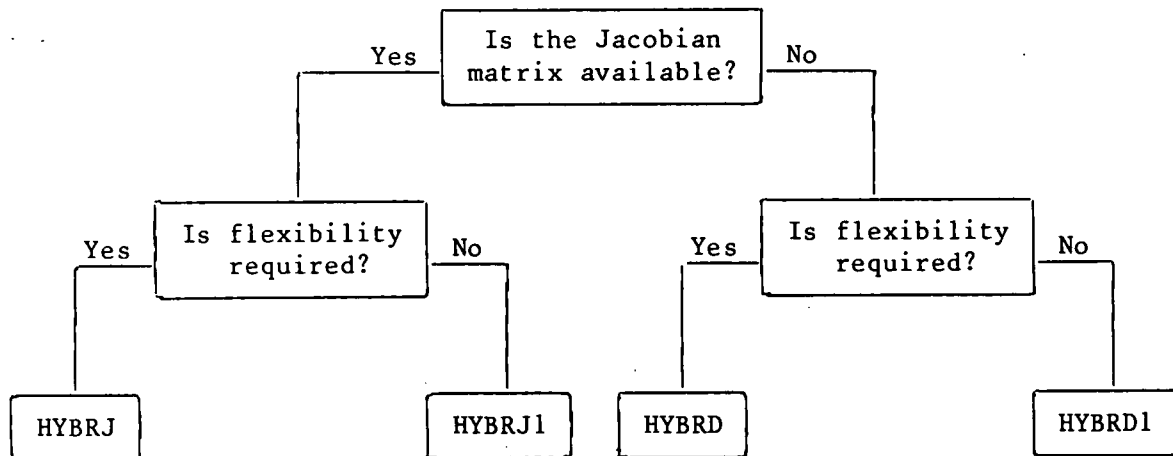


Figure 1
Decision Tree for Systems of Nonlinear Equations

1.6 MINPACK-1 Subroutines: Nonlinear Least Squares Problems

The MINPACK-1 subroutines for the numerical solution of nonlinear least squares problems are LMDIF1, LMDIF, LMDER1, LMDER, LMSTR1, and LMSTR. These subroutines provide alternative ways to solve the nonlinear least squares problem

$$\min \left\{ \sum_{i=1}^m f_i(x)^2 : x \in R^n \right\}$$

by a modification of the Levenberg-Marquardt algorithm. The principal requirements of the subroutines are as follows (see also Figure 2).

LMDIF1, LMDIF

The user must provide a subroutine to calculate the functions f_1, f_2, \dots, f_m . The Jacobian matrix is then calculated by a forward-difference approximation. LMDIF1 is the easy-to-use driver for the core subroutine LMDIF.

LMDER1, LMDER

The user must provide a subroutine to calculate the functions f_1, f_2, \dots, f_m and the Jacobian matrix

$$\left(\frac{\partial f_i(x)}{\partial x_j} \right), \quad 1 \leq i \leq m, \quad 1 \leq j \leq n.$$

(Subroutine CHKDER can be used to check the Jacobian matrix for consistency with the function values.) LMDER1 is the easy-to-use driver for the core subroutine LMDER.

LMSTR1, LMSTR

The user must provide a subroutine to calculate the functions f_1, f_2, \dots, f_m and the rows of the Jacobian matrix

$$\left(\frac{\partial f_i(x)}{\partial x_j} \right), \quad 1 \leq i \leq m, \quad i \leq j \leq n,$$

one row per call. (Subroutine CHKDER can be used to check the row of the Jacobian matrix for consistency with the corresponding function value.) LMSTR1 is the easy-to-use driver for the core subroutine LMSTR.

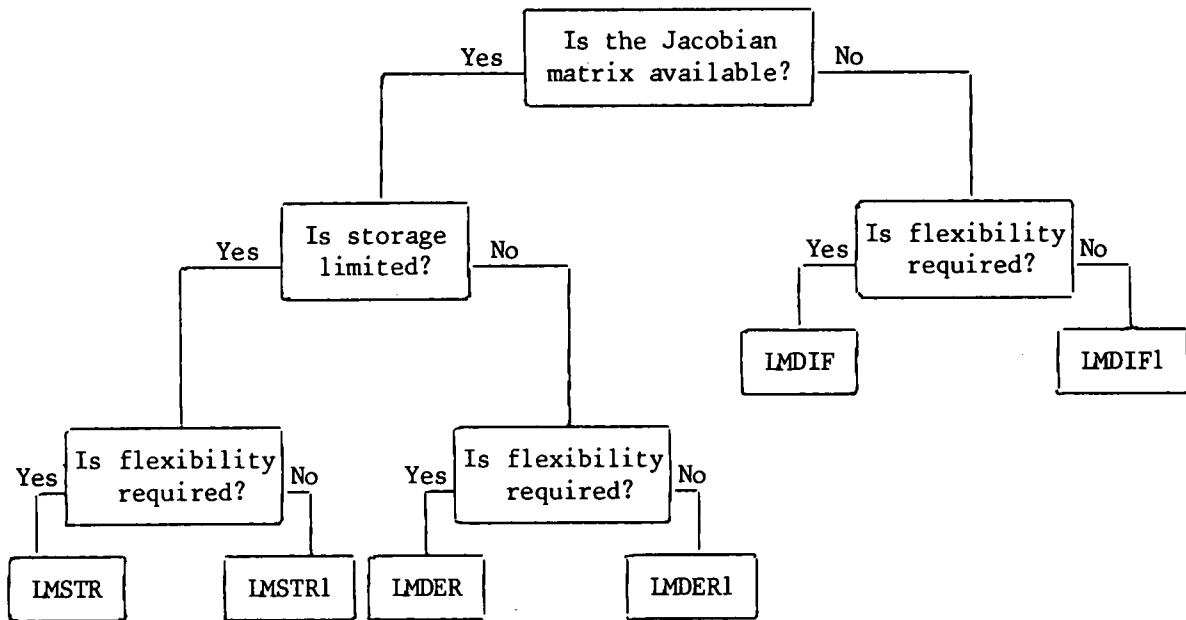


Figure 2
Decision Tree for Nonlinear Least Squares Problems

1.7 Machine-Dependent Constants

There are three machine-dependent constants that have to be set before the single or double precision version of MINPACK-1 can be used; for most machines the correct values of these constants are encoded into DATA statements in functions SPMPAR (single precision) and DPMPAR (double precision). These constants are:

- $\beta^{1-\ell}$, the machine precision ,
- $\beta^{e_{\min}-1}$, the smallest magnitude ,
- $(1 - \beta^{-\ell})\beta^{e_{\max}}$, the largest magnitude ,

where ℓ is the number of base β digits on the machine, e_{\min} is the smallest machine exponent, and e_{\max} is the largest machine exponent.

The most critical of the constants is the machine precision ϵ_M , since the MINPACK-1 subroutines treat two numbers a and b as equal if they satisfy

$$|b-a| \leq \epsilon_M |a| ,$$

and the above test forms the basis for deciding that no further improvement is possible with the algorithm.

1.8 MINPACK-1 Internal Subprograms

Most users of MINPACK-1 need only be acquainted with the core subroutines and easy-to-use drivers described in the previous sections. Some users, however, may wish to experiment by modifying an algorithmic path to improve the performance of the algorithm on a particular application. A modification to an algorithmic path can often be achieved by modifying or replacing one of the internal subprograms. Additionally, the internal subprograms may be useful independent of the MINPACK-1 algorithmic paths in which they are employed.

For these reasons brief descriptions of the MINPACK-1 internal subprograms are included below; more complete descriptions can be found in the prologue comments in the program listings of Chapter 5.

DOGLEG

Given the QR factorization of an m by n matrix A , an n by n nonsingular diagonal matrix D , an m -vector b , and a positive number Δ , this subroutine determines the convex combination of the Gauss-Newton and scaled gradient directions that solves the problem

$$\min\{\|Ax-b\| : \|Dx\| \leq \Delta\}.$$

ENORM

This function computes the Euclidean norm of a vector x .

FDJAC1

This subroutine computes a forward-difference approximation to the Jacobian matrix associated with n functions in n variables. It includes a banded Jacobian option.

FDJAC2

This subroutine computes a forward-difference approximation to the Jacobian matrix associated with m functions in n variables.

LMPAR

Given the QR factorization of an m by n matrix A , an n by n nonsingular diagonal matrix D , an m -vector b , and a positive number Δ , this subroutine is used to solve the problem

$$\min\{\|Ax-b\| : \|Dx\| \leq \Delta\}.$$

QFORM

Given the QR factorization of a rectangular matrix, this subroutine accumulates the orthogonal matrix Q from its factored form.

QRFAC

This subroutine uses Householder transformations with optional column pivoting to compute a QR factorization of an arbitrary rectangular matrix.

QRSOLV

Given the QR factorization of an m by n matrix A , an n by n diagonal matrix D , and an m -vector b , this subroutine solves the linear least squares problem

$$\begin{pmatrix} A \\ D \end{pmatrix} x \approx \begin{pmatrix} b \\ 0 \end{pmatrix}.$$

RWUPDT

This subroutine is used in updating the upper triangular part of the QR decomposition of a matrix A after a row is added to A .

RLMPYQ

This subroutine multiplies a matrix by an orthogonal matrix given as a product of Givens rotations.

RLUPDT

This subroutine is used in updating the lower triangular part of the LQ decomposition of a matrix A after a rank-1 matrix is added to A .

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CHAPTER 2

Algorithmic Details

The purpose of this chapter is to provide information about the algorithms and to point out some of the ways in which this information can be used to improve their performance. The first two sections are essential for the rest of the chapter since they provide the necessary background, but the other sections are independent of each other.

2.1 Mathematical Background

To describe the algorithms for the solution of systems of nonlinear equations and nonlinear least squares problems, it is necessary to introduce some notation.

Let R^n represent the n -dimensional Euclidean space of real n -vectors

$$x = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix},$$

and $\|x\|$ the Euclidean norm of x ,

$$\|x\| = \left(\sum_{j=1}^n x_j^2 \right)^{1/2}.$$

A function F with domain in R^n and range in R^m is denoted by $F: R^n \rightarrow R^m$. Such a function can be expressed as

$$F(x) = \begin{pmatrix} f_1(x) \\ f_2(x) \\ \vdots \\ f_m(x) \end{pmatrix},$$

where the component function $f_i: R^n \rightarrow R$ is sometimes called the i -th residual of F . The terminology derives from the fact that a common problem is to fit a model $g(t,x)$ to data y , in which case the f_i are of the form

$$f_i(x) = y_i - g(t_i, x) ,$$

where y_i is measured at t_i and x is the set of fit parameters.

In this notation a system of nonlinear equations is specified by a function $F: R^n \rightarrow R^n$, and a solution vector x^* in R^n is such that

$$F(x^*) = 0 .$$

Similarly, a nonlinear least squares problem is specified by a function $F: R^n \rightarrow R^m$ with $m \geq n$, and a solution vector x^* in R^n is such that

$$\|F(x^*)\| \leq \|F(x)\| \quad \text{for } x \in N(x^*) ,$$

where $N(x^*)$ is a neighborhood of x^* . If $N(x^*)$ is the entire domain of definition of the function, then x^* is a global solution; otherwise, x^* is a local solution.

Some of the MINPACK-1 algorithms require the specification of the Jacobian matrix of the mapping $F: R^n \rightarrow R^m$; that is, the m by n matrix $F'(x)$ whose (i,j) entry is

$$\frac{\partial f_i(x)}{\partial x_j} .$$

A related concept is the gradient of a function $f: R^n \rightarrow R$, which is the mapping $\nabla f: R^n \rightarrow R^n$ defined by

$$\nabla f(x) = \begin{pmatrix} \frac{\partial f(x)}{\partial x_1} \\ \frac{\partial f(x)}{\partial x_2} \\ \vdots \\ \frac{\partial f(x)}{\partial x_n} \end{pmatrix} .$$

Note that the i -th row of the Jacobian matrix $F'(x)$ is the gradient $\nabla f_i(x)$ of the i -th residual.

It is well-known that if x^* is a solution of the nonlinear least squares problem, then x^* solves the system of nonlinear equations

$$\sum_{i=1}^m f_i(x) \nabla f_i(x) = 0 .$$

In terms of the Jacobian matrix this implies that

$$F'(x^*)^T F(x^*) = 0 ,$$

and shows that at the solution the vector of residuals is orthogonal to the columns of the Jacobian matrix. This orthogonality condition is also satisfied at maximizers and saddle points, but algorithms usually take precautions to avoid these critical points.

2.2 Overview of the Algorithms

Consider a mapping $F: R^n \rightarrow R^m$, where $m = n$ for systems of nonlinear equations and $m \geq n$ for nonlinear least squares problems. The MINPACK-1 algorithms in these two problem areas seek a solution x^* of the problem

$$(1) \quad \min \{ \|F(x)\| : x \in R^n \} .$$

In particular, if $m = n$ it is expected that $F(x^*) = 0$.

Our initial description of the algorithms will be at the macroscopic level where the techniques used in each problem area are similar.

With each algorithm the user provides an initial approximation $x = x_0$ to the solution of the problem. The algorithm then determines a correction p to x that produces a sufficient decrease in the residuals of F at the new point $x+p$; it then sets

$$x_+ = x + p$$

and begins a new iteration with x_+ replacing x .

A sufficient decrease in the residuals implies, in particular, that

$$\|F(x+p)\| < \|F(x)\| ,$$

and thus the algorithms guarantee that

$$\|F(x_+)\| < \|F(x)\| .$$

The correction p depends upon a diagonal scaling matrix D , a step bound Δ , and an approximation J to the Jacobian matrix of F at x . Users of the core subroutines can specify initial values D_0 and Δ_0 ; in the easy-to-use drivers D_0 and Δ_0 are set internally. If the user is providing the Jacobian matrix, then $J_0 = F'(x_0)$; otherwise the algorithm sets J_0 to a forward difference approximation to $F'(x_0)$.

To compute p , the algorithm solves (approximately) the problem

$$(2) \quad \min\{\|f+Jp\|: \|Dp\| \leq \Delta\} ,$$

where f is the m -vector of residuals of F at x . If the solution of this problem does not provide a suitable correction, then Δ is decreased and, if appropriate, J is updated. A new problem is now solved, and this process is repeated (usually only once or twice) until a p is obtained at which there is sufficient decrease in the residuals, and then x is replaced by $x+p$. Before the start of the next iteration, D , Δ , and J are also replaced.

The motivation for using (2) to obtain the correction p is that for appropriate choices of J and Δ , the solution of (2) is an approximate solution of

$$\min\{\|F(x+p)\|: \|Dp\| \leq \Delta\} .$$

It follows that if there is a solution x^* such that

$$(3) \quad \|D(x-x^*)\| \leq \Delta ,$$

then $x+p$ is close to x^* . If this is not the case, then at least $x+p$ is a better approximation to x^* than x . Under reasonable conditions, it can be shown that (3) eventually holds.

The algorithms for systems of nonlinear equations and for nonlinear least squares problems differ, for example, in the manner in which the correction p

is obtained as an approximate solution of (2). The nonlinear equations algorithm obtains a p that minimizes $\|f+Jp\|$ in a two-dimensional subspace of the ellipsoid $\{p: \|Dp\| \leq \Delta\}$. The nonlinear least squares algorithm obtains a p that is the exact solution of (2) with a small (10%) perturbation of Δ . Other differences in the algorithms include convergence criteria (Section 2.3) and the manner in which J is computed (Section 2.4).

It is appropriate to close this overview of the algorithms by discussing two of their limitations. First, the algorithms are limited by the precision of the computations. Although the algorithms are globally convergent under reasonable conditions, the convergence proofs are only valid in exact arithmetic and the algorithms may fail in finite precision due to roundoff. This implies that the algorithms tend to perform better in higher precision. It also implies that the calculation of the function and the Jacobian matrix should be as accurate as possible and that improved performance results when the user can provide the Jacobian analytically.

Second, the algorithms are only designed to find local solutions. To illustrate this point, consider

$$F(x) = x^3 - 3x + 18 .$$

In this case, problem (1) has the global solution $x^* = -3$ with $F(x^*) = 0$ and the local solution $x^* = 1$ with $F(x^*) = 16$; depending on the starting point, the algorithms may converge either to the global solution or to the local solution.

2.3 Convergence Criteria

The convergence test in the MINPACK-1 algorithms for systems of nonlinear equations is based on an estimate of the distance between the current approximation x and an actual solution x^* of the problem. If D is the current scaling matrix, then this convergence test (X-convergence) attempts to guarantee that

$$(1) \quad \|D(x-x^*)\| \leq XTOL \cdot \|Dx^*\| ,$$

where $XTOL$ is a user-supplied tolerance.

There are three convergence tests in the MINPACK-1 algorithms for nonlinear least squares problems. One test is again for X-convergence, but the main convergence test is based on an estimate of the distance between the Euclidean norm $\|F(x)\|$ of the residuals at the current approximation x and the optimal value $\|F(x^*)\|$ at an actual solution x^* of the problem. This convergence test (F-convergence) attempts to guarantee that

$$(2) \quad \|F(x)\| \leq (1 + FTOL) \cdot \|F(x^*)\| ,$$

where FTOL is a second user-supplied tolerance.

The third convergence test for the nonlinear least squares problem (G-convergence) guarantees that

$$(3) \quad \max \left\{ \frac{|a_i^T f|}{\|a_i\| \|f\|} : 1 \leq i \leq n \right\} \leq GTOL ,$$

where a_1, a_2, \dots, a_n are the columns of the current approximation to the Jacobian matrix, f is the vector of residuals, and GTOL is a third user-supplied tolerance.

Note that individual specification of the above three tolerances for the nonlinear least squares problem requires direct user call of the appropriate core subroutine. The easy-to-use driver only accepts the single value TOL. It then internally sets $FTOL = XTOL = TOL$ and $GTOL = 0$.

The X-convergence condition (1) is a relative error test; it thus fails when $x^* = 0$ unless $x = 0$ also. Also note that if (1) is satisfied with $XTOL = 10^{-k}$, then the larger components of Dx have k significant digits, but smaller components may not be as accurate. For example, if D is the identity matrix, $XTOL = 0.001$, and

$$x^* = (2.0, 0.003) ,$$

then

$$x = (2.001, 0.002)$$

satisfies (1), yet the second component of x has no significant digits. This may or may not be important. However, note that if instead

$$D = \text{diag}(1, 1000) ,$$

then (1) is not satisfied even for $XTOL = 0.1$. These scaling considerations can make it important to choose D carefully. See Section 2.5 for more information on scaling.

Since x^* is unknown, the actual criterion for X-convergence cannot be based on (1); instead it depends on the step bound Δ . That is, the actual convergence test is

$$\Delta \leq XTOL \cdot \|Dx\| .$$

The F-convergence condition (2) is a relative error test; it thus fails when $F(x^*) = 0$ unless $F(x) = 0$ also. It is for this reason that F-convergence is not tested for systems of nonlinear equations where $F(x^*) = 0$ is the expected result. Also note that if (2) is satisfied with $FTOL = 10^{-k}$, then $\|F(x)\|$ has k significant digits, but x may not be as accurate. For example, if $FTOL = 10^{-6}$ and

$$F(x) = \begin{pmatrix} x - 1 \\ 1 \end{pmatrix} ,$$

then $x^* = 1$, $\|F(x^*)\| = 1$, and if $x = 1.001$ then (2) is satisfied with $FTOL = 10^{-6}$, but (1) is only satisfied with $XTOL = 10^{-3}$.

In many least squares problems, if $FTOL = (XTOL)^2$ then X-convergence implies F-convergence. This result, however, does not hold if $\|F(x^*)\|$ is very small. For example, if

$$F(x) = \begin{pmatrix} x - 1 \\ 0.0001 \end{pmatrix} ,$$

then $x^* = 1$ and $\|F(x^*)\| = 0.0001$, but if $x = 1.001$ then (1) is satisfied with $XTOL = 10^{-3}$ and yet

$$\|F(x)\| \geq 10\|F(x^*)\| .$$

Since $\|F(x^*)\|$ is unknown, the actual criterion for F-convergence cannot be literally (2); instead it is based on estimates of the terms in (2). If f

and f_+ are the vectors of residuals at the current solution approximation x and at $x+p$, respectively, then the (relative) actual reduction is

$$\text{ACTRED} = (\|f\| - \|f_+\|) / \|f\| ,$$

while the (relative) predicted reduction is

$$\text{PRERED} = (\|f\| - \|f+Jp\|) / \|f\| .$$

The F-convergence test then requires that

$$\begin{aligned} \text{PRERED} &\leq \text{FTOL} \\ |\text{ACTRED}| &\leq \text{FTOL} \\ \text{ACTRED} &\leq 2 \cdot \text{PRERED} \end{aligned}$$

all hold.

The X-convergence and F-convergence tests are quite reliable, but it is important to note that their validity depends critically on the correctness of the Jacobian. If the user is providing the Jacobian, he may make an error. (CHKDER can be used to check the Jacobian.) If the algorithm is estimating the Jacobian matrix, then the approximation may be incorrect if, for example, the function is subject to large errors and EPSFCN is chosen poorly. (For more details see Section 2.4.) In either case the algorithm usually terminates suspiciously near the starting point; recommended action if this occurs is to rerun the problem from a different starting point. If the algorithm also terminates near the new starting point, then it is very likely that the Jacobian is being determined incorrectly.

The X-convergence and F-convergence tests may also fail if the tolerances are too large. In general, XTOL and FTOL should be smaller than 10^{-5} ; recommended values for these tolerances are on the order of the square root of the machine precision. As described in Section 1.7, the single precision value of the machine precision can be obtained from the MINPACK-1 function SPMPAR and the double precision value from DPMPAR. Note, however, that on some machines the square root of machine precision is larger than 10^{-5} .

The G-convergence test (3) measures the angle between the residual vector and the columns of the Jacobian matrix and thus can be expected to fail if either $F(x^*) = 0$ or any column of $F'(x^*)$ is zero. Also note that there is no clear relationship between G-convergence and either X-convergence or F-convergence. Furthermore, the G-convergence test detects other critical points, namely maximizers and saddle points; therefore, termination with G-convergence should be examined carefully.

An important property of the tests described above is that they are scale invariant. (See Section 2.5 for more details on scaling.) Scale invariance is a feature not shared by many other convergence tests. For example, the convergence test

$$(4) \quad \|f\| \leq \text{AFTOL} ,$$

where AFTOL is a user-supplied tolerance, is not scale invariant, and this makes it difficult to choose an appropriate AFTOL. As an illustration of the difficulty with this test, consider the function

$$F(x) = (3x - 10)\exp(10x) .$$

On a computer with 15 decimal digits

$$|F(x^*)| \geq 1 ,$$

where x^* is the closest machine-representable number to $10/3$, and thus a suitable AFTOL is not apparent.

If the user, however, wants to use (4) as a termination test, then he can do this by setting NPRINT positive in the call to the respective core subroutine. (See Section 2.9 for more information on NPRINT.) This provides him periodic opportunity, through subroutine FCN with IFLAG = 0, to affect the iteration sequence, and in this instance he might insert the following program segment into FCN.

```

      IF (IFLAG .NE. 0) GO TO 10
      FNORM = ENORM(LFVEC,FVEC)
      IF (FNORM .LE. AFTOL) IFLAG = -1
      RETURN
10 CONTINUE

```

In this program segment it is assumed that LFVEC = N for systems of nonlinear equations and LFVEC = M for nonlinear least squares problems. It is also assumed that the MINPACK-1 function ENORM is declared to the precision of the computation.

2.4 Approximations to the Jacobian Matrix

If the user does not provide the Jacobian matrix, then the MINPACK-1 algorithms compute an approximation J. In the algorithms for nonlinear least squares problems, J is always determined by a forward difference approximation, while in the algorithms for systems of nonlinear equations, J is sometimes determined by a forward-difference approximation but more often by an update formula of Broyden. It is important to note that the update formula is also used in the algorithms for systems of nonlinear equations where the user is providing the Jacobian matrix, since the updating tends to improve the efficiency of the algorithms.

The forward-difference approximation to the j-th column of the Jacobian matrix can be written

$$(1) \quad \frac{F(x+h_j e_j) - F(x)}{h_j},$$

where e_j is the j-th column of the identity matrix and h_j is the difference parameter. The choice of h_j depends on the precision of the function evaluations, which is specified in the MINPACK-1 algorithms by the parameter EPSFCN. To be specific,

$$h_j = (\text{EPSFCN})^{1/2} |x_j|$$

unless $x_j = 0$, in which case

$$h_j = (\text{EPSFCN})^{\frac{1}{2}}.$$

In the easy-to-use drivers EPSFCN is set internally to the machine precision (see Section 1.7), since these subroutines assume that the functions can be evaluated accurately. In the core subroutines EPSFCN is a user-supplied parameter; if there are errors in the evaluations of the functions, then EPSFCN may need to be much larger than the machine precision. For example, if the specification of the function requires the numerical evaluation of an integral, then EPSFCN should probably be on the order of the tolerance in the integration routine.

One advantage of approximation (1) is that it is scale invariant. (See Section 2.5 for more details on scaling.) A disadvantage of (1) is that it assumes EPSFCN the same for each variable, for each component function of F , and for each vector x . These assumptions may make it difficult to determine a suitable value for EPSFCN. The user who is uncertain of an appropriate value of EPSFCN can run the algorithm with two or three values of EPSFCN and retain the value that gives the best results. In general, overestimates are better than underestimates.

The update formula of Broyden depends on the current approximation x , the correction p , and J . Since

$$F(x+p) - F(x) = \left[\int_0^1 F'(x+\theta p) d\theta \right] p,$$

it is natural to ask that the approximation J_+ at $x+p$ satisfy the equation

$$J_+ p = F(x+p) - F(x),$$

and among the possible choices be the one closest to J . To define an appropriate measure of distance, let D be the current diagonal scaling matrix and define the matrix norm

$$\|A\|_D = \left(\sum_{j=1}^n \left(\frac{\|a_j\|}{d_j} \right)^2 \right)^{\frac{1}{2}},$$

where a_1, a_2, \dots, a_n are the columns of A . It is now easy to verify that the solution of the problem

$$\min\{\|\tilde{J}-J\|_D: \tilde{J}_p = F(x+p)-F(x)\} ,$$

is given by

$$J_+ = J + \frac{(F(x+p)-F(x)-J_p)(D^T D p)^T}{\|D p\|^2} .$$

There are many properties of this formula that justify its use in algorithms for systems of nonlinear equations, but a discussion of these properties is beyond the scope of this work.

2.5 Scaling

Scale invariance is a desirable feature of an optimization algorithm. Algorithms for systems of nonlinear equations and nonlinear least squares problems are scale invariant if, given problems related by the change of scale

$$\begin{aligned} \tilde{F}(x) &= \alpha F(D_V x) \\ \tilde{x}_0 &= D_V^{-1} x_0 , \end{aligned}$$

where α is a positive scalar and D_V is a diagonal matrix with positive entries, the approximations x and \tilde{x} generated by the algorithms satisfy

$$\tilde{x} = D_V^{-1} x .$$

Scale invariance is a natural requirement that can have a significant effect on the implementation and performance of an algorithm. To the user scale invariance means, in particular, that he can work with either problem and obtain equivalent results.

The core subroutines in MINPACK-1 are scale invariant provided that the initial choice of the scaling matrix satisfies

$$(1) \quad \tilde{D}_0 = \alpha D_V D_0 ,$$

where D_0 and \tilde{D}_0 are the initial scaling matrices of the respective problems defined by F and x_0 and by \tilde{F} and \tilde{x}_0 . If the user of the core subroutines has

requested internal scaling (MODE = 1), then the internal scaling matrix is set to

$$\text{diag}(\|a_1\|, \|a_2\|, \dots, \|a_n\|) ,$$

where a_i is the i -th column of the initial Jacobian approximation, and (1) holds. If the user has stipulated external scaling (MODE = 2), then the initial scaling matrix is specified by the contents of the array DIAG, and scale invariance is only achieved if the user's choice satisfies (1).

There are certain cases in which scale invariance may be lost, as when the Jacobian matrix at the starting point has a column of zeroes and internal scaling is requested. In this case D_0 would have a zero element and be singular, but this possibility is not catered to in the current implementation. Instead, the zero element is arbitrarily set to 1, preserving nonsingularity but giving up scale invariance. In practice, however, these cases seldom arise and scale invariance is usually maintained.

Our experience is that internal scaling is generally preferable for nonlinear least squares problems and external scaling for systems of nonlinear equations. This experience is reflected in the settings built into the easy-to-use drivers; MODE = 1 is specified in the drivers for nonlinear least squares problems and MODE = 2 for systems of nonlinear equations. In the latter case, D_0 is set to the identity matrix, a choice that generally works out well in practice; if this choice is not appropriate, recourse to the core subroutine would be indicated.

It is important to note that scale invariance does not relieve the user of choosing an appropriate formulation of the problem or a reasonable starting point. In particular, note that an appropriate formulation may involve a scaling of the equations or a nonlinear transformation of the variables and that the performance of the MINPACK-1 algorithms can be affected by these transformations. For example, the algorithm for systems of nonlinear equations usually generates different approximations for problems defined by functions \tilde{F} and F , where

$$\begin{aligned}\tilde{F}(x) &= D_E F(x) , \\ \tilde{x}_0 &= x_0 ,\end{aligned}$$

and D_E is a diagonal matrix with positive entries. The main reason for this is that the algorithm usually decides that x_+ is a better approximation than x if

$$\|F(x_+)\| < \|F(x)\| ,$$

and it is entirely possible that

$$\|\tilde{F}(x_+)\| > \|\tilde{F}(x)\| .$$

The user should thus scale his equations (i.e., choose D_E) so that the expected errors in the residuals are of about the same order of magnitude.

2.6 Subroutine FCN: Calculation of the Function and Jacobian Matrix

The MINPACK-1 algorithms require that the user provide a subroutine with name of his choosing, say FCN, to calculate the residuals of the function $F: R^n \rightarrow R^m$, where $m = n$ for systems of nonlinear equations and $m \geq n$ for nonlinear least squares problems. Some of the algorithms also require that FCN calculate the Jacobian matrix of the mapping F .

It is important that the calculation of the function and Jacobian matrix be as accurate as possible. It is also important that the coding of FCN be as efficient as possible, since the timing of the algorithm is strongly influenced by the time spent in FCN. In particular, when the residuals f_i have common subexpressions it is usually worthwhile to organize the computation so that these subexpressions need be evaluated only once. For example, if the residuals are of the form

$$f_i(x) = g(x) + h_i(x) , \quad 1 \leq i \leq m$$

with $g(x)$ common to all of them, then the coding of FCN is best expressed in the following form.

$$\begin{aligned} \tau &= g(x) \\ \text{For } i &= 1, 2, \dots, m \\ f_i(x) &= \tau + h_i(x) . \end{aligned}$$

As another example, assume that the residuals are of the form

$$f_i(x) = \sum_{j=1}^n (\alpha_{ij} \cos(x_j) + \beta_{ij} \sin(x_j)) ,$$

where the α_{ij} and β_{ij} are given constants. The following program segment evaluates the f_i efficiently.

```

For i = 1,2,...,m
  f_i(x) = 0
For j = 1,2,...,n
  γ = cos(x_j)
  σ = sin(x_j)
  For i = 1,2,...,m
    f_i(x) = f_i(x) + γα_{ij} + σβ_{ij} .

```

If the user is providing the Jacobian matrix of the mapping F , then it is important that its calculation also be as efficient as possible. In particular, when the elements of the Jacobian matrix have common subexpressions, it is usually worthwhile to organize the computation so that these subexpressions need be evaluated only once. For example, if

$$f_i(x) = g(x) + h_i(x) , \quad 1 \leq i \leq m ,$$

then the rows of the Jacobian matrix are

$$\nabla f_i(x) = \nabla g(x) + \nabla h_i(x) , \quad 1 \leq i \leq m ,$$

and the subexpression $\nabla g(x)$ is thus common to all the rows of the Jacobian matrix.

As another example, assume that

$$f_i(x) = \sum_{j=1}^n (\alpha_{ij} \cos(x_j) + \beta_{ij} \sin(x_j)) ,$$

where the α_{ij} and β_{ij} are given constants. In this case,

$$\frac{\partial f_i(x)}{\partial x_j} = -\alpha_{ij} \sin(x_j) + \beta_{ij} \cos(x_j) ,$$

and the following program segment evaluates the Jacobian matrix efficiently.

```

For j = 1,2,...,n
  γ = cos(xj)
  σ = sin(xj)
  For i = 1,2,...,m
    
$$\frac{\partial f_i(x)}{\partial x_j} = -\sigma \alpha_{ij} + \gamma \beta_{ij} .$$


```

The previous example illustrates further the possibility of common sub-expressions between the function and the Jacobian matrix. For the nonlinear least squares algorithms advantage can be taken of this, because a call to FCN to evaluate the Jacobian matrix at x is always preceded by a call to evaluate the function at x . This is not the case for the nonlinear equations algorithms.

To specifically illustrate this possibility of sharing information between function and Jacobian matrix, assume that

$$f_i(x) = g(x)^2 + h_i(x) , \quad 1 \leq i \leq m .$$

Then the rows of the Jacobian matrix are

$$\nabla f_i(x) = 2g(x)\nabla g(x) + \nabla h_i(x) , \quad 1 \leq i \leq m ,$$

and the coding of FCN is best done as follows.

```

If FUNCTION EVALUATION then
  τ = g(x)
  Save τ in COMMON
  For i = 1,2,...,m
    fi(x) = τ2 + hi(x)
If JACOBIAN EVALUATION then
  v = ∇g(x)
  For i = 1,2,...,m
    ∇fi(x) = 2τv + ∇hi(x) .

```

2.7 Constraints

Systems of nonlinear equations and nonlinear least squares problems often impose constraints on the solution. For example, on physical grounds it is sometimes necessary that the solution vector have positive components.

At present there are no algorithms in MINPACK that formally admit constraints, but in some cases they can be effectively achieved with ad hoc strategies. In this section we describe two strategies for restricting the solution approximations to a region D of R^n .

The user has control over the initial approximation x_0 . It may happen, however, that x is in D but the algorithm computes a correction p such that $x+p$ is not in D . If this correction is permitted, the algorithm may never recover; that is, the approximations may now converge to an unacceptable solution outside of D .

The simplest strategy to restrict the corrections is to impose a penalty on the function if the algorithm attempts to step outside of D . For example, let μ be any number such that

$$|f_i(x_0)| \leq \mu, \quad 1 \leq i \leq m,$$

and in FCN define

$$f_i(x) = \mu, \quad 1 \leq i \leq m$$

whenever x does not belong to D . If FCN is coded in this way, a correction p for which $x+p$ lies outside of D will not decrease the residuals and is therefore not acceptable. It follows that this penalty on FCN forces all the approximations x to lie in D .

Note that this strategy restricts all the corrections, and as a consequence may lead to very slow convergence if the solution is near the boundary of D . It usually suffices to only restrict the initial correction, and users of the core subroutines can do this in several ways.

Recall from Section 2.2 that the initial correction p_0 satisfies a bound of the form

$$\|D_o p_o\| \leq \Delta_o ,$$

where D_o is a diagonal scaling matrix and Δ_o is a step bound. The contents of D_o are governed by the parameter MODE. If MODE = 1 then D_o is internally set, while if MODE = 2 then D_o is specified by the user through the array DIAG. The step bound Δ_o is determined from the parameter FACTOR. By definition

$$\Delta_o = \text{FACTOR} \cdot \|D_o x_o\| ,$$

unless x_o is the zero vector, in which case

$$\Delta_o = \text{FACTOR} .$$

It is clear from this definition that smaller values of FACTOR lead to smaller steps. For a sufficiently small value of FACTOR (usually 0.01 suffices), an improved point $x_o + p_o$ will be found that belongs to D.

Be aware that the step restriction is on $D_o p_o$ and not on p_o directly. A small element of D_o , which can be set by internal scaling when MODE = 1, may lead to a large component in the correction p_o . In many cases it is not necessary to control p_o directly, but if this is desired then MODE = 2 must be used.

When MODE = 2, the contents of D_o are specified by the user, and this allows direct control of p_o . If, for example, it is desired to restrict the components of p_o to small relative corrections of the corresponding components of x_o (assumed nonzero), then this can be done by setting

$$D_o = \text{diag} \left(\frac{1}{|\xi_1|}, \frac{1}{|\xi_2|}, \dots, \frac{1}{|\xi_n|} \right) ,$$

where ξ_i is the i -th component of x_o , and by choosing FACTOR appropriately. To justify this choice, note that p_o satisfies

$$\|D_o p_o\| \leq \Delta_o = \text{FACTOR} \cdot \|D_o x_o\| ,$$

and that the choice of D_o guarantees that

$$\|D_0 x_0\| = n^{1/2}.$$

Thus, if ρ_i is the i -th component of p_0 , then

$$|\rho_i| \leq n^{1/2} \text{FACTOR} \cdot |\xi_i|,$$

which justifies the choice of D_0 .

2.8 Error Bounds

A problem of general interest is the determination of error bounds on the components of a solution vector. It is beyond the scope of this work to discuss this topic in depth, so the discussion below is limited to the computation of bounds on the sensitivity of the parameters, and of the covariance matrix. The discussion is in terms of the nonlinear least squares problem, but some of the results also apply to systems of nonlinear equations.

Let $F: R^n \rightarrow R^m$ define a nonlinear least squares problem ($m \geq n$), and let x^* be a solution. Given $\varepsilon > 0$, the problem is to determine sensitivity (upper) bounds $\sigma_1, \sigma_2, \dots, \sigma_n$ such that, for each i , the condition

$$|x_i - x_i^*| \leq \sigma_i, \quad \text{with } x_j = x_j^* \text{ for } j \neq i,$$

implies that

$$\|F(x)\| \leq (1 + \varepsilon) \|F(x^*)\|.$$

Of particular interest are values of σ_i which are large relative to $|x_i|$, since then the residual norm $\|F(x)\|$ is insensitive to changes in the i -th parameter and may therefore indicate a possible deficiency in the formulation of the problem.

A first order estimate of the sensitivity bounds σ_i shows that

$$(1) \quad \sigma_i = \varepsilon^{1/2} \left(\frac{\|F(x^*)\|}{\|F'(x^*) \cdot e_i\|} \right),$$

where $F'(x^*)$ is the Jacobian matrix of F at x^* and e_i is the i -th column of the identity matrix. Note that if $\|F'(x^*) \cdot e_i\|$ is small relative to $\|F(x^*)\|$, then the residual norm is insensitive to changes in the i -th parameter.

If x is an approximation to the solution x^* and J is an approximation to $F'(x^*)$, then the bounds (1) can usually be replaced by

$$(2) \quad \sigma_i = \varepsilon^{1/2} \left(\frac{\|F(x)\|}{\|J e_i\|} \right) .$$

The MINPACK-1 nonlinear least squares programs (except LMDIF1) return enough information to compute the sensitivity bounds (2). On a normal exit, these programs return $F(x)$ and part of the QR decomposition of J ; namely, an upper triangular matrix R and a permutation matrix P such that

$$(3) \quad JP = QR$$

for some matrix Q with orthogonal columns. The vector $F(x)$ is returned in the array FVEC and the matrix R is returned in the upper triangular part of the array FJAC. The permutation matrix P is defined by the contents of the integer array IPVT; if

$$IPVT = (p(1), p(2), \dots, p(n)) ,$$

then the j -th column of P is the $p(j)$ -th column of the identity matrix.

The norms of the columns of the Jacobian matrix can be computed by noting that (3) implies that

$$J e_{p(j)} = Q R e_j ,$$

and hence,

$$\|J e_{p(j)}\| = \|R e_j\| .$$

The following loop uses this relationship to store $\|J e_\ell\|$ in the ℓ -th position of an array FJNORM; with this information it is then easy to compute the sensitivity bounds (2).

```

DO 10 J = 1, N
  L = IPVT(J)
  FJNORM(L) = ENORM(J, FJAC(1, J))
10  CONTINUE
```


This loop assumes that ENORM and FJNORM have been declared to the precision of the computation.

In addition to sensitivity bounds for the individual parameters, it is sometimes desirable to determine a bound for the sensitivity of the residual norm to changes in some linear combination of the parameters. Given $\epsilon > 0$ and a vector v with $\|v\| = 1$, the problem is to determine a bound σ such that

$$\|F(x^* + \sigma v)\| \leq (1 + \epsilon) \|F(x^*)\| .$$

A first order estimate of σ is now

$$\sigma = \epsilon^{\frac{1}{2}} \left(\frac{\|F(x^*)\|}{\|F'(x^*) \cdot v\|} \right) ;$$

if $\|F'(x^*) \cdot v\|$ is small relative to $\|F(x^*)\|$, then σ is large and the residual norm is insensitive to changes in the linear combination of the parameters specified by v .

For example, if the level set

$$\{x: \|F(x)\| \leq (1 + \epsilon) \|F(x^*)\|\}$$

is as in Figure 3, then the residual norm, although sensitive to changes in x_1 and x_2 , is relatively insensitive to changes along $v = (1,1)$.

If the residual norm is relatively insensitive to changes in some linear combination of the parameters, then the Jacobian matrix at the solution is nearly rank-deficient, and in these cases it may be worthwhile to attempt to determine a set of linearly independent parameters. In some statistical applications, the covariance matrix

$$(J^T J)^{-1}$$

is used for this purpose.

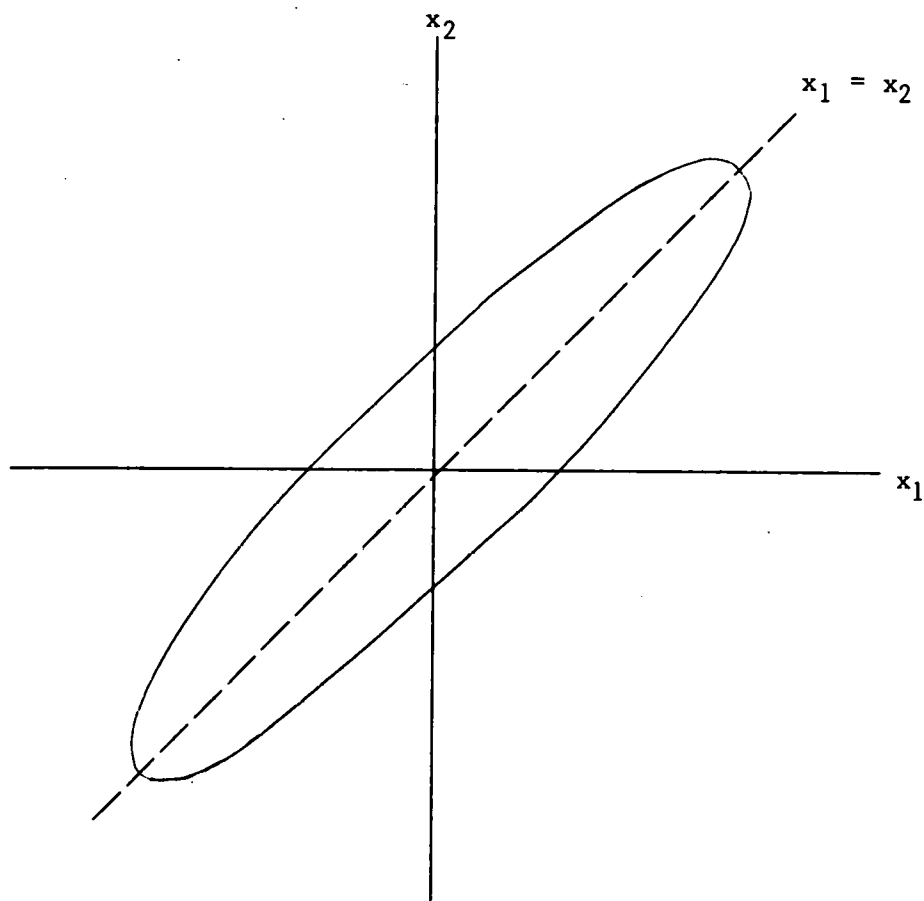


Figure 3

Subroutine COVAR, which appears at the end of this section, will compute the covariance matrix. The computation of the covariance matrix from the QR factorization of J depends on the relationship

$$(4) \quad (J^T J)^{-1} = P(R^T R)^{-1} P^T,$$

which is an easy consequence of (3). Subroutine COVAR overwrites R with the upper triangular part of $(R^T R)^{-1}$ and then computes the covariance matrix from (4).

Note that for proper execution of COVAR the QR factorization of J must have used column pivoting. This guarantees that for the resulting R

$$(5) \quad |r_{kk}| \geq |r_{ij}|, \quad k \leq i \leq j,$$

thereby allowing a reasonable determination of the numerical rank of J. Most of the MINPACK-1 nonlinear least squares subroutines return the correct factorization; the QR factorization in LMSTR1 and LMSTR, however, satisfies

$$JP_1 = Q_1 R_1$$

but R_1 does not usually satisfy (5). To obtain the correct factorization, note that the QR factorization with column pivoting of R_1 satisfies

$$R_1 P_2 = Q_2 R_2$$

where R_2 satisfies (5), and therefore

$$J(P_1 P_2) = (Q_1 Q_2) R_2$$

is the desired factorization of J. The program segment below uses the MINPACK-1 subroutine QRFAC to compute R_2 from R_1 .

```

      DO 30 J = 1, N
        JP1 = J + 1
        IF (N .LT. JP1) GO TO 20
        DO 10 I = JP1, N
          FJAC(I,J) = ZERO
10      CONTINUE
20      CONTINUE
30      CONTINUE
      CALL QRFAC(N,N,FJAC,LDFJAC,.TRUE.,IPVT2,N,WA1,WA2,WA3)
      DO 40 J = 1, N
        FJAC(J,J) = WA1(J)
        L = IPVT2(J)
        IPVT2(J) = IPVT1(L)
40      CONTINUE

```

Note that QRFAC sets the contents of the array IPVT2 to define the permutation matrix P_2 , and the final loop in the program segment overwrites IPVT2 to define the permutation matrix $P_1 P_2$.

SUBROUTINE COVAR(N,R,LDR,IPVT,TOL,WA)	COVR0010
INTEGER N,LDR	COVR0020
INTEGER IPVT(N)	COVR0030
DOUBLE PRECISION TOL	COVR0040
DOUBLE PRECISION R(LDR,N),WA(N)	COVR0050
*****	COVR0060
	COVR0070
SUBROUTINE COVAR	COVR0080
	COVR0090
GIVEN AN M BY N MATRIX A, THE PROBLEM IS TO DETERMINE	COVR0100
THE COVARIANCE MATRIX CORRESPONDING TO A, DEFINED AS	COVR0110
	COVR0120
T	COVR0130
INVERSE(A *A) .	COVR0140
	COVR0150
THIS SUBROUTINE COMPLETES THE SOLUTION OF THE PROBLEM	COVR0160
IF IT IS PROVIDED WITH THE NECESSARY INFORMATION FROM THE	COVR0170
QR FACTORIZATION, WITH COLUMN PIVOTING, OF A. THAT IS, IF	COVR0180
A*P = Q*R, WHERE P IS A PERMUTATION MATRIX, Q HAS ORTHOGONAL	COVR0190
COLUMNS, AND R IS AN UPPER TRIANGULAR MATRIX WITH DIAGONAL	COVR0200
ELEMENTS OF NONINCREASING MAGNITUDE, THEN COVAR EXPECTS	COVR0210
THE FULL UPPER TRIANGLE OF R AND THE PERMUTATION MATRIX P.	COVR0220
THE COVARIANCE MATRIX IS THEN COMPUTED AS	COVR0230
	COVR0240
	COVR0250
T T	COVR0260
P*INVERSE(R *R)*P .	COVR0270
	COVR0280
IF A IS NEARLY RANK DEFICIENT, IT MAY BE DESIRABLE TO COMPUTE	COVR0290
THE COVARIANCE MATRIX CORRESPONDING TO THE LINEARLY INDEPENDENT	COVR0300
COLUMNS OF A. TO DEFINE THE NUMERICAL RANK OF A, COVAR USES	COVR0310
THE TOLERANCE TOL. IF L IS THE LARGEST INTEGER SUCH THAT	COVR0320
	COVR0330
ABS(R(L,L)) .GT. TOL*ABS(R(1,1)) ,	COVR0340
	COVR0350
THEN COVAR COMPUTES THE COVARIANCE MATRIX CORRESPONDING TO	COVR0360
THE FIRST L COLUMNS OF R. FOR K GREATER THAN L, COLUMN	COVR0370
AND ROW IPVT(K) OF THE COVARIANCE MATRIX ARE SET TO ZERO.	COVR0380
	COVR0390
THE SUBROUTINE STATEMENT IS	COVR0400
	COVR0410
SUBROUTINE COVAR(N,R,LDR,IPVT,TOL,WA)	COVR0420
	COVR0430
WHERE	COVR0440
	COVR0450
N IS A POSITIVE INTEGER INPUT VARIABLE SET TO THE ORDER OF R.	COVR0460
	COVR0470
R IS AN N BY N ARRAY. ON INPUT THE FULL UPPER TRIANGLE MUST	COVR0480
CONTAIN THE FULL UPPER TRIANGLE OF THE MATRIX R. ON OUTPUT	COVR0490
R CONTAINS THE SQUARE SYMMETRIC COVARIANCE MATRIX.	COVR0500
	COVR0510
LDR IS A POSITIVE INTEGER INPUT VARIABLE NOT LESS THAN N	COVR0520
WHICH SPECIFIES THE LEADING DIMENSION OF THE ARRAY R.	COVR0530
	COVR0540
IPVT IS AN INTEGER INPUT ARRAY OF LENGTH N WHICH DEFINES THE	

C	PERMUTATION MATRIX P SUCH THAT $A \cdot P = Q \cdot R$. COLUMN J OF P	COVR0550
C	IS COLUMN IPVT(J) OF THE IDENTITY MATRIX.	COVR0560
C		COVR0570
C	TOL IS A NONNEGATIVE INPUT VARIABLE USED TO DEFINE THE	COVR0580
C	NUMERICAL RANK OF A IN THE MANNER DESCRIBED ABOVE.	COVR0590
C		COVR0600
C	WA IS A WORK ARRAY OF LENGTH N.	COVR0610
C		COVR0620
C	SUBPROGRAMS CALLED	COVR0630
C		COVR0640
C	FORTTRAN-SUPPLIED ... DABS	COVR0650
C		COVR0660
C	ARGONNE NATIONAL LABORATORY. MINPACK PROJECT. AUGUST 1980.	COVR0670
C	BURTON S. GARBOW, KENNETH E. HILLSTROM, JORGE J. MORE	COVR0680
C		COVR0690
C	*****	COVR0700
	INTEGER I,II,J,JJ,K,KM1,L	COVR0710
	LOGICAL SING	COVR0720
	DOUBLE PRECISION ONE,TEMP,TOLR,ZERO	COVR0730
	DATA ONE,ZERO /1.0D0,0.0D0/	COVR0740
C		COVR0750
C	FORM THE INVERSE OF R IN THE FULL UPPER TRIANGLE OF R.	COVR0760
C		COVR0770
	TOLR = TOL*DABS(R(1,1))	COVR0780
	L = 0	COVR0790
	DO 40 K = 1, N	COVR0800
	IF (DABS(R(K,K)) .LE. TOLR) GO TO 50	COVR0810
	R(K,K) = ONE/R(K,K)	COVR0820
	KM1 = K - 1	COVR0830
	IF (KM1 .LT. 1) GO TO 30	COVR0840
	DO 20 J = 1, KM1	COVR0850
	TEMP = R(K,K)*R(J,K)	COVR0860
	R(J,K) = ZERO	COVR0870
	DO 10 I = 1, J	COVR0880
	R(I,K) = R(I,K) - TEMP*R(I,J)	COVR0890
10	CONTINUE	COVR0900
20	CONTINUE	COVR0910
30	CONTINUE	COVR0920
	L = K	COVR0930
40	CONTINUE	COVR0940
50	CONTINUE	COVR0950
C		COVR0960
C	FORM THE FULL UPPER TRIANGLE OF THE INVERSE OF (R TRANSPOSE)*R	COVR0970
C	IN THE FULL UPPER TRIANGLE OF R.	COVR0980
C		COVR0990
	IF (L .LT. 1) GO TO 110	COVR1000
	DO 100 K = 1, L	COVR1010
	KM1 = K - 1	COVR1020
	IF (KM1 .LT. 1) GO TO 80	COVR1030
	DO 70 J = 1, KM1	COVR1040
	TEMP = R(J,K)	COVR1050
	DO 60 I = 1, J	COVR1060
	R(I,J) = R(I,J) + TEMP*R(I,K)	COVR1070
60	CONTINUE	COVR1080

70	CONTINUE	COVR1090
80	CONTINUE	COVR1100
	TEMP = R(K,K)	COVR1110
	DO 90 I = 1, K	COVR1120
	R(I,K) = TEMP*R(I,K)	COVR1130
90	CONTINUE	COVR1140
100	CONTINUE	COVR1150
110	CONTINUE	COVR1160
C		COVR1170
C	FORM THE FULL LOWER TRIANGLE OF THE COVARIANCE MATRIX	COVR1180
C	IN THE STRICT LOWER TRIANGLE OF R AND IN WA.	COVR1190
C		COVR1200
	DO 130 J = 1, N	COVR1210
	JJ = IPVT(J)	COVR1220
	SING = J .GT. L	COVR1230
	DO 120 I = 1, J	COVR1240
	IF (SING) R(I,J) = ZERO	COVR1250
	II = IPVT(I)	COVR1260
	IF (II .GT. JJ) R(II,JJ) = R(I,J)	COVR1270
	IF (II .LT. JJ) R(JJ,II) = R(I,J)	COVR1280
120	CONTINUE	COVR1290
	WA(JJ) = R(J,J)	COVR1300
130	CONTINUE	COVR1310
C		COVR1320
C	SYMMETRIZE THE COVARIANCE MATRIX IN R.	COVR1330
C		COVR1340
	DO 150 J = 1, N	COVR1350
	DO 140 I = 1, J	COVR1360
	R(I,J) = R(J,I)	COVR1370
140	CONTINUE	COVR1380
	R(J,J) = WA(J)	COVR1390
150	CONTINUE	COVR1400
	RETURN	COVR1410
C		COVR1420
C	LAST CARD OF SUBROUTINE COVAR.	COVR1430
C		COVR1440
	END	COVR1450

2.9 Printing

No printing is done in any of the MINPACK-1 subroutines. However, printing of certain parameters through FCN can be facilitated with the integer parameter NPRINT that is available to users of the core subroutines. For these subroutines, setting NPRINT positive results in special calls to FCN with IFLAG = 0 at the beginning of the first iteration and every NPRINT iterations thereafter and immediately prior to return. On these calls to FCN, the parameters X and FVEC are available for printing; FJAC is additionally available if using LMDER.

Often it suffices to print some simple measure of the iteration progress, and the Euclidean norm of the residuals is usually a good choice. This norm can be printed by inserting the following program segment into FCN.

```

      IF (IFLAG .NE. 0) GO TO 10
      FNORM = ENORM(LFVEC,FVEC)
      WRITE (---,1000) FNORM
1000 FORMAT (---)
      RETURN
10 CONTINUE

```

In this program segment it is assumed that LFVEC = N for systems of nonlinear equations and LFVEC = M for nonlinear least squares problems. It is also assumed that the MINPACK-1 function ENORM is declared to the precision of the computation.

CHAPTER 3

Notes and References

This chapter provides notes relating the MINPACK-1 algorithms and software to other work. The list of references appears at the end.

Powell's Hybrid Method

The MINPACK-1 version of Powell's [1970] hybrid method differs in many respects from the original version. For example, the "special iterations" used in the original algorithm proved to be inefficient and have been replaced. The updating method used is due to Broyden [1965]; the MINPACK-1 algorithm is a scaled version of the original. A comparison of an earlier version of the MINPACK-1 algorithm with other algorithms for systems of nonlinear equations has been made by Hiebert [1980].

The Levenberg-Marquardt Algorithm

There are many versions of the algorithm proposed by Levenberg [1944] and modified by Marquardt [1963]. An advantage of the MINPACK-1 version is that it avoids the difficulties associated with choosing the Levenberg-Marquardt parameter, and this allows a very strong global convergence result. The MINPACK-1 algorithm is based on the work of Hebden [1973] and follows the ideas of Moré [1977]. A comparison of an earlier version of the MINPACK-1 algorithm with other algorithms for nonlinear least squares problems has been made by Hiebert [1979].

Derivative Checking

Subroutine CHKDER is new, but similar routines exist in the Numerical Algorithms Group (NAG) library. An advantage of CHKDER is its generality; it can be used to check Jacobians, gradients, and Hessians (second derivatives). To enable this generality, CHKDER presumes no specific parameter sequence for the function evaluation program, returning control instead to the user. This in turn makes necessary a second call to CHKDER for each check.

MINPACK-1 Internal Subprograms

Subroutines DOGLEG and LMPAR are used to generate search directions in the algorithms for systems of nonlinear equations and nonlinear least squares problems, respectively. The algorithm used in DOGLEG is a fairly straightforward implementation of the ideas of Powell [1970], while LMPAR is a refined version of the algorithm described by Moré [1977]. The LMPAR algorithm is the more complicated; in particular, it requires the solution of a sequence of linear least squares problems of special form. It is for this purpose that subroutine QRSOLV is used.

The algorithm used in ENORM is a simplified version of Blue's [1978] algorithm. An advantage of the MINPACK-1 version is that it does not require machine constants; a disadvantage is that nondestructive underflows are allowed.

The banded Jacobian option in FDJAC1 is based on the work of Curtis, Powell, and Reid [1974].

QRFAC and RWUPDT are based on the corresponding algorithms in LINPACK (Dongarra, Bunch, Moler, and Stewart [1979]).

The algorithm used in RLUPDT is based on the work of Gill, Golub, Murray, and Saunders [1974].

References

- Blue, J. L. [1978]. A portable Fortran program to find the Euclidean norm of a vector, ACM Transactions on Mathematical Software 4, 15-23.
- Boyle, J. M. and Dritz, K. W. [1974]. An automated programming system to facilitate the development of quality mathematical software, Proceedings IFIP Congress, North-Holland.
- Broyden, C. G. [1965]. A class of methods for solving nonlinear simultaneous equations, Math. Comp. 19, 577-593.
- Curtis, A. R., Powell, M. J. D., and Reid, J. K. [1974]. On the estimation of sparse Jacobian matrices, J. Inst. Maths Applics 13, 117-119.
- Dongarra, J. J., Bunch, J. R., Moler, C. B., and Stewart, G. W. [1979]. LINPACK users' guide, SIAM Publications.

- Fosdick, L. D. [1974]. BRNANL, A Fortran program to identify basic blocks in Fortran programs, University of Colorado, Computer Science report CU-CS-040-74.
- Fox, P. A., Hall, A. D., and Schryer, N. L. [1978]. The PORT mathematical subroutine library, ACM Transactions on Mathematical Software 4, 104-126.
- Garbow, B. S., Hillstom, K. E., and Moré, J. J. [1980]. Implementation guide for MINPACK-1, Argonne National Laboratory report ANL-80-68.
- Gill, P. E., Golub, G. H., Murray, W., and Saunders, M. A. [1974]. Methods for modifying matrix factorizations, Math. Comp. 28, 505-535.
- Hebden, M. D. [1973]. An algorithm for minimization using exact second derivatives, Atomic Energy Research Establishment report TP 515, Harwell, England.
- Hiebert, K. L. [1979]. A comparison of nonlinear least squares software, Sandia Laboratories report SAND 79-0483, Albuquerque, New Mexico.
- Hiebert, K. L. [1980]. A comparison of software which solves systems of nonlinear equations, Sandia Laboratories report SAND 80-0181, Albuquerque, New Mexico.
- Levenberg, K. [1944]. A method for the solution of certain nonlinear problems in least squares, Quart. Appl. Math. 2, 164-168.
- Marquardt, D. W. [1963]. An algorithm for least-squares estimation of nonlinear parameters, SIAM J. Appl. Math. 11, 431-441.
- Moré, J. J. [1977]. The Levenberg-Marquardt algorithm: Implementation and Theory, Numerical Analysis, G. A. Watson, ed., Lecture Notes in Mathematics 630, Springer-Verlag.
- Moré, J. J., Garbow, B. S., and Hillstom, K. E. [1978]. Testing unconstrained optimization software, Argonne National Laboratory, Applied Mathematics Division Technical Memorandum 324 (to appear in ACM Transactions on Mathematical Software).
- Powell, M. J. D. [1970]. A hybrid method for nonlinear equations, in Numerical Methods for Nonlinear Algebraic Equations, P. Rabinowitz, ed., Gordon and Breach.
- Ryder, B. G. [1974]. The PFORT verifier, Software Practice and Experience 4, 359-377.

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CHAPTER 4

Documentation

This chapter contains the double precision version of the MINPACK-1 documentation; both single and double precision versions of the documentation are available in machine-readable form with the MINPACK-1 package. The documentation appears in the following order:

Systems of nonlinear equations

HYBRD1, HYBRD, HYBRJ1, HYBRJ

Nonlinear least squares problems

LMDF1, LMDIF, LMDER1, LMDER, LMSTR1, LMSTR

Derivative checking

CHKDER

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Documentation for MINPACK subroutine HYBRD1

Double precision version

Argonne National Laboratory

Burton S. Garbow, Kenneth E. Hillstom, Jorge J. More

March 1980

1. Purpose.

The purpose of HYBRD1 is to find a zero of a system of N non-linear functions in N variables by a modification of the Powell hybrid method. This is done by using the more general nonlinear equation solver HYBRD. The user must provide a subroutine which calculates the functions. The Jacobian is then calculated by a forward-difference approximation.

2. Subroutine and type statements.

```
SUBROUTINE HYBRD1(FCN,N,X,FVEC,TOL,INFO,WA,LWA)
INTEGER N,INFO,LWA
DOUBLE PRECISION TOL
DOUBLE PRECISION X(N),FVEC(N),WA(LWA)
EXTERNAL FCN
```

3. Parameters.

Parameters designated as input parameters must be specified on entry to HYBRD1 and are not changed on exit, while parameters designated as output parameters need not be specified on entry and are set to appropriate values on exit from HYBRD1.

FCN is the name of the user-supplied subroutine which calculates the functions. FCN must be declared in an EXTERNAL statement in the user calling program, and should be written as follows.

```
SUBROUTINE FCN(N,X,FVEC,IFLAG)
INTEGER N,IFLAG
DOUBLE PRECISION X(N),FVEC(N)
-----
CALCULATE THE FUNCTIONS AT X AND
RETURN THIS VECTOR IN FVEC.
-----
RETURN
END
```

The value of IFLAG should not be changed by FCN unless the user wants to terminate execution of HYBRD1. In this case set IFLAG to a negative integer.

N is a positive integer input variable set to the number of functions and variables.

X is an array of length N. On input X must contain an initial estimate of the solution vector. On output X contains the final estimate of the solution vector.

FVEC is an output array of length N which contains the functions evaluated at the output X.

TOL is a nonnegative input variable. Termination occurs when the algorithm estimates that the relative error between X and the solution is at most TOL. Section 4 contains more details about TOL.

INFO is an integer output variable. If the user has terminated execution, INFO is set to the (negative) value of IFLAG. See description of FCN. Otherwise, INFO is set as follows.

INFO = 0 Improper input parameters.

INFO = 1 Algorithm estimates that the relative error between X and the solution is at most TOL.

INFO = 2 Number of calls to FCN has reached or exceeded $200*(N+1)$.

INFO = 3 TOL is too small. No further improvement in the approximate solution X is possible.

INFO = 4 Iteration is not making good progress.

Sections 4 and 5 contain more details about INFO.

WA is a work array of length LWA.

LWA is a positive integer input variable not less than $(N*(3*N+13))/2$.

4. Successful completion.

The accuracy of HYBRD1 is controlled by the convergence parameter TOL. This parameter is used in a test which makes a comparison between the approximation X and a solution XSOL. HYBRD1 terminates when the test is satisfied. If TOL is less than the machine precision (as defined by the MINPACK function `DPMPAR(1)`), then HYBRD1 only attempts to satisfy the test defined by the machine precision. Further progress is not usually possible. Unless high precision solutions are required, the recommended value for TOL is the square root of the machine precision.

The test assumes that the functions are reasonably well behaved.

If this condition is not satisfied, then HYBRD1 may incorrectly indicate convergence. The validity of the answer can be checked, for example, by rerunning HYBRD1 with a tighter tolerance.

Convergence test. If $ENORM(Z)$ denotes the Euclidean norm of a vector Z , then this test attempts to guarantee that

$$ENORM(X-XSOL) \leq TOL * ENORM(XSOL).$$

If this condition is satisfied with $TOL = 10^{*(-K)}$, then the larger components of X have K significant decimal digits and INFO is set to 1. There is a danger that the smaller components of X may have large relative errors, but the fast rate of convergence of HYBRD1 usually avoids this possibility.

5. Unsuccessful completion.

Unsuccessful termination of HYBRD1 can be due to improper input parameters, arithmetic interrupts, an excessive number of function evaluations, errors in the functions, or lack of good progress.

Improper input parameters. INFO is set to 0 if $N \leq 0$, or $TOL < 0.00$, or $LWA < (N*(3*N+13))/2$.

Arithmetic interrupts. If these interrupts occur in the FCN subroutine during an early stage of the computation, they may be caused by an unacceptable choice of X by HYBRD1. In this case, it may be possible to remedy the situation by not evaluating the functions here, but instead setting the components of FVEC to numbers that exceed those in the initial FVEC, thereby indirectly reducing the step length. The step length can be more directly controlled by using instead HYBRD, which includes in its calling sequence the step-length-governing parameter FACTOR.

Excessive number of function evaluations. If the number of calls to FCN reaches $200*(N+1)$, then this indicates that the routine is converging very slowly as measured by the progress of FVEC, and INFO is set to 2. This situation should be unusual because, as indicated below, lack of good progress is usually diagnosed earlier by HYBRD1, causing termination with INFO = 4.

Errors in the functions. The choice of step length in the forward-difference approximation to the Jacobian assumes that the relative errors in the functions are of the order of the machine precision. If this is not the case, HYBRD1 may fail (usually with INFO = 4). The user should then use HYBRD instead, or one of the programs which require the analytic Jacobian (HYBRJ1 and HYBRJ).

Lack of good progress. HYBRD1 searches for a zero of the system by minimizing the sum of the squares of the functions. In so doing, it can become trapped in a region where the minimum does not correspond to a zero of the system and, in this situation, the iteration eventually fails to make good progress. In particular, this will happen if the system does not have a zero. If the system has a zero, rerunning HYBRD1 from a different starting point may be helpful.

6. Characteristics of the algorithm.

HYBRD1 is a modification of the Powell hybrid method. Two of its main characteristics involve the choice of the correction as a convex combination of the Newton and scaled gradient directions, and the updating of the Jacobian by the rank-1 method of Broyden. The choice of the correction guarantees (under reasonable conditions) global convergence for starting points far from the solution and a fast rate of convergence. The Jacobian is approximated by forward differences at the starting point, but forward differences are not used again until the rank-1 method fails to produce satisfactory progress.

Timing. The time required by HYBRD1 to solve a given problem depends on N , the behavior of the functions, the accuracy requested, and the starting point. The number of arithmetic operations needed by HYBRD1 is about $11.5 \cdot (N^2)$ to process each call to FCN. Unless FCN can be evaluated quickly, the timing of HYBRD1 will be strongly influenced by the time spent in FCN.

Storage. HYBRD1 requires $(3 \cdot N^2 + 17 \cdot N)/2$ double precision storage locations, in addition to the storage required by the program. There are no internally declared storage arrays.

7. Subprograms required.

USER-supplied FCN

MINPACK-supplied ... DOGLEG, DPMPAR, ENORM, FDJAC1, HYBRD,
QFORM, QRFAC, R1MPYQ, R1UPDT

FORTTRAN-supplied ... DABS, DMAX1, DMIN1, DSQRT, MINO, MOD

8. References.

M. J. D. Powell, A Hybrid Method for Nonlinear Equations. Numerical Methods for Nonlinear Algebraic Equations, P. Rabinowitz, editor. Gordon and Breach, 1970.

9. Example.

The problem is to determine the values of $x(1)$, $x(2)$, ..., $x(9)$, which solve the system of tridiagonal equations

$$\begin{aligned} (3-2*x(1))*x(1) & -2*x(2) & & = -1 \\ -x(i-1) + (3-2*x(i))*x(i) & & -2*x(i+1) & = -1, \quad i=2-8 \\ & -x(8) + (3-2*x(9))*x(9) & & = -1 \end{aligned}$$

```

C *****
C
C DRIVER FOR HYBRD1 EXAMPLE.
C DOUBLE PRECISION VERSION
C
C *****
C INTEGER J,N,INFO,LWA,NWRITE
C DOUBLE PRECISION TOL,FNORM
C DOUBLE PRECISION X(9),FVEC(9),WA(180)
C DOUBLE PRECISION ENORM,DPMPAR
C EXTERNAL FCN
C
C LOGICAL OUTPUT UNIT IS ASSUMED TO BE NUMBER 6.
C
C DATA NWRITE /6/
C
C N = 9
C
C THE FOLLOWING STARTING VALUES PROVIDE A ROUGH SOLUTION.
C
C DO 10 J = 1, 9
C   X(J) = -1.DO
10  CONTINUE
C
C LWA = 180
C
C SET TOL TO THE SQUARE ROOT OF THE MACHINE PRECISION.
C UNLESS HIGH PRECISION SOLUTIONS ARE REQUIRED,
C THIS IS THE RECOMMENDED SETTING.
C
C TOL = DSQRT(DPMPAR(1))
C
C CALL HYBRD1(FCN,N,X,FVEC,TOL,INFO,WA,LWA)
C FNORM = ENORM(N,FVEC)
C WRITE (NWRITE,1000) FNORM,INFO,(X(J),J=1,N)
C STOP
1000 FORMAT (5X,31H FINAL L2 NORM OF THE RESIDUALS,D15.7 //
*          5X,15H EXIT PARAMETER,16X,I10 //
*          5X,27H FINAL APPROXIMATE SOLUTION // (5X,3D15.7))
C
C LAST CARD OF DRIVER FOR HYBRD1 EXAMPLE.
C
C END
C SUBROUTINE FCN(N,X,FVEC,IFLAG)
C INTEGER N,IFLAG
C DOUBLE PRECISION X(N),FVEC(N)
C

```

```

C      SUBROUTINE FCN FOR HYBRD1 EXAMPLE.
C
      INTEGER K
      DOUBLE PRECISION ONE,TEMP,TEMP1,TEMP2,THREE,TWO,ZERO
      DATA ZERO,ONE,TWO,THREE /0.DO,1.DO,2.DO,3.DO/
C
      DO 10 K = 1, N
        TEMP = (THREE - TWO*X(K))*X(K)
        TEMP1 = ZERO
        IF (K .NE. 1) TEMP1 = X(K-1)
        TEMP2 = ZERO
        IF (K .NE. N) TEMP2 = X(K+1)
        FVEC(K) = TEMP - TEMP1 - TWO*TEMP2 + ONE
10      CONTINUE
      RETURN
C
C      LAST CARD OF SUBROUTINE FCN.
C
      END

```

Results obtained with different compilers or machines
may be slightly different.

FINAL L2 NORM OF THE RESIDUALS 0.1192636D-07

EXIT PARAMETER 1

FINAL APPROXIMATE SOLUTION

```

-0.5706545D+00 -0.6816283D+00 -0.7017325D+00
-0.7042129D+00 -0.7013690D+00 -0.6918656D+00
-0.6657920D+00 -0.5960342D+00 -0.4164121D+00

```

Documentation for MINPACK subroutine HYBRD

Double precision version

Argonne National Laboratory

Burton S. Garbow, Kenneth E. Hillstom, Jorge J. More

March 1980

1. Purpose.

The purpose of HYBRD is to find a zero of a system of N non-linear functions in N variables by a modification of the Powell hybrid method. The user must provide a subroutine which calculates the functions. The Jacobian is then calculated by a forward-difference approximation.

2. Subroutine and type statements.

```

SUBROUTINE HYBRD(FCN,N,X,FVEC,XTOL,MAXFEV,ML,MU,EPSEFCN,DIAG,
*               MODE,FACTOR,NPRINT,INFO,NFEV,FJAC,LDFJAC,
*               R,LR,QTF,WA1,WA2,WA3,WA4)
  INTEGER N,MAXFEV,ML,MU,MODE,NPRINT,INFO,NFEV,LDFJAC,LR
  DOUBLE PRECISION XTOL,EPSEFCN,FACTOR
  DOUBLE PRECISION X(N),FVEC(N),DIAG(N),FJAC(LDFJAC,N),R(LR),QTF(N),
*               WA1(N),WA2(N),WA3(N),WA4(N)
  EXTERNAL FCN

```

3. Parameters.

Parameters designated as input parameters must be specified on entry to HYBRD and are not changed on exit, while parameters designated as output parameters need not be specified on entry and are set to appropriate values on exit from HYBRD.

FCN is the name of the user-supplied subroutine which calculates the functions. FCN must be declared in an EXTERNAL statement in the user calling program, and should be written as follows.

```

SUBROUTINE FCN(N,X,FVEC,IFLAG)
  INTEGER N,IFLAG
  DOUBLE PRECISION X(N),FVEC(N)
  -----
  CALCULATE THE FUNCTIONS AT X AND
  RETURN THIS VECTOR IN FVEC.
  -----
  RETURN
  END

```

The value of IFLAG should not be changed by FCN unless the

user wants to terminate execution of HYBRD. In this case set IFLAG to a negative integer.

N is a positive integer input variable set to the number of functions and variables.

X is an array of length N. On input X must contain an initial estimate of the solution vector. On output X contains the final estimate of the solution vector.

FVEC is an output array of length N which contains the functions evaluated at the output X.

XTOL is a nonnegative input variable. Termination occurs when the relative error between two consecutive iterates is at most XTOL. Therefore, XTOL measures the relative error desired in the approximate solution. Section 4 contains more details about XTOL.

MAXFEV is a positive integer input variable. Termination occurs when the number of calls to FCN is at least MAXFEV by the end of an iteration.

ML is a nonnegative integer input variable which specifies the number of subdiagonals within the band of the Jacobian matrix. If the Jacobian is not banded, set ML to at least $N - 1$.

MU is a nonnegative integer input variable which specifies the number of superdiagonals within the band of the Jacobian matrix. If the Jacobian is not banded, set MU to at least $N - 1$.

EPSFCN is an input variable used in determining a suitable step for the forward-difference approximation. This approximation assumes that the relative errors in the functions are of the order of EPSFCN. If EPSFCN is less than the machine precision, it is assumed that the relative errors in the functions are of the order of the machine precision.

DIAG is an array of length N. If $\text{MODE} = 1$ (see below), DIAG is internally set. If $\text{MODE} = 2$, DIAG must contain positive entries that serve as multiplicative scale factors for the variables.

MODE is an integer input variable. If $\text{MODE} = 1$, the variables will be scaled internally. If $\text{MODE} = 2$, the scaling is specified by the input DIAG. Other values of MODE are equivalent to $\text{MODE} = 1$.

FACTOR is a positive input variable used in determining the initial step bound. This bound is set to the product of FACTOR and the Euclidean norm of $\text{DIAG} \cdot X$ if nonzero, or else to FACTOR itself. In most cases FACTOR should lie in the interval $(.1, 100.)$. 100. is a generally recommended value.

NPRINT is an integer input variable that enables controlled printing of iterates if it is positive. In this case, FCN is called with IFLAG = 0 at the beginning of the first iteration and every NPRINT iterations thereafter and immediately prior to return, with X and FVEC available for printing. If NPRINT is not positive, no special calls of FCN with IFLAG = 0 are made.

INFO is an integer output variable. If the user has terminated execution, INFO is set to the (negative) value of IFLAG. See description of FCN. Otherwise, INFO is set as follows.

INFO = 0 Improper input parameters.

INFO = 1 Relative error between two consecutive iterates is at most XTOL.

INFO = 2 Number of calls to FCN has reached or exceeded MAXFEV.

INFO = 3 XTOL is too small. No further improvement in the approximate solution X is possible.

INFO = 4 Iteration is not making good progress, as measured by the improvement from the last five Jacobian evaluations.

INFO = 5 Iteration is not making good progress, as measured by the improvement from the last ten iterations.

Sections 4 and 5 contain more details about INFO.

NFEV is an integer output variable set to the number of calls to FCN.

FJAC is an output N by N array which contains the orthogonal matrix Q produced by the QR factorization of the final approximate Jacobian.

LDFJAC is a positive integer input variable not less than N which specifies the leading dimension of the array FJAC.

R is an output array of length LR which contains the upper triangular matrix produced by the QR factorization of the final approximate Jacobian, stored rowwise.

LR is a positive integer input variable not less than $(N*(N+1))/2$.

QTF is an output array of length N which contains the vector $(Q \text{ transpose}) * FVEC$.

WA1, WA2, WA3, and WA4 are work arrays of length N.

4. Successful completion.

The accuracy of HYBRD is controlled by the convergence parameter XTOL. This parameter is used in a test which makes a comparison between the approximation X and a solution XSOL. HYBRD terminates when the test is satisfied. If the convergence parameter is less than the machine precision (as defined by the MINPACK function DPMPAR(1)), then HYBRD only attempts to satisfy the test defined by the machine precision. Further progress is not usually possible.

The test assumes that the functions are reasonably well behaved. If this condition is not satisfied, then HYBRD may incorrectly indicate convergence. The validity of the answer can be checked, for example, by rerunning HYBRD with a tighter tolerance.

Convergence test. If $ENORM(Z)$ denotes the Euclidean norm of a vector Z and D is the diagonal matrix whose entries are defined by the array DIAG, then this test attempts to guarantee that

$$ENORM(D*(X-XSOL)) \leq XTOL * ENORM(D*XSOL).$$

If this condition is satisfied with $XTOL = 10^{*(-K)}$, then the larger components of D*X have K significant decimal digits and INFO is set to 1. There is a danger that the smaller components of D*X may have large relative errors, but the fast rate of convergence of HYBRD usually avoids this possibility. Unless high precision solutions are required, the recommended value for XTOL is the square root of the machine precision.

5. Unsuccessful completion.

Unsuccessful termination of HYBRD can be due to improper input parameters, arithmetic interrupts, an excessive number of function evaluations, or lack of good progress.

Improper input parameters. INFO is set to 0 if N \leq 0, or XTOL \leq 0.0, or MAXFEV \leq 0, or ML \leq 0, or MU \leq 0, or FACTOR \leq 0.0, or LDFJAC \leq N, or LR \leq (N*(N+1))/2.

Arithmetic interrupts. If these interrupts occur in the FCN subroutine during an early stage of the computation, they may be caused by an unacceptable choice of X by HYBRD. In this case, it may be possible to remedy the situation by rerunning HYBRD with a smaller value of FACTOR.

Excessive number of function evaluations. A reasonable value for MAXFEV is $200*(N+1)$. If the number of calls to FCN reaches MAXFEV, then this indicates that the routine is converging very slowly as measured by the progress of FVEC, and

INFO is set to 2. This situation should be unusual because, as indicated below, lack of good progress is usually diagnosed earlier by HYBRD, causing termination with INFO = 4 or INFO = 5.

Lack of good progress. HYBRD searches for a zero of the system by minimizing the sum of the squares of the functions. In so doing, it can become trapped in a region where the minimum does not correspond to a zero of the system and, in this situation, the iteration eventually fails to make good progress. In particular, this will happen if the system does not have a zero. If the system has a zero, rerunning HYBRD from a different starting point may be helpful.

6. Characteristics of the algorithm.

HYBRD is a modification of the Powell hybrid method. Two of its main characteristics involve the choice of the correction as a convex combination of the Newton and scaled gradient directions, and the updating of the Jacobian by the rank-1 method of Broyden. The choice of the correction guarantees (under reasonable conditions) global convergence for starting points far from the solution and a fast rate of convergence. The Jacobian is approximated by forward differences at the starting point, but forward differences are not used again until the rank-1 method fails to produce satisfactory progress.

Timing. The time required by HYBRD to solve a given problem depends on N , the behavior of the functions, the accuracy requested, and the starting point. The number of arithmetic operations needed by HYBRD is about $11.5 \cdot (N^2)$ to process each call to FCN. Unless FCN can be evaluated quickly, the timing of HYBRD will be strongly influenced by the time spent in FCN.

Storage. HYBRD requires $(3 \cdot N^2 + 17 \cdot N)/2$ double precision storage locations, in addition to the storage required by the program. There are no internally declared storage arrays.

7. Subprograms required.

USER-supplied FCN

MINPACK-supplied ... DOGLEG, DPMPAR, ENORM, FDJAC1,
QFORM, QRFAC, R1MPYQ, R1UPDT

FORTTRAN-supplied ... DABS, DMAX1, DMIN1, DSQRT, MINO, MOD

8. References.

M. J. D. Powell, A Hybrid Method for Nonlinear Equations.

Numerical Methods for Nonlinear Algebraic Equations,
P. Rabinowitz, editor. Gordon and Breach, 1970.

9. Example.

The problem is to determine the values of $x(1)$, $x(2)$, ..., $x(9)$, which solve the system of tridiagonal equations

$$\begin{aligned} (3-2x(1))x(1) & \quad -2x(2) & & = -1 \\ -x(i-1) + (3-2x(i))x(i) & \quad -2x(i+1) & = -1, & i=2-8 \\ & -x(8) + (3-2x(9))x(9) & = -1 \end{aligned}$$

```

C *****
C
C DRIVER FOR HYBRD EXAMPLE.
C DOUBLE PRECISION VERSION
C
C *****
C INTEGER J,N,MAXFEV,ML,MU,MODE,NPRINT,INFO,NFEV,LDFJAC,LR,NWRITE
C DOUBLE PRECISION XTOL,EPSFCN,FACTOR,FNORM
C DOUBLE PRECISION X(9),FVEC(9),DIAG(9),FJAC(9,9),R(45),QTF(9),
*      WA1(9),WA2(9),WA3(9),WA4(9)
C DOUBLE PRECISION ENORM,DPMPAR
C EXTERNAL FCN
C
C LOGICAL OUTPUT UNIT IS ASSUMED TO BE NUMBER 6.
C
C DATA NWRITE /6/
C
C N = 9
C
C THE FOLLOWING STARTING VALUES PROVIDE A ROUGH SOLUTION.
C
C DO 10 J = 1, 9
C   X(J) = -1.DO
10 CONTINUE
C
C LDFJAC = 9
C LR = 45
C
C SET XTOL TO THE SQUARE ROOT OF THE MACHINE PRECISION.
C UNLESS HIGH PRECISION SOLUTIONS ARE REQUIRED,
C THIS IS THE RECOMMENDED SETTING.
C
C XTOL = DSQRT(DPMPAR(1))
C
C MAXFEV = 2000
C ML = 1
C MU = 1
C EPSFCN = 0.DO
C MODE = 2
C DO 20 J = 1, 9
C   DIAG(J) = 1.DO

```

```

20    CONTINUE
    FACTOR = 1.D2
    NPRINT = 0
C
    CALL HYBRD(FCN,N,X,FVEC,XTOL,MAXFEV,ML,MU,EPSFCN,DIAG,
*             MODE,FACTOR,NPRINT,INFO,NFEV,FJAC,LDFJAC,
*             R,LR,QTF,WA1,WA2,WA3,WA4)
    FNORM = ENORM(N,FVEC)
    WRITE (NWRITE,1000) FNORM,NFEV,INFO,(X(J),J=1,N)
    STOP
1000 FORMAT (5X,31H FINAL L2 NORM OF THE RESIDUALS,D15.7 //
*          5X,31H NUMBER OF FUNCTION EVALUATIONS,I10 //
*          5X,15H EXIT PARAMETER,16X,I10 //
*          5X,27H FINAL APPROXIMATE SOLUTION // (5X,3D15.7))
C
C    LAST CARD OF DRIVER FOR HYBRD EXAMPLE.
C
    END
    SUBROUTINE FCN(N,X,FVEC,IFLAG)
    INTEGER N,IFLAG
    DOUBLE PRECISION X(N),FVEC(N)
C
C    SUBROUTINE FCN FOR HYBRD EXAMPLE.
C
    INTEGER K
    DOUBLE PRECISION ONE,TEMP,TEMP1,TEMP2,THREE,TWO,ZERO
    DATA ZERO,ONE,TWO,THREE /0.D0,1.D0,2.D0,3.D0/
C
    IF (IFLAG .NE. 0) GO TO 5
C
C    INSERT PRINT STATEMENTS HERE WHEN NPRINT IS POSITIVE.
C
    RETURN
5    CONTINUE
    DO 10 K = 1, N
        TEMP = (THREE - TWO*X(K))*X(K)
        TEMP1 = ZERO
        IF (K .NE. 1) TEMP1 = X(K-1)
        TEMP2 = ZERO
        IF (K .NE. N) TEMP2 = X(K+1)
        FVEC(K) = TEMP - TEMP1 - TWO*TEMP2 + ONE
10    CONTINUE
    RETURN
C
C    LAST CARD OF SUBROUTINE FCN.
C
    END

```

Results obtained with different compilers or machines
may be slightly different.

FINAL L2 NORM OF THE RESIDUALS 0.1192636D-07

NUMBER OF FUNCTION EVALUATIONS 14

EXIT PARAMETER

1

FINAL APPROXIMATE SOLUTION

-0.5706545D+00 -0.6816283D+00 -0.7017325D+00
-0.7042129D+00 -0.7013690D+00 -0.6918656D+00
-0.6657920D+00 -0.5960342D+00 -0.4164121D+00

Documentation for MINPACK subroutine HYBRJ1

Double precision version

Argonne National Laboratory

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March 1980

1. Purpose.

The purpose of HYBRJ1 is to find a zero of a system of N non-linear functions in N variables by a modification of the Powell hybrid method. This is done by using the more general nonlinear equation solver HYBRJ. The user must provide a subroutine which calculates the functions and the Jacobian.

2. Subroutine and type statements.

```
SUBROUTINE HYBRJ1(FCN,N,X,FVEC,FJAC,LDFJAC,TOL,INFO,WA,LWA)
INTEGER N,LDFJAC,INFO,LWA
DOUBLE PRECISION TOL
DOUBLE PRECISION X(N),FVEC(N),FJAC(LDFJAC,N),WA(LWA)
EXTERNAL FCN
```

3. Parameters.

Parameters designated as input parameters must be specified on entry to HYBRJ1 and are not changed on exit, while parameters designated as output parameters need not be specified on entry and are set to appropriate values on exit from HYBRJ1.

FCN is the name of the user-supplied subroutine which calculates the functions and the Jacobian. FCN must be declared in an EXTERNAL statement in the user calling program, and should be written as follows.

```
SUBROUTINE FCN(N,X,FVEC,FJAC,LDFJAC,IFLAG)
INTEGER N,LDFJAC,IFLAG
DOUBLE PRECISION X(N),FVEC(N),FJAC(LDFJAC,N)
-----
IF IFLAG = 1 CALCULATE THE FUNCTIONS AT X AND
RETURN THIS VECTOR IN FVEC. DO NOT ALTER FJAC.
IF IFLAG = 2 CALCULATE THE JACOBIAN AT X AND
RETURN THIS MATRIX IN FJAC. DO NOT ALTER FVEC.
-----
RETURN
END
```

The value of IFLAG should not be changed by FCN unless the

user wants to terminate execution of HYBRJ1. In this case set IFLAG to a negative integer.

N is a positive integer input variable set to the number of functions and variables.

X is an array of length N. On input X must contain an initial estimate of the solution vector. On output X contains the final estimate of the solution vector.

FVEC is an output array of length N which contains the functions evaluated at the output X.

FJAC is an output N by N array which contains the orthogonal matrix Q produced by the QR factorization of the final approximate Jacobian. Section 6 contains more details about the approximation to the Jacobian.

LDFJAC is a positive integer input variable not less than N which specifies the leading dimension of the array FJAC.

TOL is a nonnegative input variable. Termination occurs when the algorithm estimates that the relative error between X and the solution is at most TOL. Section 4 contains more details about TOL.

INFO is an integer output variable. If the user has terminated execution, INFO is set to the (negative) value of IFLAG. See description of FCN. Otherwise, INFO is set as follows.

INFO = 0 Improper input parameters.

INFO = 1 Algorithm estimates that the relative error between X and the solution is at most TOL.

INFO = 2 Number of calls to FCN with IFLAG = 1 has reached $100 \cdot (N+1)$.

INFO = 3 TOL is too small. No further improvement in the approximate solution X is possible.

INFO = 4 Iteration is not making good progress.

Sections 4 and 5 contain more details about INFO.

WA is a work array of length LWA.

LWA is a positive integer input variable not less than $(N \cdot (N+13))/2$.

4. Successful completion.

The accuracy of HYBRJ1 is controlled by the convergence

parameter TOL. This parameter is used in a test which makes a comparison between the approximation X and a solution XSOL. HYBRJ1 terminates when the test is satisfied. If TOL is less than the machine precision (as defined by the MINPACK function DPMPAR(1)), then HYBRJ1 only attempts to satisfy the test defined by the machine precision. Further progress is not usually possible. Unless high precision solutions are required, the recommended value for TOL is the square root of the machine precision.

The test assumes that the functions and the Jacobian are coded consistently, and that the functions are reasonably well behaved. If these conditions are not satisfied, then HYBRJ1 may incorrectly indicate convergence. The coding of the Jacobian can be checked by the MINPACK subroutine CHKDER. If the Jacobian is coded correctly, then the validity of the answer can be checked, for example, by rerunning HYBRJ1 with a tighter tolerance.

Convergence test. If $ENORM(Z)$ denotes the Euclidean norm of a vector Z, then this test attempts to guarantee that

$$ENORM(X-XSOL) \leq TOL * ENORM(XSOL).$$

If this condition is satisfied with $TOL = 10^{*(-K)}$, then the larger components of X have K significant decimal digits and INFO is set to 1. There is a danger that the smaller components of X may have large relative errors, but the fast rate of convergence of HYBRJ1 usually avoids this possibility.

5. Unsuccessful completion.

Unsuccessful termination of HYBRJ1 can be due to improper input parameters, arithmetic interrupts, an excessive number of function evaluations, or lack of good progress.

Improper input parameters. INFO is set to 0 if $N \leq 0$, or $LDFJAC \leq N$, or $TOL \leq 0.0$, or $LWA \leq (N*(N+13))/2$.

Arithmetic interrupts. If these interrupts occur in the FCN subroutine during an early stage of the computation, they may be caused by an unacceptable choice of X by HYBRJ1. In this case, it may be possible to remedy the situation by not evaluating the functions here, but instead setting the components of FVEC to numbers that exceed those in the initial FVEC, thereby indirectly reducing the step length. The step length can be more directly controlled by using instead HYBRJ, which includes in its calling sequence the step-length-governing parameter FACTOR.

Excessive number of function evaluations. If the number of calls to FCN with IFLAG = 1 reaches $100*(N+1)$, then this indicates that the routine is converging very slowly as measured

by the progress of FVEC, and INFO is set to 2. This situation should be unusual because, as indicated below, lack of good progress is usually diagnosed earlier by HYBRJ1, causing termination with INFO = 4.

Lack of good progress. HYBRJ1 searches for a zero of the system by minimizing the sum of the squares of the functions. In so doing, it can become trapped in a region where the minimum does not correspond to a zero of the system and, in this situation, the iteration eventually fails to make good progress. In particular, this will happen if the system does not have a zero. If the system has a zero, rerunning HYBRJ1 from a different starting point may be helpful.

6. Characteristics of the algorithm.

HYBRJ1 is a modification of the Powell hybrid method. Two of its main characteristics involve the choice of the correction as a convex combination of the Newton and scaled gradient directions, and the updating of the Jacobian by the rank-1 method of Broyden. The choice of the correction guarantees (under reasonable conditions) global convergence for starting points far from the solution and a fast rate of convergence. The Jacobian is calculated at the starting point, but it is not recalculated until the rank-1 method fails to produce satisfactory progress.

Timing. The time required by HYBRJ1 to solve a given problem depends on N, the behavior of the functions, the accuracy requested, and the starting point. The number of arithmetic operations needed by HYBRJ1 is about $11.5*(N^2)$ to process each evaluation of the functions (call to FCN with IFLAG = 1) and $1.3*(N^3)$ to process each evaluation of the Jacobian (call to FCN with IFLAG = 2). Unless FCN can be evaluated quickly, the timing of HYBRJ1 will be strongly influenced by the time spent in FCN.

Storage. HYBRJ1 requires $(3*N^2 + 17*N)/2$ double precision storage locations, in addition to the storage required by the program. There are no internally declared storage arrays.

7. Subprograms required.

USER-supplied FCN

MINPACK-supplied ... DOGLEG, DPMPAR, ENORM, HYBRJ,
QFORM, QRFAC, R1MPYQ, R1UPDT

FORTTRAN-supplied ... DABS, DMAX1, DMIN1, DSQRT, MINO, MOD

8. References.

M. J. D. Powell, A Hybrid Method for Nonlinear Equations.
 Numerical Methods for Nonlinear Algebraic Equations,
 P. Rabinowitz, editor. Gordon and Breach, 1970.

9. Example.

The problem is to determine the values of $x(1)$, $x(2)$, ..., $x(9)$, which solve the system of tridiagonal equations

$$\begin{aligned} (3-2*x(1))*x(1) & \quad -2*x(2) & & = -1 \\ -x(i-1) + (3-2*x(i))*x(i) & & -2*x(i+1) & = -1, \quad i=2-8 \\ & -x(8) + (3-2*x(9))*x(9) & & = -1 \end{aligned}$$

```

C *****
C
C DRIVER FOR HYBRJ1 EXAMPLE.
C DOUBLE PRECISION VERSION
C
C *****
C INTEGER J,N,LDFJAC,INFO,LWA,NWRITE
C DOUBLE PRECISION TOL,FNORM
C DOUBLE PRECISION X(9),FVEC(9),FJAC(9,9),WA(99)
C DOUBLE PRECISION ENORM,DPMPAR
C EXTERNAL FCN
C
C LOGICAL OUTPUT UNIT IS ASSUMED TO BE NUMBER 6.
C
C DATA NWRITE /6/
C
C N = 9
C
C THE FOLLOWING STARTING VALUES PROVIDE A ROUGH SOLUTION.
C
C DO 10 J = 1, 9
C   X(J) = -1.DO
10 CONTINUE
C
C LDFJAC = 9
C LWA = 99
C
C SET TOL TO THE SQUARE ROOT OF THE MACHINE PRECISION.
C UNLESS HIGH PRECISION SOLUTIONS ARE REQUIRED,
C THIS IS THE RECOMMENDED SETTING.
C
C TOL = DSQRT(DPMPAR(1))
C
C CALL HYBRJ1(FCN,N,X,FVEC,FJAC,LDFJAC,TOL,INFO,WA,LWA)
C FNORM = ENORM(N,FVEC)
C WRITE (NWRITE,1000) FNORM,INFO,(X(J),J=1,N)
C STOP
1000 FORMAT (5X,31H FINAL L2 NORM OF THE RESIDUALS,D15.7 //
*          5X,15H EXIT PARAMETER,16X,I10 //
*          5X,27H FINAL APPROXIMATE SOLUTION // (5X,3D15.7))

```



```

C
C LAST CARD OF DRIVER FOR HYBRJ1 EXAMPLE.
C
END
SUBROUTINE FCN(N,X,FVEC,FJAC,LDFJAC,IFLAG)
INTEGER N,LDFJAC,IFLAG
DOUBLE PRECISION X(N),FVEC(N),FJAC(LDFJAC,N)
C
C SUBROUTINE FCN FOR HYBRJ1 EXAMPLE.
C
INTEGER J,K
DOUBLE PRECISION ONE,TEMP,TEMP1,TEMP2,THREE,TWO,ZERO
DATA ZERO,ONE,TWO,THREE,FOUR /0.DO,1.DO,2.DO,3.DO,4.DO/
C
IF (IFLAG .EQ. 2) GO TO 20
DO 10 K = 1, N
  TEMP = (THREE - TWO*X(K))*X(K)
  TEMP1 = ZERO
  IF (K .NE. 1) TEMP1 = X(K-1)
  TEMP2 = ZERO
  IF (K .NE. N) TEMP2 = X(K+1)
  FVEC(K) = TEMP - TEMP1 - TWO*TEMP2 + ONE
10 CONTINUE
GO TO 50
20 CONTINUE
DO 40 K = 1, N
  DO 30 J = 1, N
    FJAC(K,J) = ZERO
30 CONTINUE
  FJAC(K,K) = THREE - FOUR*X(K)
  IF (K .NE. 1) FJAC(K,K-1) = -ONE
  IF (K .NE. N) FJAC(K,K+1) = -TWO
40 CONTINUE
50 CONTINUE
RETURN
C
C LAST CARD OF SUBROUTINE FCN.
C
END

```

Results obtained with different compilers or machines
may be slightly different.

FINAL L2 NORM OF THE RESIDUALS 0.1192636D-07

EXIT PARAMETER 1

FINAL APPROXIMATE SOLUTION

```

-0.5706545D+00 -0.6816283D+00 -0.7017325D+00
-0.7042129D+00 -0.7013690D+00 -0.6918656D+00
-0.6657920D+00 -0.5960342D+00 -0.4164121D+00

```

Documentation for MINPACK subroutine HYBRJ

Double precision version

Argonne National Laboratory

Burton S. Garbow, Kenneth E. Hillstom, Jorge J. More

March 1980

1. Purpose.

The purpose of HYBRJ is to find a zero of a system of N non-linear functions in N variables by a modification of the Powell hybrid method. The user must provide a subroutine which calculates the functions and the Jacobian.

2. Subroutine and type statements.

```

SUBROUTINE HYBRJ(FCN,N,X,FVEC,FJAC,LDFJAC,XTOL,MAXFEV,DIAG,
*              MODE,FACTOR,NPRINT,INFO,NFEV,NJEV,R,LR,QTF,
*              WA1,WA2,WA3,WA4)
  INTEGER N,LDFJAC,MAXFEV,MODE,NPRINT,INFO,NFEV,NJEV,LR
  DOUBLE PRECISION XTOL,FACTOR
  DOUBLE PRECISION X(N),FVEC(N),FJAC(LDFJAC,N),DIAG(N),R(LR),QTF(N),
*              WA1(N),WA2(N),WA3(N),WA4(N)

```

3. Parameters.

Parameters designated as input parameters must be specified on entry to HYBRJ and are not changed on exit, while parameters designated as output parameters need not be specified on entry and are set to appropriate values on exit from HYBRJ.

FCN is the name of the user-supplied subroutine which calculates the functions and the Jacobian. FCN must be declared in an EXTERNAL statement in the user calling program, and should be written as follows.

```

SUBROUTINE FCN(N,X,FVEC,FJAC,LDFJAC,IFLAG)
  INTEGER N,LDFJAC,IFLAG
  DOUBLE PRECISION X(N),FVEC(N),FJAC(LDFJAC,N)
  -----
  IF IFLAG = 1 CALCULATE THE FUNCTIONS AT X AND
  RETURN THIS VECTOR IN FVEC.  DO NOT ALTER FJAC.
  IF IFLAG = 2 CALCULATE THE JACOBIAN AT X AND
  RETURN THIS MATRIX IN FJAC.  DO NOT ALTER FVEC.
  -----
  RETURN
  END

```

The value of IFLAG should not be changed by FCN unless the user wants to terminate execution of HYBRJ. In this case set IFLAG to a negative integer.

N is a positive integer input variable set to the number of functions and variables.

X is an array of length N. On input X must contain an initial estimate of the solution vector. On output X contains the final estimate of the solution vector.

FVEC is an output array of length N which contains the functions evaluated at the output X.

FJAC is an output N by N array which contains the orthogonal matrix Q produced by the QR factorization of the final approximate Jacobian. Section 6 contains more details about the approximation to the Jacobian.

LDFJAC is a positive integer input variable not less than N which specifies the leading dimension of the array FJAC.

XTOL is a nonnegative input variable. Termination occurs when the relative error between two consecutive iterates is at most XTOL. Therefore, XTOL measures the relative error desired in the approximate solution. Section 4 contains more details about XTOL.

MAXFEV is a positive integer input variable. Termination occurs when the number of calls to FCN with IFLAG = 1 has reached MAXFEV.

DIAG is an array of length N. If MODE = 1 (see below), DIAG is internally set. If MODE = 2, DIAG must contain positive entries that serve as multiplicative scale factors for the variables.

MODE is an integer input variable. If MODE = 1, the variables will be scaled internally. If MODE = 2, the scaling is specified by the input DIAG. Other values of MODE are equivalent to MODE = 1.

FACTOR is a positive input variable used in determining the initial step bound. This bound is set to the product of FACTOR and the Euclidean norm of DIAG*X if nonzero, or else to FACTOR itself. In most cases FACTOR should lie in the interval (.1,100.). 100. is a generally recommended value.

NPRINT is an integer input variable that enables controlled printing of iterates if it is positive. In this case, FCN is called with IFLAG = 0 at the beginning of the first iteration and every NPRINT iterations thereafter and immediately prior to return, with X and FVEC available for printing. FVEC and FJAC should not be altered. If NPRINT is not positive, no

special calls of FCN with IFLAG = 0 are made.

INFO is an integer output variable. If the user has terminated execution, INFO is set to the (negative) value of IFLAG. See description of FCN. Otherwise, INFO is set as follows.

INFO = 0 Improper input parameters.

INFO = 1 Relative error between two consecutive iterates is at most XTOL.

INFO = 2 Number of calls to FCN with IFLAG = 1 has reached MAXFEV.

INFO = 3 XTOL is too small. No further improvement in the approximate solution X is possible.

INFO = 4 Iteration is not making good progress, as measured by the improvement from the last five Jacobian evaluations.

INFO = 5 Iteration is not making good progress, as measured by the improvement from the last ten iterations.

Sections 4 and 5 contain more details about INFO.

NFEV is an integer output variable set to the number of calls to FCN with IFLAG = 1.

NJEV is an integer output variable set to the number of calls to FCN with IFLAG = 2.

R is an output array of length LR which contains the upper triangular matrix produced by the QR factorization of the final approximate Jacobian, stored rowwise.

LR is a positive integer input variable not less than $(N*(N+1))/2$.

QTF is an output array of length N which contains the vector $(Q \text{ transpose}) * FVEC$.

WA1, WA2, WA3, and WA4 are work arrays of length N.

4. Successful completion.

The accuracy of HYBRJ is controlled by the convergence parameter XTOL. This parameter is used in a test which makes a comparison between the approximation X and a solution XSOL. HYBRJ terminates when the test is satisfied. If the convergence parameter is less than the machine precision (as defined by the MINPACK function DPMPPAR(1)), then HYBRJ only attempts to satisfy the test defined by the machine precision. Further progress is not

usually possible.

The test assumes that the functions and the Jacobian are coded consistently, and that the functions are reasonably well behaved. If these conditions are not satisfied, then HYBRJ may incorrectly indicate convergence. The coding of the Jacobian can be checked by the MINPACK subroutine CHKDER. If the Jacobian is coded correctly, then the validity of the answer can be checked, for example, by rerunning HYBRJ with a tighter tolerance.

Convergence test. If $ENORM(Z)$ denotes the Euclidean norm of a vector Z and D is the diagonal matrix whose entries are defined by the array $DIAG$, then this test attempts to guarantee that

$$ENORM(D*(X-XSOL)) \leq XTOL*ENORM(D*XSOL).$$

If this condition is satisfied with $XTOL = 10^{*(-K)}$, then the larger components of $D*X$ have K significant decimal digits and $INFO$ is set to 1. There is a danger that the smaller components of $D*X$ may have large relative errors, but the fast rate of convergence of HYBRJ usually avoids this possibility. Unless high precision solutions are required, the recommended value for $XTOL$ is the square root of the machine precision.

5. Unsuccessful completion.

Unsuccessful termination of HYBRJ can be due to improper input parameters, arithmetic interrupts, an excessive number of function evaluations, or lack of good progress.

Improper input parameters. $INFO$ is set to 0 if $N \leq 0$, or $LDFJAC \leq N$, or $XTOL \leq 0.00$, or $MAXFEV \leq 0$, or $FACTOR \leq 0.00$, or $LR \leq (N*(N+1))/2$.

Arithmetic interrupts. If these interrupts occur in the FCN subroutine during an early stage of the computation, they may be caused by an unacceptable choice of X by HYBRJ. In this case, it may be possible to remedy the situation by rerunning HYBRJ with a smaller value of $FACTOR$.

Excessive number of function evaluations. A reasonable value for $MAXFEV$ is $100*(N+1)$. If the number of calls to FCN with $IFLAG = 1$ reaches $MAXFEV$, then this indicates that the routine is converging very slowly as measured by the progress of $FVEC$, and $INFO$ is set to 2. This situation should be unusual because, as indicated below, lack of good progress is usually diagnosed earlier by HYBRJ, causing termination with $INFO = 4$ or $INFO = 5$.

Lack of good progress. HYBRJ searches for a zero of the system by minimizing the sum of the squares of the functions. In so

doing, it can become trapped in a region where the minimum does not correspond to a zero of the system and, in this situation, the iteration eventually fails to make good progress. In particular, this will happen if the system does not have a zero. If the system has a zero, rerunning HYBRJ from a different starting point may be helpful.

6. Characteristics of the algorithm.

HYBRJ is a modification of the Powell hybrid method. Two of its main characteristics involve the choice of the correction as a convex combination of the Newton and scaled gradient directions, and the updating of the Jacobian by the rank-1 method of Broyden. The choice of the correction guarantees (under reasonable conditions) global convergence for starting points far from the solution and a fast rate of convergence. The Jacobian is calculated at the starting point, but it is not recalculated until the rank-1 method fails to produce satisfactory progress.

Timing. The time required by HYBRJ to solve a given problem depends on N , the behavior of the functions, the accuracy requested, and the starting point. The number of arithmetic operations needed by HYBRJ is about $11.5*(N^2)$ to process each evaluation of the functions (call to FCN with IFLAG = 1) and $1.3*(N^3)$ to process each evaluation of the Jacobian (call to FCN with IFLAG = 2). Unless FCN can be evaluated quickly, the timing of HYBRJ will be strongly influenced by the time spent in FCN.

Storage. HYBRJ requires $(3*N^2 + 17*N)/2$ double precision storage locations, in addition to the storage required by the program. There are no internally declared storage arrays.

7. Subprograms required.

USER-supplied FCN

MINPACK-supplied ... DOGLEG, DPMPAR, ENORM,
QFORM, QRFAC, R1MPYQ, R1UPDT

FORTTRAN-supplied ... DABS, DMAX1, DMIN1, DSQRT, MIN0, MOD

8. References.

M. J. D. Powell, A Hybrid Method for Nonlinear Equations.
Numerical Methods for Nonlinear Algebraic Equations,
P. Rabinowitz, editor. Gordon and Breach, 1970.

9. Example.

The problem is to determine the values of $x(1)$, $x(2)$, ..., $x(9)$, which solve the system of tridiagonal equations

$$\begin{aligned} (3-2x(1))x(1) & -2x(2) & & = -1 \\ -x(i-1) + (3-2x(i))x(i) & & -2x(i+1) & = -1, \quad i=2-8 \\ & -x(8) + (3-2x(9))x(9) & & = -1 \end{aligned}$$

DRIVER FOR HYBRJ EXAMPLE.
DOUBLE PRECISION VERSION

INTEGER J,N,LDFJAC,MAXFEV,MODE,NPRINT,INFO,NFEV,NJEV,LR,NWRITE
DOUBLE PRECISION XTOL,FACTOR,FNORM
DOUBLE PRECISION X(9),FVEC(9),FJAC(9,9),DIAG(9),R(45),QTF(9),
* WA1(9),WA2(9),WA3(9),WA4(9)
DOUBLE PRECISION ENORM,DPMPAR
EXTERNAL FCN

LOGICAL OUTPUT UNIT IS ASSUMED TO BE NUMBER 6.

DATA NWRITE /6/

N = 9

THE FOLLOWING STARTING VALUES PROVIDE A ROUGH SOLUTION.

DO 10 J = 1, 9
X(J) = -1.DO

10 CONTINUE

LDFJAC = 9
LR = 45

SET XTOL TO THE SQUARE ROOT OF THE MACHINE PRECISION.
UNLESS HIGH PRECISION SOLUTIONS ARE REQUIRED,
THIS IS THE RECOMMENDED SETTING.

XTOL = DSQRT(DPMPAR(1))

MAXFEV = 1000
MODE = 2
DO 20 J = 1, 9
DIAG(J) = 1.DO
20 CONTINUE
FACTOR = 1.D2
NPRINT = 0

CALL HYBRJ(FCN,N,X,FVEC,FJAC,LDFJAC,XTOL,MAXFEV,DIAG,
* MODE,FACTOR,NPRINT,INFO,NFEV,NJEV,R,LR,QTF,
* WA1,WA2,WA3,WA4)
FNORM = ENORM(N,FVEC)
WRITE (NWRITE,1000) FNORM,NFEV,NJEV,INFO,(X(J),J=1,N)

```

      STOP
1000 FORMAT (5X,31H FINAL L2 NORM OF THE RESIDUALS,D15.7 //
*          5X,31H NUMBER OF FUNCTION EVALUATIONS,I10 //
*          5X,31H NUMBER OF JACOBIAN EVALUATIONS,I10 //
*          5X,15H EXIT PARAMETER,16X,I10 //
*          5X,27H FINAL APPROXIMATE SOLUTION // (5X,3D15.7))

C
C      LAST CARD OF DRIVER FOR HYBRJ EXAMPLE.
C

      END
      SUBROUTINE FCN(N,X,FVEC,FJAC,LDFJAC,IFLAG)
      INTEGER N,LDFJAC,IFLAG
      DOUBLE PRECISION X(N),FVEC(N),FJAC(LDFJAC,N)

C
C      SUBROUTINE FCN FOR HYBRJ EXAMPLE.
C

      INTEGER J,K
      DOUBLE PRECISION ONE,TEMP,TEMP1,TEMP2,THREE,TWO,ZERO
      DATA ZERO,ONE,TWO,THREE,FOUR /0.DO,1.DO,2.DO,3.DO,4.DO/

C
      IF (IFLAG .NE. 0) GO TO 5

C
C      INSERT PRINT STATEMENTS HERE WHEN NPRINT IS POSITIVE.
C

      RETURN
5  CONTINUE
      IF (IFLAG .EQ. 2) GO TO 20
      DO 10 K = 1, N
          TEMP = (THREE - TWO*X(K))*X(K)
          TEMP1 = ZERO
          IF (K .NE. 1) TEMP1 = X(K-1)
          TEMP2 = ZERO
          IF (K .NE. N) TEMP2 = X(K+1)
          FVEC(K) = TEMP - TEMP1 - TWO*TEMP2 + ONE
10     CONTINUE
          GO TO 50
20  CONTINUE
      DO 40 K = 1, N
          DO 30 J = 1, N
              FJAC(K,J) = ZERO
30     CONTINUE
          FJAC(K,K) = THREE - FOUR*X(K)
          IF (K .NE. 1) FJAC(K,K-1) = -ONE
          IF (K .NE. N) FJAC(K,K+1) = -TWO
40     CONTINUE
50  CONTINUE
      RETURN

C
C      LAST CARD OF SUBROUTINE FCN.
C

      END

```

Results obtained with different compilers or machines
may be slightly different.

FINAL L2 NORM OF THE RESIDUALS 0.1192636D-07

NUMBER OF FUNCTION EVALUATIONS 11

NUMBER OF JACOBIAN EVALUATIONS 1

EXIT PARAMETER 1

FINAL APPROXIMATE SOLUTION

-0.5706545D+00 -0.6816283D+00 -0.7017325D+00

-0.7042129D+00 -0.7013690D+00 -0.6918656D+00

-0.6657920D+00 -0.5960342D+00 -0.4164121D+00

Documentation for MINPACK subroutine LMDER1

Double precision version

Argonne National Laboratory

Burton S. Garbow, Kenneth E. Hillstom, Jorge J. More

March 1980

1. Purpose.

The purpose of LMDER1 is to minimize the sum of the squares of M nonlinear functions in N variables by a modification of the Levenberg-Marquardt algorithm. This is done by using the more general least-squares solver LMDER. The user must provide a subroutine which calculates the functions and the Jacobian.

2. Subroutine and type statements.

```
SUBROUTINE LMDER1(FCN,M,N,X,FVEC,FJAC,LDFJAC,TOL,
*                INFO,IPVT,WA,LWA)
INTEGER M,N,LDFJAC,INFO,LWA
INTEGER IPVT(N)
DOUBLE PRECISION TOL
DOUBLE PRECISION X(N),FVEC(M),FJAC(LDFJAC,N),WA(LWA)
EXTERNAL FCN
```

3. Parameters.

Parameters designated as input parameters must be specified on entry to LMDER1 and are not changed on exit, while parameters designated as output parameters need not be specified on entry and are set to appropriate values on exit from LMDER1.

FCN is the name of the user-supplied subroutine which calculates the functions and the Jacobian. FCN must be declared in an EXTERNAL statement in the user calling program, and should be written as follows.

```
SUBROUTINE FCN(M,N,X,FVEC,FJAC,LDFJAC,IFLAG)
INTEGER M,N,LDFJAC,IFLAG
DOUBLE PRECISION X(N),FVEC(M),FJAC(LDFJAC,N)
-----
IF IFLAG = 1 CALCULATE THE FUNCTIONS AT X AND
RETURN THIS VECTOR IN FVEC. DO NOT ALTER FJAC.
IF IFLAG = 2 CALCULATE THE JACOBIAN AT X AND
RETURN THIS MATRIX IN FJAC. DO NOT ALTER FVEC.
-----
RETURN
END
```

The value of IFLAG should not be changed by FCN unless the user wants to terminate execution of LMDER1. In this case set IFLAG to a negative integer.

M is a positive integer input variable set to the number of functions.

N is a positive integer input variable set to the number of variables. N must not exceed M.

X is an array of length N. On input X must contain an initial estimate of the solution vector. On output X contains the final estimate of the solution vector.

FVEC is an output array of length M which contains the functions evaluated at the output X.

FJAC is an output M by N array. The upper N by N submatrix of FJAC contains an upper triangular matrix R with diagonal elements of nonincreasing magnitude such that

$$P^T (JAC^T JAC) P = R^T R,$$

where P is a permutation matrix and JAC is the final calculated Jacobian. Column j of P is column IPVT(j) (see below) of the identity matrix. The lower trapezoidal part of FJAC contains information generated during the computation of R.

LDFJAC is a positive integer input variable not less than M which specifies the leading dimension of the array FJAC.

TOL is a nonnegative input variable. Termination occurs when the algorithm estimates either that the relative error in the sum of squares is at most TOL or that the relative error between X and the solution is at most TOL. Section 4 contains more details about TOL.

INFO is an integer output variable. If the user has terminated execution, INFO is set to the (negative) value of IFLAG. See description of FCN. Otherwise, INFO is set as follows.

INFO = 0 Improper input parameters.

INFO = 1 Algorithm estimates that the relative error in the sum of squares is at most TOL.

INFO = 2 Algorithm estimates that the relative error between X and the solution is at most TOL.

INFO = 3 Conditions for INFO = 1 and INFO = 2 both hold.

INFO = 4 FVEC is orthogonal to the columns of the Jacobian to machine precision.

INFO = 5 Number of calls to FCN with IFLAG = 1 has reached $100*(N+1)$.

INFO = 6 TOL is too small. No further reduction in the sum of squares is possible.

INFO = 7 TOL is too small. No further improvement in the approximate solution X is possible.

Sections 4 and 5 contain more details about INFO.

IPVT is an integer output array of length N. IPVT defines a permutation matrix P such that $JAC*P = Q*R$, where JAC is the final calculated Jacobian, Q is orthogonal (not stored), and R is upper triangular with diagonal elements of nonincreasing magnitude. Column j of P is column IPVT(j) of the identity matrix.

WA is a work array of length LWA.

LWA is a positive integer input variable not less than $5*N+M$.

4. Successful completion.

The accuracy of LMDER1 is controlled by the convergence parameter TOL. This parameter is used in tests which make three types of comparisons between the approximation X and a solution XSOL. LMDER1 terminates when any of the tests is satisfied. If TOL is less than the machine precision (as defined by the MINPACK function DPMPAR(1)), then LMDER1 only attempts to satisfy the test defined by the machine precision. Further progress is not usually possible. Unless high precision solutions are required, the recommended value for TOL is the square root of the machine precision.

The tests assume that the functions and the Jacobian are coded consistently, and that the functions are reasonably well behaved. If these conditions are not satisfied, then LMDER1 may incorrectly indicate convergence. The coding of the Jacobian can be checked by the MINPACK subroutine CHKDER. If the Jacobian is coded correctly, then the validity of the answer can be checked, for example, by rerunning LMDER1 with a tighter tolerance.

First convergence test. If ENORM(Z) denotes the Euclidean norm of a vector Z, then this test attempts to guarantee that

$$ENORM(FVEC) \leq (1+TOL)*ENORM(FVECS),$$

where FVECS denotes the functions evaluated at XSOL. If this condition is satisfied with $TOL = 10^{*-K}$, then the final residual norm ENORM(FVEC) has K significant decimal digits and INFO is set to 1 (or to 3 if the second test is also

satisfied).

Second convergence test. If D is a diagonal matrix (implicitly generated by LMDER1) whose entries contain scale factors for the variables, then this test attempts to guarantee that

$$\text{ENORM}(D*(X-XSOL)) \leq \text{TOL} * \text{ENORM}(D*XSOL).$$

If this condition is satisfied with $\text{TOL} = 10^{*(-K)}$, then the larger components of $D*X$ have K significant decimal digits and INFO is set to 2 (or to 3 if the first test is also satisfied). There is a danger that the smaller components of $D*X$ may have large relative errors, but the choice of D is such that the accuracy of the components of X is usually related to their sensitivity.

Third convergence test. This test is satisfied when FVEC is orthogonal to the columns of the Jacobian to machine precision. There is no clear relationship between this test and the accuracy of LMDER1, and furthermore, the test is equally well satisfied at other critical points, namely maximizers and saddle points. Therefore, termination caused by this test (INFO = 4) should be examined carefully.

5. Unsuccessful completion.

Unsuccessful termination of LMDER1 can be due to improper input parameters, arithmetic interrupts, or an excessive number of function evaluations.

Improper input parameters. INFO is set to 0 if N \leq 0, or M \leq N, or LDFJAC \leq M, or TOL \leq 0.00, or LWA \leq 5*N+M.

Arithmetic interrupts. If these interrupts occur in the FCN subroutine during an early stage of the computation, they may be caused by an unacceptable choice of X by LMDER1. In this case, it may be possible to remedy the situation by not evaluating the functions here, but instead setting the components of FVEC to numbers that exceed those in the initial FVEC, thereby indirectly reducing the step length. The step length can be more directly controlled by using instead LMDER, which includes in its calling sequence the step-length-governing parameter FACTOR.

Excessive number of function evaluations. If the number of calls to FCN with IFLAG = 1 reaches $100*(N+1)$, then this indicates that the routine is converging very slowly as measured by the progress of FVEC, and INFO is set to 5. In this case, it may be helpful to restart LMDER1, thereby forcing it to disregard old (and possibly harmful) information.

6. Characteristics of the algorithm.

LMDER1 is a modification of the Levenberg-Marquardt algorithm. Two of its main characteristics involve the proper use of implicitly scaled variables and an optimal choice for the correction. The use of implicitly scaled variables achieves scale invariance of LMDER1 and limits the size of the correction in any direction where the functions are changing rapidly. The optimal choice of the correction guarantees (under reasonable conditions) global convergence from starting points far from the solution and a fast rate of convergence for problems with small residuals.

Timing. The time required by LMDER1 to solve a given problem depends on M and N, the behavior of the functions, the accuracy requested, and the starting point. The number of arithmetic operations needed by LMDER1 is about N^3 to process each evaluation of the functions (call to FCN with IFLAG = 1) and $M(N^2)$ to process each evaluation of the Jacobian (call to FCN with IFLAG = 2). Unless FCN can be evaluated quickly, the timing of LMDER1 will be strongly influenced by the time spent in FCN.

Storage. LMDER1 requires $M \cdot N + 2 \cdot M + 6 \cdot N$ double precision storage locations and N integer storage locations, in addition to the storage required by the program. There are no internally declared storage arrays.

7. Subprograms required.

USER-supplied FCN

MINPACK-supplied ... DPMPAR, ENORM, LMDER, LMPAR, QRFAC, QRSOLV

FORTTRAN-supplied ... DABS, DMAX1, DMIN1, DSQRT, MOD

8. References.

Jorge J. More, The Levenberg-Marquardt Algorithm, Implementation and Theory. Numerical Analysis, G. A. Watson, editor. Lecture Notes in Mathematics 630, Springer-Verlag, 1977.

9. Example.

The problem is to determine the values of $x(1)$, $x(2)$, and $x(3)$ which provide the best fit (in the least squares sense) of

$$x(1) + u(i)/(v(i)*x(2) + w(i)*x(3)), \quad i = 1, 15$$

to the data

$$y = (0.14, 0.18, 0.22, 0.25, 0.29, 0.32, 0.35, 0.39, \\ 0.37, 0.58, 0.73, 0.96, 1.34, 2.10, 4.39),$$

where $u(i) = i$, $v(i) = 16 - i$, and $w(i) = \min(u(i), v(i))$. The i -th component of FVEC is thus defined by

$$y(i) = (x(1) + u(i)/(v(i)*x(2) + w(i)*x(3))).$$

```

C *****
C
C DRIVER FOR LMDER1 EXAMPLE.
C DOUBLE PRECISION VERSION
C
C *****
C INTEGER J,M,N,LDFJAC,INFO,LWA,NWRITE
C INTEGER IPV(3)
C DOUBLE PRECISION TOL,FNORM
C DOUBLE PRECISION X(3),FVEC(15),FJAC(15,3),WA(30)
C DOUBLE PRECISION ENORM,DPMPAR
C EXTERNAL FCN
C
C LOGICAL OUTPUT UNIT IS ASSUMED TO BE NUMBER 6.
C
C DATA NWRITE /6/
C
C M = 15
C N = 3
C
C THE FOLLOWING STARTING VALUES PROVIDE A ROUGH FIT.
C
C X(1) = 1.DO
C X(2) = 1.DO
C X(3) = 1.DO
C
C LDFJAC = 15
C LWA = 30
C
C SET TOL TO THE SQUARE ROOT OF THE MACHINE PRECISION.
C UNLESS HIGH PRECISION SOLUTIONS ARE REQUIRED,
C THIS IS THE RECOMMENDED SETTING.
C
C TOL = DSQRT(DPMPAR(1))
C
C CALL LMDER1(FCN,M,N,X,FVEC,FJAC,LDFJAC,TOL,
*          INFO,IPVT,WA,LWA)
C FNORM = ENORM(M,FVEC)
C WRITE (NWRITE,1000) FNORM,INFO,(X(J),J=1,N)
C STOP
1000 FORMAT (5X,31H FINAL L2 NORM OF THE RESIDUALS,D15.7 //
*          5X,15H EXIT PARAMETER,16X,I10 //
*          5X,27H FINAL APPROXIMATE SOLUTION // 5X,3D15.7)
C
C LAST CARD OF DRIVER FOR LMDER1 EXAMPLE.
C
C
```

END

SUBROUTINE FCN(M,N,X,FVEC,FJAC,LDFJAC,IFLAG)

INTEGER M,N,LDFJAC,IFLAG

DOUBLE PRECISION X(N),FVEC(M),FJAC(LDFJAC,N)

SUBROUTINE FCN FOR LMDER1 EXAMPLE.

INTEGER I

DOUBLE PRECISION TMP1,TMP2,TMP3,TMP4

DOUBLE PRECISION Y(15)

DATA Y(1),Y(2),Y(3),Y(4),Y(5),Y(6),Y(7),Y(8),

* Y(9),Y(10),Y(11),Y(12),Y(13),Y(14),Y(15)

* /1.4D-1,1.8D-1,2.2D-1,2.5D-1,2.9D-1,3.2D-1,3.5D-1,3.9D-1,

* 3.7D-1,5.8D-1,7.3D-1,9.6D-1,1.34D0,2.1D0,4.39D0/

IF (IFLAG .EQ. 2) GO TO 20

DO 10 I = 1, 15

 TMP1 = I

 TMP2 = 16 - I

 TMP3 = TMP1

 IF (I .GT. 8) TMP3 = TMP2

 FVEC(I) = Y(I) - (X(1) + TMP1/(X(2)*TMP2 + X(3)*TMP3))

10 CONTINUE

GO TO 40

20 CONTINUE

DO 30 I = 1, 15

 TMP1 = I

 TMP2 = 16 - I

 TMP3 = TMP1

 IF (I .GT. 8) TMP3 = TMP2

 TMP4 = (X(2)*TMP2 + X(3)*TMP3)**2

 FJAC(I,1) = -1.D0

 FJAC(I,2) = TMP1*TMP2/TMP4

 FJAC(I,3) = TMP1*TMP3/TMP4

30 CONTINUE

40 CONTINUE

RETURN

LAST CARD OF SUBROUTINE FCN.

END

Results obtained with different compilers or machines
may be slightly different.

FINAL L2 NORM OF THE RESIDUALS 0.9063596D-01

EXIT PARAMETER 1

FINAL APPROXIMATE SOLUTION

0.8241058D-01 0.1133037D+01 0.2343695D+01

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Documentation for MINPACK subroutine LMDER

Double precision version

Argonne National Laboratory

Burton S. Garbow, Kenneth E. Hillstom, Jorge J. More

March 1980

1. Purpose.

The purpose of LMDER is to minimize the sum of the squares of M nonlinear functions in N variables by a modification of the Levenberg-Marquardt algorithm. The user must provide a subroutine which calculates the functions and the Jacobian.

2. Subroutine and type statements.

```

SUBROUTINE LMDER(FCN,M,N,X,FVEC,FJAC,LDFJAC,FTOL,XTOL,GTOL,
*               MAXFEV,DIAG,MODE,FACTOR,NPRINT,INFO,NFEV,NJEV,
*               IPVT,QTF,WA1,WA2,WA3,WA4)
INTEGER M,N,LDFJAC,MAXFEV,MODE,NPRINT,INFO,NFEV,NJEV
INTEGER IPVT(N)
DOUBLE PRECISION FTOL,XTOL,GTOL,FACTOR
DOUBLE PRECISION X(N),FVEC(M),FJAC(LDFJAC,N),DIAG(N),QTF(N),
*               WA1(N),WA2(N),WA3(N),WA4(M)

```

3. Parameters.

Parameters designated as input parameters must be specified on entry to LMDER and are not changed on exit, while parameters designated as output parameters need not be specified on entry and are set to appropriate values on exit from LMDER.

FCN is the name of the user-supplied subroutine which calculates the functions and the Jacobian. FCN must be declared in an EXTERNAL statement in the user calling program, and should be written as follows.

```

SUBROUTINE FCN(M,N,X,FVEC,FJAC,LDFJAC,IFLAG)
INTEGER M,N,LDFJAC,IFLAG
DOUBLE PRECISION X(N),FVEC(M),FJAC(LDFJAC,N)
-----
IF IFLAG = 1 CALCULATE THE FUNCTIONS AT X AND
RETURN THIS VECTOR IN FVEC. DO NOT ALTER FJAC.
IF IFLAG = 2 CALCULATE THE JACOBIAN AT X AND
RETURN THIS MATRIX IN FJAC. DO NOT ALTER FVEC.
-----
RETURN
END

```

The value of IFLAG should not be changed by FCN unless the user wants to terminate execution of LMDER. In this case set IFLAG to a negative integer.

M is a positive integer input variable set to the number of functions.

N is a positive integer input variable set to the number of variables. N must not exceed M.

X is an array of length N. On input X must contain an initial estimate of the solution vector. On output X contains the final estimate of the solution vector.

FVEC is an output array of length M which contains the functions evaluated at the output X.

FJAC is an output M by N array. The upper N by N submatrix of FJAC contains an upper triangular matrix R with diagonal elements of nonincreasing magnitude such that

$$P^T (JAC^T JAC) P = R^T R,$$

where P is a permutation matrix and JAC is the final calculated Jacobian. Column j of P is column IPVT(j) (see below) of the identity matrix. The lower trapezoidal part of FJAC contains information generated during the computation of R.

LDFJAC is a positive integer input variable not less than M which specifies the leading dimension of the array FJAC.

FTOL is a nonnegative input variable. Termination occurs when both the actual and predicted relative reductions in the sum of squares are at most FTOL. Therefore, FTOL measures the relative error desired in the sum of squares. Section 4 contains more details about FTOL.

XTOL is a nonnegative input variable. Termination occurs when the relative error between two consecutive iterates is at most XTOL. Therefore, XTOL measures the relative error desired in the approximate solution. Section 4 contains more details about XTOL.

GTOL is a nonnegative input variable. Termination occurs when the cosine of the angle between FVEC and any column of the Jacobian is at most GTOL in absolute value. Therefore, GTOL measures the orthogonality desired between the function vector and the columns of the Jacobian. Section 4 contains more details about GTOL.

MAXFEV is a positive integer input variable. Termination occurs when the number of calls to FCN with IFLAG = 1 has reached MAXFEV.

DIAG is an array of length N. If MODE = 1 (see below), DIAG is internally set. If MODE = 2, DIAG must contain positive entries that serve as multiplicative scale factors for the variables.

MODE is an integer input variable. If MODE = 1, the variables will be scaled internally. If MODE = 2, the scaling is specified by the input DIAG. Other values of MODE are equivalent to MODE = 1.

FACTOR is a positive input variable used in determining the initial step bound. This bound is set to the product of FACTOR and the Euclidean norm of $\text{DIAG} \cdot X$ if nonzero, or else to FACTOR itself. In most cases FACTOR should lie in the interval (.1,100.). 100. is a generally recommended value.

NPRINT is an integer input variable that enables controlled printing of iterates if it is positive. In this case, FCN is called with IFLAG = 0 at the beginning of the first iteration and every NPRINT iterations thereafter and immediately prior to return, with X, FVEC, and FJAC available for printing. FVEC and FJAC should not be altered. If NPRINT is not positive, no special calls of FCN with IFLAG = 0 are made.

INFO is an integer output variable. If the user has terminated execution, INFO is set to the (negative) value of IFLAG. See description of FCN. Otherwise, INFO is set as follows.

INFO = 0 Improper input parameters.

INFO = 1 Both actual and predicted relative reductions in the sum of squares are at most FTOL.

INFO = 2 Relative error between two consecutive iterates is at most XTOL.

INFO = 3 Conditions for INFO = 1 and INFO = 2 both hold.

INFO = 4 The cosine of the angle between FVEC and any column of the Jacobian is at most GTOL in absolute value.

INFO = 5 Number of calls to FCN with IFLAG = 1 has reached MAXFEV.

INFO = 6 FTOL is too small. No further reduction in the sum of squares is possible.

INFO = 7 XTOL is too small. No further improvement in the approximate solution X is possible.

INFO = 8 GTOL is too small. FVEC is orthogonal to the columns of the Jacobian to machine precision.

Sections 4 and 5 contain more details about INFO.

NFEV is an integer output variable set to the number of calls to FCN with IFLAG = 1.

NJEV is an integer output variable set to the number of calls to FCN with IFLAG = 2.

IPVT is an integer output array of length N. IPVT defines a permutation matrix P such that $JAC * P = Q * R$, where JAC is the final calculated Jacobian, Q is orthogonal (not stored), and R is upper triangular with diagonal elements of nonincreasing magnitude. Column j of P is column IPVT(j) of the identity matrix.

QTF is an output array of length N which contains the first N elements of the vector $(Q \text{ transpose}) * FVEC$.

WA1, WA2, and WA3 are work arrays of length N.

WA4 is a work array of length M.

4. Successful completion.

The accuracy of LMDER is controlled by the convergence parameters FTOL, XTOL, and GTOL. These parameters are used in tests which make three types of comparisons between the approximation X and a solution XSOL. LMDER terminates when any of the tests is satisfied. If any of the convergence parameters is less than the machine precision (as defined by the MINPACK function DPMPAR(1)), then LMDER only attempts to satisfy the test defined by the machine precision. Further progress is not usually possible.

The tests assume that the functions and the Jacobian are coded consistently, and that the functions are reasonably well behaved. If these conditions are not satisfied, then LMDER may incorrectly indicate convergence. The coding of the Jacobian can be checked by the MINPACK subroutine CHKDER. If the Jacobian is coded correctly, then the validity of the answer can be checked, for example, by rerunning LMDER with tighter tolerances.

First convergence test. If $ENORM(Z)$ denotes the Euclidean norm of a vector Z, then this test attempts to guarantee that

$$ENORM(FVEC) \leq (1+FTOL) * ENORM(FVECS),$$

where FVECS denotes the functions evaluated at XSOL. If this condition is satisfied with $FTOL = 10^{*(-K)}$, then the final residual norm $ENORM(FVEC)$ has K significant decimal digits and INFO is set to 1 (or to 3 if the second test is also satisfied). Unless high precision solutions are required, the recommended value for FTOL is the square root of the machine precision.

Second convergence test. If D is the diagonal matrix whose entries are defined by the array DIAG, then this test attempts to guarantee that

$$\text{ENORM}(D*(X-XSOL)) \leq \text{XTOL} * \text{ENORM}(D*XSOL).$$

If this condition is satisfied with $\text{XTOL} = 10^{**}(-K)$, then the larger components of $D*X$ have K significant decimal digits and INFO is set to 2 (or to 3 if the first test is also satisfied). There is a danger that the smaller components of $D*X$ may have large relative errors, but if $\text{MODE} = 1$, then the accuracy of the components of X is usually related to their sensitivity. Unless high precision solutions are required, the recommended value for XTOL is the square root of the machine precision.

Third convergence test. This test is satisfied when the cosine of the angle between FVEC and any column of the Jacobian at X is at most GTOL in absolute value. There is no clear relationship between this test and the accuracy of LMDER, and furthermore, the test is equally well satisfied at other critical points, namely maximizers and saddle points. Therefore, termination caused by this test ($\text{INFO} = 4$) should be examined carefully. The recommended value for GTOL is zero.

5. Unsuccessful completion.

Unsuccessful termination of LMDER can be due to improper input parameters, arithmetic interrupts, or an excessive number of function evaluations.

Improper input parameters. INFO is set to 0 if $N \leq 0$, or $M \leq N$, or $\text{LDFJAC} \leq M$, or $\text{FTOL} \leq 0.00$, or $\text{XTOL} \leq 0.00$, or $\text{GTOL} \leq 0.00$, or $\text{MAXFEV} \leq 0$, or $\text{FACTOR} \leq 0.00$.

Arithmetic interrupts. If these interrupts occur in the FCN subroutine during an early stage of the computation, they may be caused by an unacceptable choice of X by LMDER. In this case, it may be possible to remedy the situation by rerunning LMDER with a smaller value of FACTOR.

Excessive number of function evaluations. A reasonable value for MAXFEV is $100*(N+1)$. If the number of calls to FCN with $\text{IFLAG} = 1$ reaches MAXFEV, then this indicates that the routine is converging very slowly as measured by the progress of FVEC, and INFO is set to 5. In this case, it may be helpful to restart LMDER with MODE set to 1.

6. Characteristics of the algorithm.

LMDER is a modification of the Levenberg-Marquardt algorithm.

Two of its main characteristics involve the proper use of implicitly scaled variables (if `MODE = 1`) and an optimal choice for the correction. The use of implicitly scaled variables achieves scale invariance of `LMDER` and limits the size of the correction in any direction where the functions are changing rapidly. The optimal choice of the correction guarantees (under reasonable conditions) global convergence from starting points far from the solution and a fast rate of convergence for problems with small residuals.

Timing. The time required by `LMDER` to solve a given problem depends on `M` and `N`, the behavior of the functions, the accuracy requested, and the starting point. The number of arithmetic operations needed by `LMDER` is about N^3 to process each evaluation of the functions (call to `FCN` with `IFLAG = 1`) and $M(N^2)$ to process each evaluation of the Jacobian (call to `FCN` with `IFLAG = 2`). Unless `FCN` can be evaluated quickly, the timing of `LMDER` will be strongly influenced by the time spent in `FCN`.

Storage. `LMDER` requires $M \cdot N + 2 \cdot M + 6 \cdot N$ double precision storage locations and `N` integer storage locations, in addition to the storage required by the program. There are no internally declared storage arrays.

7. Subprograms required.

USER-supplied `FCN`

MINPACK-supplied ... `DPMPAR`, `ENORM`, `LMPAR`, `QRFAC`, `QRSOLV`

FORTTRAN-supplied ... `DABS`, `DMAX1`, `DMIN1`, `DSQRT`, `MOD`

8. References.

Jorge J. More, The Levenberg-Marquardt Algorithm, Implementation and Theory. Numerical Analysis, G. A. Watson, editor. Lecture Notes in Mathematics 630, Springer-Verlag, 1977.

9. Example.

The problem is to determine the values of `x(1)`, `x(2)`, and `x(3)` which provide the best fit (in the least squares sense) of

$$x(1) + u(i)/(v(i) \cdot x(2) + w(i) \cdot x(3)), \quad i = 1, 15$$

to the data

$$y = (0.14, 0.18, 0.22, 0.25, 0.29, 0.32, 0.35, 0.39, \\ 0.37, 0.58, 0.73, 0.96, 1.34, 2.10, 4.39),$$

where $u(i) = i$, $v(i) = 16 - i$, and $w(i) = \min(u(i), v(i))$. The i -th component of FVEC is thus defined by

$$y(i) = (x(1) + u(i)/(v(i)*x(2) + w(i)*x(3))).$$

DRIVER FOR LMDER EXAMPLE.
DOUBLE PRECISION VERSION

INTEGER J,M,N,LDFJAC,MAXFEV,MODE,NPRINT,INFO,NFEV,NJEV,NWRITE
INTEGER IPVT(3)
DOUBLE PRECISION FTOL,XTOL,GTOL,FACTOR,ENORM
DOUBLE PRECISION X(3),FVEC(15),FJAC(15,3),DIAG(3),QTF(3),
* WA1(3),WA2(3),WA3(3),WA4(15)
DOUBLE PRECISION ENORM,DPMPAR
EXTERNAL FCN

LOGICAL OUTPUT UNIT IS ASSUMED TO BE NUMBER 6.

DATA NWRITE /6/

M = 15
N = 3

THE FOLLOWING STARTING VALUES PROVIDE A ROUGH FIT.

X(1) = 1.D0
X(2) = 1.D0
X(3) = 1.D0

LDFJAC = 15

SET FTOL AND XTOL TO THE SQUARE ROOT OF THE MACHINE PRECISION
AND GTOL TO ZERO. UNLESS HIGH PRECISION SOLUTIONS ARE
REQUIRED, THESE ARE THE RECOMMENDED SETTINGS.

FTOL = DSQRT(DPMPAR(1))
XTOL = DSQRT(DPMPAR(1))
GTOL = 0.D0

MAXFEV = 400
MODE = 1
FACTOR = 1.D2
NPRINT = 0

CALL LMDER(FCN,M,N,X,FVEC,FJAC,LDFJAC,FTOL,XTOL,GTOL,
* MAXFEV,DIAG,MODE,FACTOR,NPRINT,INFO,NFEV,NJEV,
* IPVT,QTF,WA1,WA2,WA3,WA4)
ENORM = ENORM(M,FVEC)
WRITE (NWRITE,1000) ENORM,NFEV,NJEV,INFO,(X(J),J=1,N)
STOP

1000 FORMAT (5X,31H FINAL L2 NORM OF THE RESIDUALS,D15.7 //


```

*      5X,31H NUMBER OF FUNCTION EVALUATIONS,I10 //
*      5X,31H NUMBER OF JACOBIAN EVALUATIONS,I10 //
*      5X,15H EXIT PARAMETER,16X,I10 //
*      5X,27H FINAL APPROXIMATE SOLUTION // 5X,3D15.7)

```

C
C
C

LAST CARD OF DRIVER FOR LMDER EXAMPLE.

END

```

SUBROUTINE FCN(M,N,X,FVEC,FJAC,LDFJAC,IFLAG)
INTEGER M,N,LDFJAC,IFLAG
DOUBLE PRECISION X(N),FVEC(M),FJAC(LDFJAC,N)

```

C
C
C

SUBROUTINE FCN FOR LMDER EXAMPLE.

```

INTEGER I
DOUBLE PRECISION TMP1,TMP2,TMP3,TMP4
DOUBLE PRECISION Y(15)
DATA Y(1),Y(2),Y(3),Y(4),Y(5),Y(6),Y(7),Y(8),
*      Y(9),Y(10),Y(11),Y(12),Y(13),Y(14),Y(15)
*      /1.4D-1,1.8D-1,2.2D-1,2.5D-1,2.9D-1,3.2D-1,3.5D-1,3.9D-1,
*      3.7D-1,5.8D-1,7.3D-1,9.6D-1,1.34D0,2.1D0,4.39D0/

```

C
C
C
C

IF (IFLAG .NE. 0) GO TO 5

INSERT PRINT STATEMENTS HERE WHEN NPRINT IS POSITIVE.

RETURN

5 CONTINUE

IF (IFLAG .EQ. 2) GO TO 20

DO 10 I = 1, 15

 TMP1 = I

 TMP2 = 16 - I

 TMP3 = TMP1

 IF (I .GT. 8) TMP3 = TMP2

 FVEC(I) = Y(I) - (X(1) + TMP1/(X(2)*TMP2 + X(3)*TMP3))

10 CONTINUE

GO TO 40

20 CONTINUE

DO 30 I = 1, 15

 TMP1 = I

 TMP2 = 16 - I

 TMP3 = TMP1

 IF (I .GT. 8) TMP3 = TMP2

 TMP4 = (X(2)*TMP2 + X(3)*TMP3)**2

 FJAC(I,1) = -1.D0

 FJAC(I,2) = TMP1*TMP2/TMP4

 FJAC(I,3) = TMP1*TMP3/TMP4

30 CONTINUE

40 CONTINUE

RETURN

C
C
C

LAST CARD OF SUBROUTINE FCN.

END

Results obtained with different compilers or machines may be slightly different.

FINAL L2 NORM OF THE RESIDUALS 0.9063596D-01

NUMBER OF FUNCTION EVALUATIONS 6

NUMBER OF JACOBIAN EVALUATIONS 5

EXIT PARAMETER 1

FINAL APPROXIMATE SOLUTION

0.8241058D-01 0.1133037D+01 0.2343695D+01

Documentation for MINPACK subroutine LMSTR1

Double precision version

Argonne National Laboratory

Burton S. Garbow, Kenneth E. Hillstom, Jorge J. More

March 1980

1. Purpose.

The purpose of LMSTR1 is to minimize the sum of the squares of M nonlinear functions in N variables by a modification of the Levenberg-Marquardt algorithm which uses minimal storage. This is done by using the more general least-squares solver LMSTR. The user must provide a subroutine which calculates the functions and the rows of the Jacobian.

2. Subroutine and type statements.

```

SUBROUTINE LMSTR1(FCN,M,N,X,FVEC,FJAC,LDFJAC,TOL,
*               INFO,IPVT,WA,LWA)
INTEGER M,N,LDFJAC,INFO,LWA
INTEGER IPVT(N)
DOUBLE PRECISION TOL
DOUBLE PRECISION X(N),FVEC(M),FJAC(LDFJAC,N),WA(LWA)
EXTERNAL FCN

```

3. Parameters.

Parameters designated as input parameters must be specified on entry to LMSTR1 and are not changed on exit, while parameters designated as output parameters need not be specified on entry and are set to appropriate values on exit from LMSTR1.

FCN is the name of the user-supplied subroutine which calculates the functions and the rows of the Jacobian. FCN must be declared in an EXTERNAL statement in the user calling program, and should be written as follows.

```

SUBROUTINE FCN(M,N,X,FVEC,FJROW,IFLAG)
INTEGER M,N,IFLAG
DOUBLE PRECISION X(N),FVEC(M),FJROW(N)
-----
IF IFLAG = 1 CALCULATE THE FUNCTIONS AT X AND
RETURN THIS VECTOR IN FVEC.
IF IFLAG = I CALCULATE THE (I-1)-ST ROW OF THE
JACOBIAN AT X AND RETURN THIS VECTOR IN FJROW.
-----
RETURN

```

END

The value of IFLAG should not be changed by FCN unless the user wants to terminate execution of LMSTR1. In this case set IFLAG to a negative integer.

M is a positive integer input variable set to the number of functions.

N is a positive integer input variable set to the number of variables. N must not exceed M.

X is an array of length N. On input X must contain an initial estimate of the solution vector. On output X contains the final estimate of the solution vector.

FVEC is an output array of length M which contains the functions evaluated at the output X.

FJAC is an output N by N array. The upper triangle of FJAC contains an upper triangular matrix R such that

$$P^T (JAC^T JAC) P = R^T R,$$

where P is a permutation matrix and JAC is the final calculated Jacobian. Column j of P is column IPV(j) (see below) of the identity matrix. The lower triangular part of FJAC contains information generated during the computation of R.

LDFJAC is a positive integer input variable not less than N which specifies the leading dimension of the array FJAC.

TOL is a nonnegative input variable. Termination occurs when the algorithm estimates either that the relative error in the sum of squares is at most TOL or that the relative error between X and the solution is at most TOL. Section 4 contains more details about TOL.

INFO is an integer output variable. If the user has terminated execution, INFO is set to the (negative) value of IFLAG. See description of FCN. Otherwise, INFO is set as follows.

INFO = 0 Improper input parameters.

INFO = 1 Algorithm estimates that the relative error in the sum of squares is at most TOL.

INFO = 2 Algorithm estimates that the relative error between X and the solution is at most TOL.

INFO = 3 Conditions for INFO = 1 and INFO = 2 both hold.

INFO = 4 FVEC is orthogonal to the columns of the Jacobian to

machine precision.

INFO = 5 Number of calls to FCN with IFLAG = 1 has reached $100*(N+1)$.

INFO = 6 TOL is too small. No further reduction in the sum of squares is possible.

INFO = 7 TOL is too small. No further improvement in the approximate solution X is possible.

Sections 4 and 5 contain more details about INFO.

IPVT is an integer output array of length N. IPVT defines a permutation matrix P such that $JAC*P = Q*R$, where JAC is the final calculated Jacobian, Q is orthogonal (not stored), and R is upper triangular. Column j of P is column IPVT(j) of the identity matrix.

WA is a work array of length LWA.

LWA is a positive integer input variable not less than $5*N+M$.

4. Successful completion.

The accuracy of LMSTR1 is controlled by the convergence parameter TOL. This parameter is used in tests which make three types of comparisons between the approximation X and a solution XSOL. LMSTR1 terminates when any of the tests is satisfied. If TOL is less than the machine precision (as defined by the MINPACK function DPMPAR(1)), then LMSTR1 only attempts to satisfy the test defined by the machine precision. Further progress is not usually possible. Unless high precision solutions are required, the recommended value for TOL is the square root of the machine precision.

The tests assume that the functions and the Jacobian are coded consistently, and that the functions are reasonably well behaved. If these conditions are not satisfied, then LMSTR1 may incorrectly indicate convergence. The coding of the Jacobian can be checked by the MINPACK subroutine CHKDER. If the Jacobian is coded correctly, then the validity of the answer can be checked, for example, by rerunning LMSTR1 with a tighter tolerance.

First convergence test. If ENORM(Z) denotes the Euclidean norm of a vector Z, then this test attempts to guarantee that

$$ENORM(FVEC) \leq (1+TOL)*ENORM(FVECS),$$

where FVECS denotes the functions evaluated at XSOL. If this condition is satisfied with $TOL = 10^{*(-K)}$, then the final residual norm ENORM(FVEC) has K significant decimal digits and

INFO is set to 1 (or to 3 if the second test is also satisfied).

Second convergence test. If D is a diagonal matrix (implicitly generated by LMSTR1) whose entries contain scale factors for the variables, then this test attempts to guarantee that

$$\text{ENORM}(D*(X-XSOL)) \leq \text{TOL} * \text{ENORM}(D*XSOL).$$

If this condition is satisfied with $\text{TOL} = 10^{*(-K)}$, then the larger components of $D*X$ have K significant decimal digits and INFO is set to 2 (or to 3 if the first test is also satisfied). There is a danger that the smaller components of $D*X$ may have large relative errors, but the choice of D is such that the accuracy of the components of X is usually related to their sensitivity.

Third convergence test. This test is satisfied when FVEC is orthogonal to the columns of the Jacobian to machine precision. There is no clear relationship between this test and the accuracy of LMSTR1, and furthermore, the test is equally well satisfied at other critical points, namely maximizers and saddle points. Therefore, termination caused by this test (INFO = 4) should be examined carefully.

5. Unsuccessful completion.

Unsuccessful termination of LMSTR1 can be due to improper input parameters, arithmetic interrupts, or an excessive number of function evaluations.

Improper input parameters. INFO is set to 0 if $N \leq 0$, or $M \leq N$, or $\text{LDFJAC} \leq N$, or $\text{TOL} \leq 0$, or $\text{LWA} \leq 5*N+M$.

Arithmetic interrupts. If these interrupts occur in the FCN subroutine during an early stage of the computation, they may be caused by an unacceptable choice of X by LMSTR1. In this case, it may be possible to remedy the situation by not evaluating the functions here, but instead setting the components of FVEC to numbers that exceed those in the initial FVEC, thereby indirectly reducing the step length. The step length can be more directly controlled by using instead LMSTR, which includes in its calling sequence the step-length-governing parameter FACTOR.

Excessive number of function evaluations. If the number of calls to FCN with IFLAG = 1 reaches $100*(N+1)$, then this indicates that the routine is converging very slowly as measured by the progress of FVEC, and INFO is set to 5. In this case, it may be helpful to restart LMSTR1, thereby forcing it to disregard old (and possibly harmful) information.

6. Characteristics of the algorithm.

LMSTR1 is a modification of the Levenberg-Marquardt algorithm. Two of its main characteristics involve the proper use of implicitly scaled variables and an optimal choice for the correction. The use of implicitly scaled variables achieves scale invariance of LMSTR1 and limits the size of the correction in any direction where the functions are changing rapidly. The optimal choice of the correction guarantees (under reasonable conditions) global convergence from starting points far from the solution and a fast rate of convergence for problems with small residuals.

Timing. The time required by LMSTR1 to solve a given problem depends on M and N, the behavior of the functions, the accuracy requested, and the starting point. The number of arithmetic operations needed by LMSTR1 is about N^3 to process each evaluation of the functions (call to FCN with IFLAG = 1) and $1.5(N^2)$ to process each row of the Jacobian (call to FCN with IFLAG .GE. 2). Unless FCN can be evaluated quickly, the timing of LMSTR1 will be strongly influenced by the time spent in FCN.

Storage. LMSTR1 requires $N^2 + 2M + 6N$ double precision storage locations and N integer storage locations, in addition to the storage required by the program. There are no internally declared storage arrays.

7. Subprograms required.

USER-supplied FCN

MINPACK-supplied ... DMPAR, ENORM, LMSTR, LMPAR, QRFAC, QRSOLV, RWUPDT

FORTTRAN-supplied ... DABS, DMAX1, DMIN1, DSQRT, MOD

8. References.

Jorge J. More, The Levenberg-Marquardt Algorithm, Implementation and Theory. Numerical Analysis, G. A. Watson, editor. Lecture Notes in Mathematics 630, Springer-Verlag, 1977.

9. Example.

The problem is to determine the values of $x(1)$, $x(2)$, and $x(3)$ which provide the best fit (in the least squares sense) of

$$x(1) + u(i)/(v(i)*x(2) + w(i)*x(3)), \quad i = 1, 15$$

to the data

$$y = (0.14, 0.18, 0.22, 0.25, 0.29, 0.32, 0.35, 0.39, \\ 0.37, 0.58, 0.73, 0.96, 1.34, 2.10, 4.39),$$

where $u(i) = i$, $v(i) = 16 - i$, and $w(i) = \min(u(i), v(i))$. The i -th component of FVEC is thus defined by

$$y(i) - (x(1) + u(i)/(v(i)*x(2) + w(i)*x(3))).$$

```

C *****
C
C DRIVER FOR LMSTR1 EXAMPLE.
C DOUBLE PRECISION VERSION
C
C *****
C INTEGER J,M,N,LDFJAC,INFO,LWA,NWRITE
C INTEGER IPVT(3)
C DOUBLE PRECISION TOL,FNORM
C DOUBLE PRECISION X(3),FVEC(15),FJAC(3,3),WA(30)
C DOUBLE PRECISION ENORM,DPMPAR
C EXTERNAL FCN
C
C LOGICAL OUTPUT UNIT IS ASSUMED TO BE NUMBER 6.
C
C DATA NWRITE /6/
C
C M = 15
C N = 3
C
C THE FOLLOWING STARTING VALUES PROVIDE A ROUGH FIT.
C
C X(1) = 1.D0
C X(2) = 1.D0
C X(3) = 1.D0
C
C LDFJAC = 3
C LWA = 30
C
C SET TOL TO THE SQUARE ROOT OF THE MACHINE PRECISION.
C UNLESS HIGH PRECISION SOLUTIONS ARE REQUIRED,
C THIS IS THE RECOMMENDED SETTING.
C
C TOL = DSQRT(DPMPAR(1))
C
C CALL LMSTR1(FCN,M,N,X,FVEC,FJAC,LDFJAC,TOL,
*          INFO,IPVT,WA,LWA)
C FNORM = ENORM(M,FVEC)
C WRITE (NWRITE,1000) FNORM,INFO,(X(J),J=1,N)
C STOP
1000 FORMAT (5X,31H FINAL L2 NORM OF THE RESIDUALS,D15.7 //
*          5X,15H EXIT PARAMETER,16X,I10 //
*          5X,27H FINAL APPROXIMATE SOLUTION // 5X,3D15.7)
C

```



```

C      LAST CARD OF DRIVER FOR LMSTR1 EXAMPLE.
      END
      SUBROUTINE FCN(M,N,X,FVEC,FJROW,IFLAG)
      INTEGER M,N,IFLAG
      DOUBLE PRECISION X(N),FVEC(M),FJROW(N)
C
C      SUBROUTINE FCN FOR LMSTR1 EXAMPLE.
C
      INTEGER I
      DOUBLE PRECISION TMP1,TMP2,TMP3,TMP4
      DOUBLE PRECISION Y(15)
      DATA Y(1),Y(2),Y(3),Y(4),Y(5),Y(6),Y(7),Y(8),
*          Y(9),Y(10),Y(11),Y(12),Y(13),Y(14),Y(15)
*          /1.4D-1,1.8D-1,2.2D-1,2.5D-1,2.9D-1,3.2D-1,3.5D-1,3.9D-1,
*          3.7D-1,5.8D-1,7.3D-1,9.6D-1,1.34D0,2.1D0,4.39D0/
C
      IF (IFLAG .GE. 2) GO TO 20
      DO 10 I = 1, 15
          TMP1 = I
          TMP2 = 16 - I
          TMP3 = TMP1
          IF (I .GT. 8) TMP3 = TMP2
          FVEC(I) = Y(I) - (X(1) + TMP1/(X(2)*TMP2 + X(3)*TMP3))
10      CONTINUE
      GO TO 40
20      CONTINUE
      I = IFLAG - 1
          TMP1 = I
          TMP2 = 16 - I
          TMP3 = TMP1
          IF (I .GT. 8) TMP3 = TMP2
          TMP4 = (X(2)*TMP2 + X(3)*TMP3)**2
          FJROW(1) = -1.D0
          FJROW(2) = TMP1*TMP2/TMP4
          FJROW(3) = TMP1*TMP3/TMP4
30      CONTINUE
40      CONTINUE
      RETURN
C
C      LAST CARD OF SUBROUTINE FCN.
C
      END

Results obtained with different compilers or machines
may be slightly different.

FINAL L2 NORM OF THE RESIDUALS   0.9063596D-01

EXIT PARAMETER                    1

FINAL APPROXIMATE SOLUTION

0.8241058D-01  0.1133037D+01  0.2343695D+01

```

Documentation for MINPACK subroutine LMSTR

Double precision version

Argonne National Laboratory

Burton S. Garbow, Kenneth E. Hillstom, Jorge J. More

March 1980

1. Purpose.

The purpose of LMSTR is to minimize the sum of the squares of M nonlinear functions in N variables by a modification of the Levenberg-Marquardt algorithm which uses minimal storage. The user must provide a subroutine which calculates the functions and the rows of the Jacobian.

2. Subroutine and type statements.

```

SUBROUTINE LMSTR(FCN,M,N,X,FVEC,FJAC,LDFJAC,FTOL,XTOL,GTOL,
*               MAXFEV,DIAG,MODE,FACTOR,NPRINT,INFO,NFEV,NJEV,
*               IPV,T,QTF,WA1,WA2,WA3,WA4)
  INTEGER M,N,LDFJAC,MAXFEV,MODE,NPRINT,INFO,NFEV,NJEV
  INTEGER IPV(T,N)
  DOUBLE PRECISION FTOL,XTOL,GTOL,FACTOR
  DOUBLE PRECISION X(N),FVEC(M),FJAC(LDFJAC,N),DIAG(N),QTF(N),
*               WA1(N),WA2(N),WA3(N),WA4(M)

```

3. Parameters.

Parameters designated as input parameters must be specified on entry to LMSTR and are not changed on exit, while parameters designated as output parameters need not be specified on entry and are set to appropriate values on exit from LMSTR.

FCN is the name of the user-supplied subroutine which calculates the functions and the rows of the Jacobian. FCN must be declared in an EXTERNAL statement in the user calling program, and should be written as follows.

```

SUBROUTINE FCN(M,N,X,FVEC,FJROW,IFLAG)
  INTEGER M,N,IFLAG
  DOUBLE PRECISION X(N),FVEC(M),FJROW(N)
  -----
  IF IFLAG = 1 CALCULATE THE FUNCTIONS AT X AND
  RETURN THIS VECTOR IN FVEC.
  IF IFLAG = I CALCULATE THE (I-1)-ST ROW OF THE
  JACOBIAN AT X AND RETURN THIS VECTOR IN FJROW.
  -----
  RETURN

```

END

The value of IFLAG should not be changed by FCN unless the user wants to terminate execution of LMSTR. In this case set IFLAG to a negative integer.

M is a positive integer input variable set to the number of functions.

N is a positive integer input variable set to the number of variables. N must not exceed M.

X is an array of length N. On input X must contain an initial estimate of the solution vector. On output X contains the final estimate of the solution vector.

FVEC is an output array of length M which contains the functions evaluated at the output X.

FJAC is an output N by N array. The upper triangle of FJAC contains an upper triangular matrix R such that

$$P^T (JAC^T JAC) P = R^T R,$$

where P is a permutation matrix and JAC is the final calculated Jacobian. Column j of P is column IPVT(j) (see below) of the identity matrix. The lower triangular part of FJAC contains information generated during the computation of R.

LDEFJAC is a positive integer input variable not less than N which specifies the leading dimension of the array FJAC.

FTOL is a nonnegative input variable. Termination occurs when both the actual and predicted relative reductions in the sum of squares are at most FTOL. Therefore, FTOL measures the relative error desired in the sum of squares. Section 4 contains more details about FTOL.

XTOL is a nonnegative input variable. Termination occurs when the relative error between two consecutive iterates is at most XTOL. Therefore, XTOL measures the relative error desired in the approximate solution. Section 4 contains more details about XTOL.

GTOL is a nonnegative input variable. Termination occurs when the cosine of the angle between FVEC and any column of the Jacobian is at most GTOL in absolute value. Therefore, GTOL measures the orthogonality desired between the function vector and the columns of the Jacobian. Section 4 contains more details about GTOL.

MAXFEV is a positive integer input variable. Termination occurs when the number of calls to FCN with IFLAG = 1 has reached

MAXFEV.

DIAG is an array of length N. If MODE = 1 (see below), DIAG is internally set. If MODE = 2, DIAG must contain positive entries that serve as multiplicative scale factors for the variables.

MODE is an integer input variable. If MODE = 1, the variables will be scaled internally. If MODE = 2, the scaling is specified by the input DIAG. Other values of MODE are equivalent to MODE = 1.

FACTOR is a positive input variable used in determining the initial step bound. This bound is set to the product of FACTOR and the Euclidean norm of DIAG*X if nonzero, or else to FACTOR itself. In most cases FACTOR should lie in the interval (.1,100.). 100. is a generally recommended value.

NPRINT is an integer input variable that enables controlled printing of iterates if it is positive. In this case, FCN is called with IFLAG = 0 at the beginning of the first iteration and every NPRINT iterations thereafter and immediately prior to return, with X and FVEC available for printing. If NPRINT is not positive, no special calls of FCN with IFLAG = 0 are made.

INFO is an integer output variable. If the user has terminated execution, INFO is set to the (negative) value of IFLAG. See description of FCN. Otherwise, INFO is set as follows.

INFO = 0 Improper input parameters.

INFO = 1 Both actual and predicted relative reductions in the sum of squares are at most FTOL.

INFO = 2 Relative error between two consecutive iterates is at most XTOL.

INFO = 3 Conditions for INFO = 1 and INFO = 2 both hold.

INFO = 4 The cosine of the angle between FVEC and any column of the Jacobian is at most GTOL in absolute value.

INFO = 5 Number of calls to FCN with IFLAG = 1 has reached MAXFEV.

INFO = 6 FTOL is too small. No further reduction in the sum of squares is possible.

INFO = 7 XTOL is too small. No further improvement in the approximate solution X is possible.

INFO = 8 GTOL is too small. FVEC is orthogonal to the columns of the Jacobian to machine precision.

Sections 4 and 5 contain more details about INFO.

NFEV is an integer output variable set to the number of calls to FCN with IFLAG = 1.

NJEV is an integer output variable set to the number of calls to FCN with IFLAG = 2.

IPVT is an integer output array of length N. IPVT defines a permutation matrix P such that $JAC * P = Q * R$, where JAC is the final calculated Jacobian, Q is orthogonal (not stored), and R is upper triangular. Column j of P is column IPVT(j) of the identity matrix.

QTF is an output array of length N which contains the first N elements of the vector $(Q \text{ transpose}) * FVEC$.

WA1, WA2, and WA3 are work arrays of length N.

WA4 is a work array of length M.

4. Successful completion.

The accuracy of LMSTR is controlled by the convergence parameters FTOL, XTOL, and GTOL. These parameters are used in tests which make three types of comparisons between the approximation X and a solution XSOL. LMSTR terminates when any of the tests is satisfied. If any of the convergence parameters is less than the machine precision (as defined by the MINPACK function DPMPAR(1)), then LMSTR only attempts to satisfy the test defined by the machine precision. Further progress is not usually possible.

The tests assume that the functions and the Jacobian are coded consistently, and that the functions are reasonably well behaved. If these conditions are not satisfied, then LMSTR may incorrectly indicate convergence. The coding of the Jacobian can be checked by the MINPACK subroutine CHKDER. If the Jacobian is coded correctly, then the validity of the answer can be checked, for example, by rerunning LMSTR with tighter tolerances.

First convergence test. If ENORM(Z) denotes the Euclidean norm of a vector Z, then this test attempts to guarantee that

$$ENORM(FVEC) \leq (1+FTOL) * ENORM(FVECS),$$

where FVECS denotes the functions evaluated at XSOL. If this condition is satisfied with $FTOL = 10^{*(-K)}$, then the final residual norm ENORM(FVEC) has K significant decimal digits and INFO is set to 1 (or to 3 if the second test is also satisfied). Unless high precision solutions are required, the recommended value for FTOL is the square root of the machine

precision.

Second convergence test. If D is the diagonal matrix whose entries are defined by the array DIAG, then this test attempts to guarantee that

$$\text{ENORM}(D*(X-XSOL)) \leq \text{XTOL} * \text{ENORM}(D*XSOL).$$

If this condition is satisfied with $\text{XTOL} = 10^{*(-K)}$, then the larger components of $D*X$ have K significant decimal digits and INFO is set to 2 (or to 3 if the first test is also satisfied). There is a danger that the smaller components of $D*X$ may have large relative errors, but if $\text{MODE} = 1$, then the accuracy of the components of X is usually related to their sensitivity. Unless high precision solutions are required, the recommended value for XTOL is the square root of the machine precision.

Third convergence test. This test is satisfied when the cosine of the angle between FVEC and any column of the Jacobian at X is at most GTOL in absolute value. There is no clear relationship between this test and the accuracy of LMSTR, and furthermore, the test is equally well satisfied at other critical points, namely maximizers and saddle points. Therefore, termination caused by this test ($\text{INFO} = 4$) should be examined carefully. The recommended value for GTOL is zero.

5. Unsuccessful completion.

Unsuccessful termination of LMSTR can be due to improper input parameters, arithmetic interrupts, or an excessive number of function evaluations.

Improper input parameters. INFO is set to 0 if $N \leq 0$, or $M \leq N$, or $\text{LDFJAC} \leq N$, or $\text{FTOL} \leq 0.00$, or $\text{XTOL} \leq 0.00$, or $\text{GTOL} \leq 0.00$, or $\text{MAXFEV} \leq 0$, or $\text{FACTOR} \leq 0.00$.

Arithmetic interrupts. If these interrupts occur in the FCN subroutine during an early stage of the computation, they may be caused by an unacceptable choice of X by LMSTR. In this case, it may be possible to remedy the situation by rerunning LMSTR with a smaller value of FACTOR.

Excessive number of function evaluations. A reasonable value for MAXFEV is $100*(N+1)$. If the number of calls to FCN with $\text{IFLAG} = 1$ reaches MAXFEV, then this indicates that the routine is converging very slowly as measured by the progress of FVEC, and INFO is set to 5. In this case, it may be helpful to restart LMSTR with MODE set to 1.

6. Characteristics of the algorithm.

LMSTR is a modification of the Levenberg-Marquardt algorithm. Two of its main characteristics involve the proper use of implicitly scaled variables (if `MODE = 1`) and an optimal choice for the correction. The use of implicitly scaled variables achieves scale invariance of LMSTR and limits the size of the correction in any direction where the functions are changing rapidly. The optimal choice of the correction guarantees (under reasonable conditions) global convergence from starting points far from the solution and a fast rate of convergence for problems with small residuals.

Timing. The time required by LMSTR to solve a given problem depends on M and N , the behavior of the functions, the accuracy requested, and the starting point. The number of arithmetic operations needed by LMSTR is about N^3 to process each evaluation of the functions (call to `FCN` with `IFLAG = 1`) and $1.5(N^2)$ to process each row of the Jacobian (call to `FCN` with `IFLAG .GE. 2`). Unless `FCN` can be evaluated quickly, the timing of LMSTR will be strongly influenced by the time spent in `FCN`.

Storage. LMSTR requires $N^2 + 2M + 6N$ double precision storage locations and N integer storage locations, in addition to the storage required by the program. There are no internally declared storage arrays.

7. Subprograms required.

USER-supplied `FCN`

MINPACK-supplied ... `DPMPAR, ENORM, LMPAR, QRFAC, QRSOLV, RWUPDT`

FORTTRAN-supplied ... `DABS, DMAX1, DMIN1, DSQRT, MOD`

8. References.

Jorge J. More, The Levenberg-Marquardt Algorithm, Implementation and Theory. Numerical Analysis, G. A. Watson, editor. Lecture Notes in Mathematics 630, Springer-Verlag, 1977.

9. Example.

The problem is to determine the values of $x(1)$, $x(2)$, and $x(3)$ which provide the best fit (in the least squares sense) of

$$x(1) + u(i)/(v(i)*x(2) + w(i)*x(3)), \quad i = 1, 15$$

to the data

$$y = (0.14, 0.18, 0.22, 0.25, 0.29, 0.32, 0.35, 0.39, \\ 0.37, 0.58, 0.73, 0.96, 1.34, 2.10, 4.39),$$

where $u(i) = i$, $v(i) = 16 - i$, and $w(i) = \min(u(i), v(i))$. The i -th component of FVEC is thus defined by

$$y(i) = (x(1) + u(i)/(v(i)*x(2) + w(i)*x(3))).$$

```

C *****
C
C DRIVER FOR LMSTR EXAMPLE.
C DOUBLE PRECISION VERSION
C
C *****
C INTEGER J,M,N,LDFJAC,MAXFEV,MODE,NPRINT,INFO,NFEV,NJEV,NWRITE
C INTEGER IPVT(3)
C DOUBLE PRECISION FTOL,XTOL,GTOL,FACTOR,FNORM
C DOUBLE PRECISION X(3),FVEC(15),FJAC(3,3),DIAG(3),QTF(3),
*      WA1(3),WA2(3),WA3(3),WA4(15)
C DOUBLE PRECISION ENORM,DPMPAR
C EXTERNAL FCN
C
C LOGICAL OUTPUT UNIT IS ASSUMED TO BE NUMBER 6.
C
C DATA NWRITE /6/
C
C M = 15
C N = 3
C
C THE FOLLOWING STARTING VALUES PROVIDE A ROUGH FIT.
C
C X(1) = 1.D0
C X(2) = 1.D0
C X(3) = 1.D0
C
C LDFJAC = 3
C
C SET FTOL AND XTOL TO THE SQUARE ROOT OF THE MACHINE PRECISION
C AND GTOL TO ZERO. UNLESS HIGH PRECISION SOLUTIONS ARE
C REQUIRED, THESE ARE THE RECOMMENDED SETTINGS.
C
C FTOL = DSQRT(DPMPAR(1))
C XTOL = DSQRT(DPMPAR(1))
C GTOL = 0.D0
C
C MAXFEV = 400
C MODE = 1
C FACTOR = 1.D2
C NPRINT = 0
C
C CALL LMSTR(FCN,M,N,X,FVEC,FJAC,LDFJAC,FTOL,XTOL,GTOL,
*      MAXFEV,DIAG,MODE,FACTOR,NPRINT,INFO,NFEV,NJEV,
*      IPVT,QTF,WA1,WA2,WA3,WA4)
C FNORM = ENORM(M,FVEC)
C WRITE (NWRITE,1000) FNORM,NFEV,NJEV,INFO,(X(J),J=1,N)
C STOP
1000 FORMAT (5X,31H FINAL L2 NORM OF THE RESIDUALS,D15.7 //

```



```

*      5X,31H NUMBER OF FUNCTION EVALUATIONS,I10 //
*      5X,31H NUMBER OF JACOBIAN EVALUATIONS,I10 //
*      5X,15H EXIT PARAMETER,16X,I10 //
*      5X,27H FINAL APPROXIMATE SOLUTION // 5X,3D15.7)

```

```

C      LAST CARD OF DRIVER FOR LMSTR EXAMPLE.
C
C

```

```

      END
      SUBROUTINE FCN(M,N,X,FVEC,FJROW,IFLAG)
      INTEGER M,N,IFLAG
      DOUBLE PRECISION X(N),FVEC(M),FJROW(N)

```

```

C      SUBROUTINE FCN FOR LMSTR EXAMPLE.
C
C

```

```

      INTEGER I
      DOUBLE PRECISION TMP1,TMP2,TMP3,TMP4
      DOUBLE PRECISION Y(15)
      DATA Y(1),Y(2),Y(3),Y(4),Y(5),Y(6),Y(7),Y(8),
*          Y(9),Y(10),Y(11),Y(12),Y(13),Y(14),Y(15)
*          /1.4D-1,1.8D-1,2.2D-1,2.5D-1,2.9D-1,3.2D-1,3.5D-1,3.9D-1,
*          3.7D-1,5.8D-1,7.3D-1,9.6D-1,1.34D0,2.1D0,4.39D0/

```

```

C      IF (IFLAG .NE. 0) GO TO 5
C
C

```

```

C      INSERT PRINT STATEMENTS HERE WHEN NPRINT IS POSITIVE.
C
C

```

```

      RETURN
5  CONTINUE
      IF (IFLAG .GE. 2) GO TO 20
      DO 10 I = 1, 15
          TMP1 = I
          TMP2 = 16 - I
          TMP3 = TMP1
          IF (I .GT. 8) TMP3 = TMP2
          FVEC(I) = Y(I) - (X(1) + TMP1/(X(2)*TMP2 + X(3)*TMP3))
10  CONTINUE
      GO TO 40
20  CONTINUE
      I = IFLAG - 1
      TMP1 = I
      TMP2 = 16 - I
      TMP3 = TMP1
      IF (I .GT. 8) TMP3 = TMP2
      TMP4 = (X(2)*TMP2 + X(3)*TMP3)**2
      FJROW(1) = -1.D0
      FJROW(2) = TMP1*TMP2/TMP4
      FJROW(3) = TMP1*TMP3/TMP4
30  CONTINUE
40  CONTINUE
      RETURN

```

```

C      LAST CARD OF SUBROUTINE FCN.
C
C

```

```

      END

```

Results obtained with different compilers or machines
may be slightly different.

FINAL L2 NORM OF THE RESIDUALS 0.9063596D-01

NUMBER OF FUNCTION EVALUATIONS 6

NUMBER OF JACOBIAN EVALUATIONS 5

EXIT PARAMETER 1

FINAL APPROXIMATE SOLUTION

0.8241058D-01 0.1133037D+01 0.2343695D+01

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Documentation for MINPACK subroutine LMDIF1

Double precision version

Argonne National Laboratory

Burton S. Garbow, Kenneth E. Hillstom, Jorge J. More

March 1980

1. Purpose.

The purpose of LMDIF1 is to minimize the sum of the squares of M nonlinear functions in N variables by a modification of the Levenberg-Marquardt algorithm. This is done by using the more general least-squares solver LMDIF. The user must provide a subroutine which calculates the functions. The Jacobian is then calculated by a forward-difference approximation.

2. Subroutine and type statements.

```
SUBROUTINE LMDIF1(FCN,M,N,X,FVEC,TOL,INFO,IWA,WA,LWA)
INTEGER M,N,INFO,LWA
INTEGER IWA(N)
DOUBLE PRECISION TOL
DOUBLE PRECISION X(N),FVEC(M),WA(LWA)
EXTERNAL FCN
```

3. Parameters.

Parameters designated as input parameters must be specified on entry to LMDIF1 and are not changed on exit, while parameters designated as output parameters need not be specified on entry and are set to appropriate values on exit from LMDIF1.

FCN is the name of the user-supplied subroutine which calculates the functions. FCN must be declared in an EXTERNAL statement in the user calling program, and should be written as follows.

```
SUBROUTINE FCN(M,N,X,FVEC,IFLAG)
INTEGER M,N,IFLAG
DOUBLE PRECISION X(N),FVEC(M)
-----
CALCULATE THE FUNCTIONS AT X AND
RETURN THIS VECTOR IN FVEC.
-----
RETURN
END
```

The value of IFLAG should not be changed by FCN unless the user wants to terminate execution of LMDIF1. In this case set

IFLAG to a negative integer.

M is a positive integer input variable set to the number of functions.

N is a positive integer input variable set to the number of variables. N must not exceed M.

X is an array of length N. On input X must contain an initial estimate of the solution vector. On output X contains the final estimate of the solution vector.

FVEC is an output array of length M which contains the functions evaluated at the output X.

TOL is a nonnegative input variable. Termination occurs when the algorithm estimates either that the relative error in the sum of squares is at most TOL or that the relative error between X and the solution is at most TOL. Section 4 contains more details about TOL.

INFO is an integer output variable. If the user has terminated execution, INFO is set to the (negative) value of IFLAG. See description of FCN. Otherwise, INFO is set as follows.

INFO = 0 Improper input parameters.

INFO = 1 Algorithm estimates that the relative error in the sum of squares is at most TOL.

INFO = 2 Algorithm estimates that the relative error between X and the solution is at most TOL.

INFO = 3 Conditions for INFO = 1 and INFO = 2 both hold.

INFO = 4 FVEC is orthogonal to the columns of the Jacobian to machine precision.

INFO = 5 Number of calls to FCN has reached or exceeded $200*(N+1)$.

INFO = 6 TOL is too small. No further reduction in the sum of squares is possible.

INFO = 7 TOL is too small. No further improvement in the approximate solution X is possible.

Sections 4 and 5 contain more details about INFO.

IWA is an integer work array of length N.

WA is a work array of length LWA.

LWA is a positive integer input variable not less than

$M*N+5*N+M$.

4. Successful completion.

The accuracy of LMDIF1 is controlled by the convergence parameter TOL. This parameter is used in tests which make three types of comparisons between the approximation X and a solution XSOL. LMDIF1 terminates when any of the tests is satisfied. If TOL is less than the machine precision (as defined by the MINPACK function DPMPAR(1)), then LMDIF1 only attempts to satisfy the test defined by the machine precision. Further progress is not usually possible. Unless high precision solutions are required, the recommended value for TOL is the square root of the machine precision.

The tests assume that the functions are reasonably well behaved. If this condition is not satisfied, then LMDIF1 may incorrectly indicate convergence. The validity of the answer can be checked, for example, by rerunning LMDIF1 with a tighter tolerance.

First convergence test. If $ENORM(Z)$ denotes the Euclidean norm of a vector Z, then this test attempts to guarantee that

$$ENORM(FVEC) \leq (1+TOL)*ENORM(FVECS),$$

where FVECS denotes the functions evaluated at XSOL. If this condition is satisfied with $TOL = 10^{*(-K)}$, then the final residual norm $ENORM(FVEC)$ has K significant decimal digits and INFO is set to 1 (or to 3 if the second test is also satisfied).

Second convergence test. If D is a diagonal matrix (implicitly generated by LMDIF1) whose entries contain scale factors for the variables, then this test attempts to guarantee that

$$ENORM(D*(X-XSOL)) \leq TOL*ENORM(D*XSOL).$$

If this condition is satisfied with $TOL = 10^{*(-K)}$, then the larger components of $D*X$ have K significant decimal digits and INFO is set to 2 (or to 3 if the first test is also satisfied). There is a danger that the smaller components of $D*X$ may have large relative errors, but the choice of D is such that the accuracy of the components of X is usually related to their sensitivity.

Third convergence test. This test is satisfied when FVEC is orthogonal to the columns of the Jacobian to machine precision. There is no clear relationship between this test and the accuracy of LMDIF1, and furthermore, the test is equally well satisfied at other critical points, namely maximizers and saddle points. Also, errors in the functions (see below) may result in the test being satisfied at a point not close to the

minimum. Therefore, termination caused by this test (INFO = 4) should be examined carefully.

5. Unsuccessful completion.

Unsuccessful termination of LMDIF1 can be due to improper input parameters, arithmetic interrupts, an excessive number of function evaluations, or errors in the functions.

Improper input parameters. INFO is set to 0 if N .LE. 0, or M .LT. N, or TOL .LT. 0.DO, or LWA .LT. M*N+5*N+M.

Arithmetic interrupts. If these interrupts occur in the FCN subroutine during an early stage of the computation, they may be caused by an unacceptable choice of X by LMDIF1. In this case, it may be possible to remedy the situation by not evaluating the functions here, but instead setting the components of FVEC to numbers that exceed those in the initial FVEC, thereby indirectly reducing the step length. The step length can be more directly controlled by using instead LMDIF, which includes in its calling sequence the step-length-governing parameter FACTOR.

Excessive number of function evaluations. If the number of calls to FCN reaches $200*(N+1)$, then this indicates that the routine is converging very slowly as measured by the progress of FVEC, and INFO is set to 5. In this case, it may be helpful to restart LMDIF1, thereby forcing it to disregard old (and possibly harmful) information.

Errors in the functions. The choice of step length in the forward-difference approximation to the Jacobian assumes that the relative errors in the functions are of the order of the machine precision. If this is not the case, LMDIF1 may fail (usually with INFO = 4). The user should then use LMDIF instead, or one of the programs which require the analytic Jacobian (LMDER1 and LMDER).

6. Characteristics of the algorithm.

LMDIF1 is a modification of the Levenberg-Marquardt algorithm. Two of its main characteristics involve the proper use of implicitly scaled variables and an optimal choice for the correction. The use of implicitly scaled variables achieves scale invariance of LMDIF1 and limits the size of the correction in any direction where the functions are changing rapidly. The optimal choice of the correction guarantees (under reasonable conditions) global convergence from starting points far from the solution and a fast rate of convergence for problems with small residuals.

Timing. The time required by LMDIF1 to solve a given problem

depends on M and N, the behavior of the functions, the accuracy requested, and the starting point. The number of arithmetic operations needed by LMDIF1 is about N^3 to process each evaluation of the functions (one call to FCN) and $M(N^2)$ to process each approximation to the Jacobian (N calls to FCN). Unless FCN can be evaluated quickly, the timing of LMDIF1 will be strongly influenced by the time spent in FCN.

Storage. LMDIF1 requires $M \cdot N + 2 \cdot M + 6 \cdot N$ double precision storage locations and N integer storage locations, in addition to the storage required by the program. There are no internally declared storage arrays.

7. Subprograms required.

USER-supplied FCN

MINPACK-supplied ... DPMPAR, ENORM, FDJAC2, LMDIF, LMPAR,
QRFAC, QRSOLV

FORTTRAN-supplied ... DABS, DMAX1, DMIN1, DSQRT, MOD

8. References.

Jorge J. More, The Levenberg-Marquardt Algorithm, Implementation and Theory. Numerical Analysis, G. A. Watson, editor. Lecture Notes in Mathematics 630, Springer-Verlag, 1977.

9. Example.

The problem is to determine the values of $x(1)$, $x(2)$, and $x(3)$ which provide the best fit (in the least squares sense) of

$$x(1) + u(i)/(v(i) \cdot x(2) + w(i) \cdot x(3)), \quad i = 1, 15$$

to the data

$$y = (0.14, 0.18, 0.22, 0.25, 0.29, 0.32, 0.35, 0.39, \\ 0.37, 0.58, 0.73, 0.96, 1.34, 2.10, 4.39),$$

where $u(i) = i$, $v(i) = 16 - i$, and $w(i) = \min(u(i), v(i))$. The i -th component of FVEC is thus defined by

$$y(i) - (x(1) + u(i)/(v(i) \cdot x(2) + w(i) \cdot x(3))).$$

```
C *****
C
C DRIVER FOR LMDIF1 EXAMPLE.
C DOUBLE PRECISION VERSION
C
```



```

C      *****
      INTEGER J,M,N,INFO,LWA,NWRITE
      INTEGER IWA(3)
      DOUBLE PRECISION TOL,FNORM
      DOUBLE PRECISION X(3),FVEC(15),WA(75)
      DOUBLE PRECISION ENORM,DPMPAR
      EXTERNAL FCN

C
C      LOGICAL OUTPUT UNIT IS ASSUMED TO BE NUMBER 6.
C
C      DATA NWRITE /6/

C      M = 15
      N = 3

C
C      THE FOLLOWING STARTING VALUES PROVIDE A ROUGH FIT.
C
      X(1) = 1.D0
      X(2) = 1.D0
      X(3) = 1.D0

C
      LWA = 75

C
C      SET TOL TO THE SQUARE ROOT OF THE MACHINE PRECISION.
C      UNLESS HIGH PRECISION SOLUTIONS ARE REQUIRED,
C      THIS IS THE RECOMMENDED SETTING.
C
      TOL = DSQRT(DPMPAR(1))

C
      CALL LMDIF1(FCN,M,N,X,FVEC,TOL,INFO,IWA,WA,LWA)
      FNORM = ENORM(M,FVEC)
      WRITE (NWRITE,1000) FNORM,INFO,(X(J),J=1,N)
      STOP
1000 FORMAT (5X,31H FINAL L2 NORM OF THE RESIDUALS,D15.7 //
*          5X,15H EXIT PARAMETER,16X,I10 //
*          5X,27H FINAL APPROXIMATE SOLUTION // 5X,3D15.7)

C
C      LAST CARD OF DRIVER FOR LMDIF1 EXAMPLE.
C
      END
      SUBROUTINE FCN(M,N,X,FVEC,IFLAG)
      INTEGER M,N,IFLAG
      DOUBLE PRECISION X(N),FVEC(M)

C
C      SUBROUTINE FCN FOR LMDIF1 EXAMPLE.
C
      INTEGER I
      DOUBLE PRECISION TMP1,TMP2,TMP3
      DOUBLE PRECISION Y(15)
      DATA Y(1),Y(2),Y(3),Y(4),Y(5),Y(6),Y(7),Y(8),
*          Y(9),Y(10),Y(11),Y(12),Y(13),Y(14),Y(15)
*          /1.4D-1,1.8D-1,2.2D-1,2.5D-1,2.9D-1,3.2D-1,3.5D-1,3.9D-1,
*          3.7D-1,5.8D-1,7.3D-1,9.6D-1,1.34D0,2.1D0,4.39D0/
C

```

```
DO 10 I = 1, 15
  TMP1 = I
  TMP2 = 16 - I
  TMP3 = TMP1
  IF (I .GT. 8) TMP3 = TMP2
  FVEC(I) = Y(I) - (X(1) + TMP1/(X(2)*TMP2 + X(3)*TMP3))
10  CONTINUE
  RETURN
```

C
C
C

LAST CARD OF SUBROUTINE FCN.

END

Results obtained with different compilers or machines
may be slightly different.

FINAL L2 NORM OF THE RESIDUALS 0.9063596D-01

EXIT PARAMETER 1

FINAL APPROXIMATE SOLUTION

0.8241057D-01 0.1133037D+01 0.2343695D+01

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Documentation for MINPACK subroutine LMDIF

Double precision version

Argonne National Laboratory

Burton S. Garbow, Kenneth E. Hillstom, Jorge J. More

March 1980

1. Purpose.

The purpose of LMDIF is to minimize the sum of the squares of M nonlinear functions in N variables by a modification of the Levenberg-Marquardt algorithm. The user must provide a subroutine which calculates the functions. The Jacobian is then calculated by a forward-difference approximation.

2. Subroutine and type statements.

```

SUBROUTINE LMDIF(FCN,M,N,X,FVEC,FTOL,XTOL,GTOL,MAXFEV,EPSFCN,
*              DIAG,MODE,FACTOR,NPRINT,INFO,NFEV,FJAC,LDFJAC,
*              IPVT,QTF,WA1,WA2,WA3,WA4)
  INTEGER M,N,MAXFEV,MODE,NPRINT,INFO,NFEV,LDFJAC
  INTEGER IPVT(N)
  DOUBLE PRECISION FTOL,XTOL,GTOL,EPSFCN,FACTOR
  DOUBLE PRECISION X(N),FVEC(M),DIAG(N),FJAC(LDFJAC,N),QTF(N),
*              WA1(N),WA2(N),WA3(N),WA4(M)
  EXTERNAL FCN

```

3. Parameters.

Parameters designated as input parameters must be specified on entry to LMDIF and are not changed on exit, while parameters designated as output parameters need not be specified on entry and are set to appropriate values on exit from LMDIF.

FCN is the name of the user-supplied subroutine which calculates the functions. FCN must be declared in an EXTERNAL statement in the user calling program, and should be written as follows.

```

SUBROUTINE FCN(M,N,X,FVEC,IFLAG)
  INTEGER M,N,IFLAG
  DOUBLE PRECISION X(N),FVEC(M)
  -----
  CALCULATE THE FUNCTIONS AT X AND
  RETURN THIS VECTOR IN FVEC.
  -----
  RETURN
  END

```

The value of IFLAG should not be changed by FCN unless the user wants to terminate execution of LMDIF. In this case set IFLAG to a negative integer.

M is a positive integer input variable set to the number of functions.

N is a positive integer input variable set to the number of variables. N must not exceed M.

X is an array of length N. On input X must contain an initial estimate of the solution vector. On output X contains the final estimate of the solution vector.

FVEC is an output array of length M which contains the functions evaluated at the output X.

FTOL is a nonnegative input variable. Termination occurs when both the actual and predicted relative reductions in the sum of squares are at most FTOL. Therefore, FTOL measures the relative error desired in the sum of squares. Section 4 contains more details about FTOL.

XTOL is a nonnegative input variable. Termination occurs when the relative error between two consecutive iterates is at most XTOL. Therefore, XTOL measures the relative error desired in the approximate solution. Section 4 contains more details about XTOL.

GTOL is a nonnegative input variable. Termination occurs when the cosine of the angle between FVEC and any column of the Jacobian is at most GTOL in absolute value. Therefore, GTOL measures the orthogonality desired between the function vector and the columns of the Jacobian. Section 4 contains more details about GTOL.

MAXFEV is a positive integer input variable. Termination occurs when the number of calls to FCN is at least MAXFEV by the end of an iteration.

EPSFCN is an input variable used in determining a suitable step for the forward-difference approximation. This approximation assumes that the relative errors in the functions are of the order of EPSFCN. If EPSFCN is less than the machine precision, it is assumed that the relative errors in the functions are of the order of the machine precision.

DIAG is an array of length N. If MODE = 1 (see below), DIAG is internally set. If MODE = 2, DIAG must contain positive entries that serve as multiplicative scale factors for the variables.

MODE is an integer input variable. If MODE = 1, the variables will be scaled internally. If MODE = 2, the scaling is

specified by the input DIAG. Other values of MODE are equivalent to MODE = 1.

FACTOR is a positive input variable used in determining the initial step bound. This bound is set to the product of FACTOR and the Euclidean norm of DIAG*X if nonzero, or else to FACTOR itself. In most cases FACTOR should lie in the interval (.1,100.). 100. is a generally recommended value.

NPRINT is an integer input variable that enables controlled printing of iterates if it is positive. In this case, FCN is called with IFLAG = 0 at the beginning of the first iteration and every NPRINT iterations thereafter and immediately prior to return, with X and FVEC available for printing. If NPRINT is not positive, no special calls of FCN with IFLAG = 0 are made.

INFO is an integer output variable. If the user has terminated execution, INFO is set to the (negative) value of IFLAG. See description of FCN. Otherwise, INFO is set as follows.

INFO = 0 Improper input parameters.

INFO = 1 Both actual and predicted relative reductions in the sum of squares are at most FTOL.

INFO = 2 Relative error between two consecutive iterates is at most XTOL.

INFO = 3 Conditions for INFO = 1 and INFO = 2 both hold.

INFO = 4 The cosine of the angle between FVEC and any column of the Jacobian is at most GTOL in absolute value.

INFO = 5 Number of calls to FCN has reached or exceeded MAXFEV.

INFO = 6 FTOL is too small. No further reduction in the sum of squares is possible.

INFO = 7 XTOL is too small. No further improvement in the approximate solution X is possible.

INFO = 8 GTOL is too small. FVEC is orthogonal to the columns of the Jacobian to machine precision.

Sections 4 and 5 contain more details about INFO.

NFEV is an integer output variable set to the number of calls to FCN.

FJAC is an output M by N array. The upper N by N submatrix of FJAC contains an upper triangular matrix R with diagonal elements of nonincreasing magnitude such that

$$P^T * (JAC^T * JAC) * P = R^T * R,$$

where P is a permutation matrix and JAC is the final calculated Jacobian. Column j of P is column IPVT(j) (see below) of the identity matrix. The lower trapezoidal part of FJAC contains information generated during the computation of R.

LDEFJAC is a positive integer input variable not less than M which specifies the leading dimension of the array FJAC.

IPVT is an integer output array of length N. IPVT defines a permutation matrix P such that $JAC * P = Q * R$, where JAC is the final calculated Jacobian, Q is orthogonal (not stored), and R is upper triangular with diagonal elements of nonincreasing magnitude. Column j of P is column IPVT(j) of the identity matrix.

QTF is an output array of length N which contains the first N elements of the vector $(Q \text{ transpose}) * FVEC$.

WA1, WA2, and WA3 are work arrays of length N.

WA4 is a work array of length M.

4. Successful completion.

The accuracy of LMDIF is controlled by the convergence parameters FTOL, XTOL, and GTOL. These parameters are used in tests which make three types of comparisons between the approximation X and a solution XSOL. LMDIF terminates when any of the tests is satisfied. If any of the convergence parameters is less than the machine precision (as defined by the MINPACK function DPMPAR(1)), then LMDIF only attempts to satisfy the test defined by the machine precision. Further progress is not usually possible.

The tests assume that the functions are reasonably well behaved. If this condition is not satisfied, then LMDIF may incorrectly indicate convergence. The validity of the answer can be checked, for example, by rerunning LMDIF with tighter tolerances.

First convergence test. If ENORM(Z) denotes the Euclidean norm of a vector Z, then this test attempts to guarantee that

$$ENORM(FVEC) \leq (1 + FTOL) * ENORM(FVECS),$$

where FVECS denotes the functions evaluated at XSOL. If this condition is satisfied with $FTOL = 10^{(-K)}$, then the final residual norm ENORM(FVEC) has K significant decimal digits and INFO is set to 1 (or to 3 if the second test is also satisfied). Unless high precision solutions are required, the

recommended value for FTOL is the square root of the machine precision.

Second convergence test. If D is the diagonal matrix whose entries are defined by the array DIAG, then this test attempts to guarantee that

$$\text{ENORM}(D*(X-XSOL)) \leq \text{XTOL} * \text{ENORM}(D*XSOL).$$

If this condition is satisfied with $\text{XTOL} = 10^{**(-K)}$, then the larger components of $D*X$ have K significant decimal digits and INFO is set to 2 (or to 3 if the first test is also satisfied). There is a danger that the smaller components of $D*X$ may have large relative errors, but if $\text{MODE} = 1$, then the accuracy of the components of X is usually related to their sensitivity. Unless high precision solutions are required, the recommended value for XTOL is the square root of the machine precision.

Third convergence test. This test is satisfied when the cosine of the angle between FVEC and any column of the Jacobian at X is at most GTOL in absolute value. There is no clear relationship between this test and the accuracy of LMDIF, and furthermore, the test is equally well satisfied at other critical points, namely maximizers and saddle points. Therefore, termination caused by this test ($\text{INFO} = 4$) should be examined carefully. The recommended value for GTOL is zero.

5. Unsuccessful completion.

Unsuccessful termination of LMDIF can be due to improper input parameters, arithmetic interrupts, or an excessive number of function evaluations.

Improper input parameters. INFO is set to 0 if $N \leq 0$, or $M \leq N$, or $\text{LDFJAC} \leq M$, or $\text{FTOL} \leq 0.00$, or $\text{XTOL} \leq 0.00$, or $\text{GTOL} \leq 0.00$, or $\text{MAXFEV} \leq 0$, or $\text{FACTOR} \leq 0.00$.

Arithmetic interrupts. If these interrupts occur in the FCN subroutine during an early stage of the computation, they may be caused by an unacceptable choice of X by LMDIF. In this case, it may be possible to remedy the situation by rerunning LMDIF with a smaller value of FACTOR.

Excessive number of function evaluations. A reasonable value for MAXFEV is $200*(N+1)$. If the number of calls to FCN reaches MAXFEV, then this indicates that the routine is converging very slowly as measured by the progress of FVEC, and INFO is set to 5. In this case, it may be helpful to restart LMDIF with MODE set to 1.

6. Characteristics of the algorithm.

LMDIF is a modification of the Levenberg-Marquardt algorithm. Two of its main characteristics involve the proper use of implicitly scaled variables (if `MODE = 1`) and an optimal choice for the correction. The use of implicitly scaled variables achieves scale invariance of LMDIF and limits the size of the correction in any direction where the functions are changing rapidly. The optimal choice of the correction guarantees (under reasonable conditions) global convergence from starting points far from the solution and a fast rate of convergence for problems with small residuals.

Timing. The time required by LMDIF to solve a given problem depends on M and N , the behavior of the functions, the accuracy requested, and the starting point. The number of arithmetic operations needed by LMDIF is about N^3 to process each evaluation of the functions (one call to `FCN`) and $M(N^2)$ to process each approximation to the Jacobian (N calls to `FCN`). Unless `FCN` can be evaluated quickly, the timing of LMDIF will be strongly influenced by the time spent in `FCN`.

Storage. LMDIF requires $M \cdot N + 2 \cdot M + 6 \cdot N$ double precision storage locations and N integer storage locations, in addition to the storage required by the program. There are no internally declared storage arrays.

7. Subprograms required.

USER-supplied `FCN`

MINPACK-supplied ... `DPMPAR, ENORM, FDJAC2, LMPAR, QRFAC, QRSOLV`

FORTTRAN-supplied ... `DABS, DMAX1, DMIN1, DSQRT, MOD`

8. References.

Jorge J. More, The Levenberg-Marquardt Algorithm, Implementation and Theory. Numerical Analysis, G. A. Watson, editor. Lecture Notes in Mathematics 630, Springer-Verlag, 1977.

9. Example.

The problem is to determine the values of $x(1)$, $x(2)$, and $x(3)$ which provide the best fit (in the least squares sense) of

$$x(1) + u(i)/(v(i) \cdot x(2) + w(i) \cdot x(3)), \quad i = 1, 15$$

to the data

$$y = (0.14, 0.18, 0.22, 0.25, 0.29, 0.32, 0.35, 0.39, \\ 0.37, 0.58, 0.73, 0.96, 1.34, 2.10, 4.39),$$

where $u(i) = i$, $v(i) = 16 - i$, and $w(i) = \min(u(i), v(i))$. The i -th component of FVEC is thus defined by

$$y(i) = (x(1) + u(i)/(v(i)*x(2) + w(i)*x(3))).$$

DRIVER FOR LMDIF EXAMPLE.
DOUBLE PRECISION VERSION

INTEGER J, M, N, MAXFEV, MODE, NPRINT, INFO, NFEV, LDFJAC, NWRITE
INTEGER IPVT(3)
DOUBLE PRECISION FTOL, XTOL, GTOL, EPSFCN, FACTOR, FNORM
DOUBLE PRECISION X(3), FVEC(15), DIAG(3), FJAC(15, 3), QTF(3),
* WA1(3), WA2(3), WA3(3), WA4(15)
DOUBLE PRECISION ENORM, DPMPAR
EXTERNAL FCN

LOGICAL OUTPUT UNIT IS ASSUMED TO BE NUMBER 6.

DATA NWRITE /6/

M = 15
N = 3

THE FOLLOWING STARTING VALUES PROVIDE A ROUGH FIT.

X(1) = 1.D0
X(2) = 1.D0
X(3) = 1.D0

LDFJAC = 15

SET FTOL AND XTOL TO THE SQUARE ROOT OF THE MACHINE PRECISION
AND GTOL TO ZERO. UNLESS HIGH PRECISION SOLUTIONS ARE
REQUIRED, THESE ARE THE RECOMMENDED SETTINGS.

FTOL = DSQRT(DPMPAR(1))
XTOL = DSQRT(DPMPAR(1))
GTOL = 0.D0

MAXFEV = 800
EPSFCN = 0.D0
MODE = 1
FACTOR = 1.D2
NPRINT = 0

CALL LMDIF(FCN, M, N, X, FVEC, FTOL, XTOL, GTOL, MAXFEV, EPSFCN,
* DIAG, MODE, FACTOR, NPRINT, INFO, NFEV, FJAC, LDFJAC,
* IPVT, QTF, WA1, WA2, WA3, WA4)

```

      FNORM = ENORM(M,FVEC)
      WRITE (NWRITE,1000) FNORM,NFEV,INFO,(X(J),J=1,N)
      STOP
1000 FORMAT (5X,31H FINAL L2 NORM OF THE RESIDUALS,D15.7 //
*          5X,31H NUMBER OF FUNCTION EVALUATIONS,I10 //
*          5X,15H EXIT PARAMETER,16X,I10 //
*          5X,27H FINAL APPROXIMATE SOLUTION // 5X,3D15.7)

C
C      LAST CARD OF DRIVER FOR LMDIF EXAMPLE.
C
      END
      SUBROUTINE FCN(M,N,X,FVEC,IFLAG)
      INTEGER M,N,IFLAG
      DOUBLE PRECISION X(N),FVEC(M)

C
C      SUBROUTINE FCN FOR LMDIF EXAMPLE.
C
      INTEGER I
      DOUBLE PRECISION TMP1,TMP2,TMP3
      DOUBLE PRECISION Y(15)
      DATA Y(1),Y(2),Y(3),Y(4),Y(5),Y(6),Y(7),Y(8),
*          Y(9),Y(10),Y(11),Y(12),Y(13),Y(14),Y(15)
*          /1.4D-1,1.8D-1,2.2D-1,2.5D-1,2.9D-1,3.2D-1,3.5D-1,3.9D-1,
*          3.7D-1,5.8D-1,7.3D-1,9.6D-1,1.34D0,2.1D0,4.39D0/

C
      IF (IFLAG .NE. 0) GO TO 5

C
C      INSERT PRINT STATEMENTS HERE WHEN NPRINT IS POSITIVE.
C
      RETURN
5 CONTINUE
      DO 10 I = 1, 15
          TMP1 = I
          TMP2 = 16 - I
          TMP3 = TMP1
          IF (I .GT. 8) TMP3 = TMP2
          FVEC(I) = Y(I) - (X(1) + TMP1/(X(2)*TMP2 + X(3)*TMP3))
10 CONTINUE
      RETURN

C
C      LAST CARD OF SUBROUTINE FCN.
C
      END

```

Results obtained with different compilers or machines
may be slightly different.

FINAL L2 NORM OF THE RESIDUALS 0.9063596D-01

NUMBER OF FUNCTION EVALUATIONS 21

EXIT PARAMETER 1

FINAL APPROXIMATE SOLUTION

0.8241057D-01 0.1133037D+01 0.2343695D+01

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Documentation for MINPACK subroutine CHKDER

Double precision version

Argonne National Laboratory

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March 1980

1. Purpose.

The purpose of CHKDER is to check the gradients of M nonlinear functions in N variables, evaluated at a point X , for consistency with the functions themselves. The user must call CHKDER twice, first with $MODE = 1$ and then with $MODE = 2$.

2. Subroutine and type statements.

```
SUBROUTINE CHKDER(M,N,X,FVEC,FJAC,LDFJAC,XP,FVECP,MODE,ERR)
  INTEGER M,N,LDFJAC,MODE
  DOUBLE PRECISION X(N),FVEC(M),FJAC(LDFJAC,N),XP(N),FVECP(M),
  *                ERR(M)
```

3. Parameters.

Parameters designated as input parameters must be specified on entry to CHKDER and are not changed on exit, while parameters designated as output parameters need not be specified on entry and are set to appropriate values on exit from CHKDER.

M is a positive integer input variable set to the number of functions.

N is a positive integer input variable set to the number of variables.

X is an input array of length N .

$FVEC$ is an array of length M . On input when $MODE = 2$, $FVEC$ must contain the functions evaluated at X .

$FJAC$ is an M by N array. On input when $MODE = 2$, the rows of $FJAC$ must contain the gradients of the respective functions evaluated at X .

$LDFJAC$ is a positive integer input variable not less than M which specifies the leading dimension of the array $FJAC$.

XP is an array of length N . On output when $MODE = 1$, XP is set to a neighboring point of X .

FVECP is an array of length M. On input when MODE = 2, FVECP must contain the functions evaluated at XP.

MODE is an integer input variable set to 1 on the first call and 2 on the second. Other values of MODE are equivalent to MODE = 1.

ERR is an array of length M. On output when MODE = 2, ERR contains measures of correctness of the respective gradients. If there is no severe loss of significance, then if ERR(I) is 1.0 the I-th gradient is correct, while if ERR(I) is 0.0 the I-th gradient is incorrect. For values of ERR between 0.0 and 1.0, the categorization is less certain. In general, a value of ERR(I) greater than 0.5 indicates that the I-th gradient is probably correct, while a value of ERR(I) less than 0.5 indicates that the I-th gradient is probably incorrect.

4. Successful completion.

CHKDER usually guarantees that if ERR(I) is 1.0, then the I-th gradient at X is consistent with the I-th function. This suggests that the input X be such that consistency of the gradient at X implies consistency of the gradient at all points of interest. If all the components of X are distinct and the fractional part of each one has two nonzero digits, then X is likely to be a satisfactory choice.

If ERR(I) is not 1.0 but is greater than 0.5, then the I-th gradient is probably consistent with the I-th function (the more so the larger ERR(I) is), but the conditions for ERR(I) to be 1.0 have not been completely satisfied. In this case, it is recommended that CHKDER be rerun with other input values of X. If ERR(I) is always greater than 0.5, then the I-th gradient is consistent with the I-th function.

5. Unsuccessful completion.

CHKDER does not perform reliably if cancellation or rounding errors cause a severe loss of significance in the evaluation of a function. Therefore, none of the components of X should be unusually small (in particular, zero) or any other value which may cause loss of significance. The relative differences between corresponding elements of FVECP and FVEC should be at least two orders of magnitude greater than the machine precision (as defined by the MINPACK function DPMPAR(1)). If there is a severe loss of significance in the evaluation of the I-th function, then ERR(I) may be 0.0 and yet the I-th gradient could be correct.

If ERR(I) is not 0.0 but is less than 0.5, then the I-th gradient is probably not consistent with the I-th function (the more so the smaller ERR(I) is), but the conditions for ERR(I) to

be 0.0 have not been completely satisfied. In this case, it is recommended that CHKDER be rerun with other input values of X. If ERR(I) is always less than 0.5 and if there is no severe loss of significance, then the I-th gradient is not consistent with the I-th function.

6. Characteristics of the algorithm.

CHKDER checks the I-th gradient for consistency with the I-th function by computing a forward-difference approximation along a suitably chosen direction and comparing this approximation with the user-supplied gradient along the same direction. The principal characteristic of CHKDER is its invariance to changes in scale of the variables or functions.

Timing. The time required by CHKDER depends only on M and N. The number of arithmetic operations needed by CHKDER is about N when MODE = 1 and M*N when MODE = 2.

Storage. CHKDER requires $M*N + 3*M + 2*N$ double precision storage locations, in addition to the storage required by the program. There are no internally declared storage arrays.

7. Subprograms required.

MINPACK-supplied ... DPMPAR

FORTTRAN-supplied DABS, DLOG10, DSQRT

8. References.

None.

9. Example.

This example checks the Jacobian matrix for the problem that determines the values of $x(1)$, $x(2)$, and $x(3)$ which provide the best fit (in the least squares sense) of

$$x(1) + u(i)/(v(i)*x(2) + w(i)*x(3)), \quad i = 1, 15$$

to the data

$$y = (0.14, 0.18, 0.22, 0.25, 0.29, 0.32, 0.35, 0.39, \\ 0.37, 0.58, 0.73, 0.96, 1.34, 2.10, 4.39),$$

where $u(i) = i$, $v(i) = 16 - i$, and $w(i) = \min(u(i), v(i))$. The i-th component of FVEC is thus defined by

$$y(i) - (x(1) + u(i)/(v(i)*x(2) + w(i)*x(3))).$$


```

C      *****
C
C      DRIVER FOR CHKDER EXAMPLE.
C      DOUBLE PRECISION VERSION
C
C      *****
C      INTEGER I,M,N,LDFJAC,MODE,NWRITE
C      DOUBLE PRECISION X(3),FVEC(15),FJAC(15,3),XP(3),FVECP(15),
*      ERR(15)
C
C      LOGICAL OUTPUT UNIT IS ASSUMED TO BE NUMBER 6.
C
C      DATA NWRITE /6/
C
C      M = 15
C      N = 3
C
C      THE FOLLOWING VALUES SHOULD BE SUITABLE FOR
C      CHECKING THE JACOBIAN MATRIX.
C
C      X(1) = 9.2D-1
C      X(2) = 1.3D-1
C      X(3) = 5.4D-1
C
C      LDFJAC = 15
C
C      MODE = 1
C      CALL CHKDER(M,N,X,FVEC,FJAC,LDFJAC,XP,FVECP,MODE,ERR)
C      MODE = 2
C      CALL FCN(M,N,X,FVEC,FJAC,LDFJAC,1)
C      CALL FCN(M,N,X,FVEC,FJAC,LDFJAC,2)
C      CALL FCN(M,N,XP,FVECP,FJAC,LDFJAC,1)
C      CALL CHKDER(M,N,X,FVEC,FJAC,LDFJAC,XP,FVECP,MODE,ERR)
C
C      DO 10 I = 1, M
C          FVECP(I) = FVECP(I) - FVEC(I)
10      CONTINUE
C      WRITE (NWRITE,1000) (FVEC(I),I=1,M)
C      WRITE (NWRITE,2000) (FVECP(I),I=1,M)
C      WRITE (NWRITE,3000) (ERR(I),I=1,M)
C      STOP
1000  FORMAT (/5X,5H FVEC // (5X,3D15.7))
2000  FORMAT (/5X,13H FVECP - FVEC // (5X,3D15.7))
3000  FORMAT (/5X,4H ERR // (5X,3D15.7))
C
C      LAST CARD OF DRIVER FOR CHKDER EXAMPLE.
C
C      END
C      SUBROUTINE FCN(M,N,X,FVEC,FJAC,LDFJAC,IFLAG)
C      INTEGER M,N,LDFJAC,IFLAG
C      DOUBLE PRECISION X(N),FVEC(M),FJAC(LDFJAC,N)
C
C      SUBROUTINE FCN FOR CHKDER EXAMPLE.

```

```

      INTEGER I
      DOUBLE PRECISION TMP1,TMP2,TMP3,TMP4
      DOUBLE PRECISION Y(15)
      DATA Y(1),Y(2),Y(3),Y(4),Y(5),Y(6),Y(7),Y(8),
*          Y(9),Y(10),Y(11),Y(12),Y(13),Y(14),Y(15)
*          /1.4D-1,1.8D-1,2.2D-1,2.5D-1,2.9D-1,3.2D-1,3.5D-1,3.9D-1,
*          3.7D-1,5.8D-1,7.3D-1,9.6D-1,1.34D0,2.1D0,4.39D0/

C
      IF (IFLAG .EQ. 2) GO TO 20
      DO 10 I = 1, 15
        TMP1 = I
        TMP2 = 16 - I
        TMP3 = TMP1
        IF (I .GT. 8) TMP3 = TMP2
        FVEC(I) = Y(I) - (X(1) + TMP1/(X(2)*TMP2 + X(3)*TMP3))
10     CONTINUE
      GO TO 40
20     CONTINUE
      DO 30 I = 1, 15
        TMP1 = I
        TMP2 = 16 - I

C
C      ERROR INTRODUCED INTO NEXT STATEMENT FOR ILLUSTRATION.
C      CORRECTED STATEMENT SHOULD READ      TMP3 = TMP1 .
C
        TMP3 = TMP2
        IF (I .GT. 8) TMP3 = TMP2
        TMP4 = (X(2)*TMP2 + X(3)*TMP3)**2
        FJAC(I,1) = -1.D0
        FJAC(I,2) = TMP1*TMP2/TMP4
        FJAC(I,3) = TMP1*TMP3/TMP4
30     CONTINUE
40     CONTINUE
      RETURN

C
C      LAST CARD OF SUBROUTINE FCN.
C
      END

      Results obtained with different compilers or machines
      may be different.  In particular, the differences
      FVECP - FVEC are machine dependent.

      FVEC

      -0.1181606D+01 -0.1429655D+01 -0.1606344D+01
      -0.1745269D+01 -0.1840654D+01 -0.1921586D+01
      -0.1984141D+01 -0.2022537D+01 -0.2468977D+01
      -0.2827562D+01 -0.3473582D+01 -0.4437612D+01
      -0.6047662D+01 -0.9267761D+01 -0.1891806D+02

      FVECP - FVEC

      -0.7724666D-08 -0.3432405D-08 -0.2034843D-09

```

0.2313685D-08	0.4331078D-08	0.5984096D-08
0.7363281D-08	0.8531470D-08	0.1488591D-07
0.2335850D-07	0.3522012D-07	0.5301255D-07
0.8266660D-07	0.1419747D-06	0.3198990D-06

ERR

0.1141397D+00	0.9943516D-01	0.9674474D-01
0.9980447D-01	0.1073116D+00	0.1220445D+00
0.1526814D+00	0.1000000D+01	0.1000000D+01
0.1000000D+01	0.1000000D+01	0.1000000D+01
0.1000000D+01	0.1000000D+01	0.1000000D+01

CHAPTER 5

Program Listings

This chapter contains the double precision version of the MINPACK-1 program listings; both single and double precision versions of the subprograms are available with the MINPACK-1 package. The listings appear in the following (alphanumeric) order:

CHKDER, DOGLEG, ENORM, FDJAC1, FDJAC2, HYBRD, HYBRD1,
HYBRJ, HYBRJ1, LMDER, LMDER1, LMDIF, LMDIF1, LMPAR, LMSTR,
LMSTR1, QFORM, QRFAC, QRSOLV, RWUPDT, RLMPYQ, RLUPDT.

Functions SPMPAR (single precision) and DPMPAR (double precision), which provide the machine-dependent constants, appear at the end.

SUBROUTINE CHKDER(M,N,X,FVEC,FJAC,LDFJAC,XP,FVECP,MODE,ERR)	CHDR0010
INTEGER M,N,LDFJAC,MODE	CHDR0020
DOUBLE PRECISION X(N),FVEC(M),FJAC(LDFJAC,N),XP(N),FVECP(M),	CHDR0030
* ERR(M)	CHDR0040
*****	CHDR0050
SUBROUTINE CHKDER	CHDR0060
THIS SUBROUTINE CHECKS THE GRADIENTS OF M NONLINEAR FUNCTIONS	CHDR0070
IN N VARIABLES, EVALUATED AT A POINT X, FOR CONSISTENCY WITH	CHDR0080
THE FUNCTIONS THEMSELVES. THE USER MUST CALL CHKDER TWICE,	CHDR0090
FIRST WITH MODE = 1 AND THEN WITH MODE = 2.	CHDR0100
MODE = 1. ON INPUT, X MUST CONTAIN THE POINT OF EVALUATION.	CHDR0110
ON OUTPUT, XP IS SET TO A NEIGHBORING POINT.	CHDR0120
MODE = 2. ON INPUT, FVEC MUST CONTAIN THE FUNCTIONS AND THE	CHDR0130
ROWS OF FJAC MUST CONTAIN THE GRADIENTS	CHDR0140
OF THE RESPECTIVE FUNCTIONS EACH EVALUATED	CHDR0150
AT X, AND FVECP MUST CONTAIN THE FUNCTIONS	CHDR0160
EVALUATED AT XP.	CHDR0170
ON OUTPUT, ERR CONTAINS MEASURES OF CORRECTNESS OF	CHDR0180
THE RESPECTIVE GRADIENTS.	CHDR0190
THE SUBROUTINE DOES NOT PERFORM RELIABLY IF CANCELLATION OR	CHDR0200
ROUNDING ERRORS CAUSE A SEVERE LOSS OF SIGNIFICANCE IN THE	CHDR0210
EVALUATION OF A FUNCTION. THEREFORE, NONE OF THE COMPONENTS	CHDR0220
OF X SHOULD BE UNUSUALLY SMALL (IN PARTICULAR, ZERO) OR ANY	CHDR0230
OTHER VALUE WHICH MAY CAUSE LOSS OF SIGNIFICANCE.	CHDR0240
THE SUBROUTINE STATEMENT IS	CHDR0250
SUBROUTINE CHKDER(M,N,X,FVEC,FJAC,LDFJAC,XP,FVECP,MODE,ERR)	CHDR0260
WHERE	CHDR0270
M IS A POSITIVE INTEGER INPUT VARIABLE SET TO THE NUMBER	CHDR0280
OF FUNCTIONS.	CHDR0290
N IS A POSITIVE INTEGER INPUT VARIABLE SET TO THE NUMBER	CHDR0300
OF VARIABLES.	CHDR0310
X IS AN INPUT ARRAY OF LENGTH N.	CHDR0320
FVEC IS AN ARRAY OF LENGTH M. ON INPUT WHEN MODE = 2,	CHDR0330
FVEC MUST CONTAIN THE FUNCTIONS EVALUATED AT X.	CHDR0340
FJAC IS AN M BY N ARRAY. ON INPUT WHEN MODE = 2,	CHDR0350
THE ROWS OF FJAC MUST CONTAIN THE GRADIENTS OF	CHDR0360
THE RESPECTIVE FUNCTIONS EVALUATED AT X.	CHDR0370
LDFJAC IS A POSITIVE INTEGER INPUT PARAMETER NOT LESS THAN M	CHDR0380
WHICH SPECIFIES THE LEADING DIMENSION OF THE ARRAY FJAC.	CHDR0390
	CHDR0400
	CHDR0410
	CHDR0420
	CHDR0430
	CHDR0440
	CHDR0450
	CHDR0460
	CHDR0470
	CHDR0480
	CHDR0490
	CHDR0500
	CHDR0510
	CHDR0520
	CHDR0530
	CHDR0540

C	XP IS AN ARRAY OF LENGTH N. ON OUTPUT WHEN MODE = 1,	CHDR0550
C	XP IS SET TO A NEIGHBORING POINT OF X.	CHDR0560
C		CHDR0570
C	FVECP IS AN ARRAY OF LENGTH M. ON INPUT WHEN MODE = 2,	CHDR0580
C	FVECP MUST CONTAIN THE FUNCTIONS EVALUATED AT XP.	CHDR0590
C		CHDR0600
C	MODE IS AN INTEGER INPUT VARIABLE SET TO 1 ON THE FIRST CALL	CHDR0610
C	AND 2 ON THE SECOND. OTHER VALUES OF MODE ARE EQUIVALENT	CHDR0620
C	TO MODE = 1.	CHDR0630
C		CHDR0640
C	ERR IS AN ARRAY OF LENGTH M. ON OUTPUT WHEN MODE = 2,	CHDR0650
C	ERR CONTAINS MEASURES OF CORRECTNESS OF THE RESPECTIVE	CHDR0660
C	GRADIENTS. IF THERE IS NO SEVERE LOSS OF SIGNIFICANCE,	CHDR0670
C	THEN IF ERR(I) IS 1.0 THE I-TH GRADIENT IS CORRECT,	CHDR0680
C	WHILE IF ERR(I) IS 0.0 THE I-TH GRADIENT IS INCORRECT.	CHDR0690
C	FOR VALUES OF ERR BETWEEN 0.0 AND 1.0, THE CATEGORIZATION	CHDR0700
C	IS LESS CERTAIN. IN GENERAL, A VALUE OF ERR(I) GREATER	CHDR0710
C	THAN 0.5 INDICATES THAT THE I-TH GRADIENT IS PROBABLY	CHDR0720
C	CORRECT, WHILE A VALUE OF ERR(I) LESS THAN 0.5 INDICATES	CHDR0730
C	THAT THE I-TH GRADIENT IS PROBABLY INCORRECT.	CHDR0740
C		CHDR0750
C	SUBPROGRAMS CALLED	CHDR0760
C		CHDR0770
C	MINPACK SUPPLIED ... DPMPAR	CHDR0780
C		CHDR0790
C	FORTRAN SUPPLIED ... DABS,DLOG10,DSQRT	CHDR0800
C		CHDR0810
C	ARGONNE-NATIONAL LABORATORY. MINPACK PROJECT. MARCH 1980.	CHDR0820
C	BURTON S. GARBOW, KENNETH E. HILLSTROM, JORGE J. MORE	CHDR0830
C		CHDR0840
C	*****	CHDR0850
C	INTEGER I,J	CHDR0860
C	DOUBLE PRECISION EPS,EPSF,EPSLOG,EPSMCH,FACTOR,ONE,TEMP,ZERO	CHDR0870
C	DOUBLE PRECISION DPMPAR	CHDR0880
C	DATA FACTOR,ONE,ZERO /1.0D2,1.0D0,0.0D0/	CHDR0890
C		CHDR0900
C	EPSMCH IS THE MACHINE PRECISION.	CHDR0910
C		CHDR0920
C	EPSMCH = DPMPAR(1)	CHDR0930
C		CHDR0940
C	EPS = DSQRT(EPSMCH)	CHDR0950
C		CHDR0960
C	IF (MODE .EQ. 2) GO TO 20	CHDR0970
C		CHDR0980
C	MODE = 1.	CHDR0990
C		CHDR1000
C	DO 10 J = 1, N	CHDR1010
	TEMP = EPS*DABS(X(J))	CHDR1020
	IF (TEMP .EQ. ZERO) TEMP = EPS	CHDR1030
	XP(J) = X(J) + TEMP	CHDR1040
10	CONTINUE	CHDR1050
	GO TO 70	CHDR1060
20	CONTINUE	CHDR1070
C		CHDR1080

C	MODE = 2.	CHDR1090
C		CHDR1100
	EPSF = FACTOR*EPSMCH	CHDR1110
	EPSLOG = DLOG10(EPS)	CHDR1120
	DO 30 I = 1, M	CHDR1130
	ERR(I) = ZERO	CHDR1140
30	CONTINUE	CHDR1150
	DO 50 J = 1, N	CHDR1160
	TEMP = DABS(X(J))	CHDR1170
	IF (TEMP .EQ. ZERO) TEMP = ONE	CHDR1180
	DO 40 I = 1, M	CHDR1190
	ERR(I) = ERR(I) + TEMP*FJAC(I,J)	CHDR1200
40	CONTINUE	CHDR1210
50	CONTINUE	CHDR1220
	DO 60 I = 1, M	CHDR1230
	TEMP = ONE	CHDR1240
	IF (FVEC(I) .NE. ZERO .AND. FVECP(I) .NE. ZERO	CHDR1250
*	AND. DABS(FVECP(I)-FVEC(I)) .GE. EPSF*DABS(FVEC(I)))	CHDR1260
*	TEMP = EPS*DABS((FVECP(I)-FVEC(I))/EPS-ERR(I))	CHDR1270
*	/(DABS(FVEC(I)) + DABS(FVECP(I)))	CHDR1280
	ERR(I) = ONE	CHDR1290
	IF (TEMP .GT. EPSMCH .AND. TEMP .LT. EPS)	CHDR1300
*	ERR(I) = (DLOG10(TEMP) - EPSLOG)/EPSLOG	CHDR1310
	IF (TEMP .GE. EPS) ERR(I) = ZERO	CHDR1320
60	CONTINUE	CHDR1330
70	CONTINUE	CHDR1340
C		CHDR1350
	RETURN	CHDR1360
C		CHDR1370
C	LAST CARD OF SUBROUTINE CHKDER.	CHDR1380
C		CHDR1390
	END	CHDR1400

SUBROUTINE DOGLEG(N,R,LR,DIAG,QTB,DELTA,X,WA1,WA2)	DOGL0010
INTEGER N,LR	DOGL0020
DOUBLE PRECISION DELTA	DOGL0030
DOUBLE PRECISION R(LR),DIAG(N),QTB(N),X(N),WA1(N),WA2(N)	DOGL0040
*****	DOGL0050
SUBROUTINE DOGLEG	DOGL0060
GIVEN AN M BY N MATRIX A, AN N BY N NONSINGULAR DIAGONAL	DOGL0070
MATRIX D, AN M-VECTOR B, AND A POSITIVE NUMBER DELTA, THE	DOGL0080
PROBLEM IS TO DETERMINE THE CONVEX COMBINATION X OF THE	DOGL0090
GAUSS-NEWTON AND SCALED GRADIENT DIRECTIONS THAT MINIMIZES	DOGL0100
(A*X - B) IN THE LEAST SQUARES SENSE, SUBJECT TO THE	DOGL0110
RESTRICTION THAT THE EUCLIDEAN NORM OF D*X BE AT MOST DELTA.	DOGL0120
THIS SUBROUTINE COMPLETES THE SOLUTION OF THE PROBLEM	DOGL0130
IF IT IS PROVIDED WITH THE NECESSARY INFORMATION FROM THE	DOGL0140
QR FACTORIZATION OF A. THAT IS, IF $A = Q \cdot R$, WHERE Q HAS	DOGL0150
ORTHOGONAL COLUMNS AND R IS AN UPPER TRIANGULAR MATRIX,	DOGL0160
THEN DOGLEG EXPECTS THE FULL UPPER TRIANGLE OF R AND	DOGL0170
THE FIRST N COMPONENTS OF $(Q \text{ TRANSPOSE}) \cdot B$.	DOGL0180
THE SUBROUTINE STATEMENT IS	DOGL0190
SUBROUTINE DOGLEG(N,R,LR,DIAG,QTB,DELTA,X,WA1,WA2)	DOGL0200
WHERE	DOGL0210
N IS A POSITIVE INTEGER INPUT VARIABLE SET TO THE ORDER OF R.	DOGL0220
R IS AN INPUT ARRAY OF LENGTH LR WHICH MUST CONTAIN THE UPPER	DOGL0230
TRIANGULAR MATRIX R STORED BY ROWS.	DOGL0240
LR IS A POSITIVE INTEGER INPUT VARIABLE NOT LESS THAN	DOGL0250
$(N \cdot (N+1))/2$.	DOGL0260
DIAG IS AN INPUT ARRAY OF LENGTH N WHICH MUST CONTAIN THE	DOGL0270
DIAGONAL ELEMENTS OF THE MATRIX D.	DOGL0280
QTB IS AN INPUT ARRAY OF LENGTH N WHICH MUST CONTAIN THE FIRST	DOGL0290
N ELEMENTS OF THE VECTOR $(Q \text{ TRANSPOSE}) \cdot B$.	DOGL0300
DELTA IS A POSITIVE INPUT VARIABLE WHICH SPECIFIES AN UPPER	DOGL0310
BOUND ON THE EUCLIDEAN NORM OF D*X.	DOGL0320
X IS AN OUTPUT ARRAY OF LENGTH N WHICH CONTAINS THE DESIRED	DOGL0330
CONVEX COMBINATION OF THE GAUSS-NEWTON DIRECTION AND THE	DOGL0340
SCALED GRADIENT DIRECTION.	DOGL0350
WA1 AND WA2 ARE WORK ARRAYS OF LENGTH N.	DOGL0360
SUBPROGRAMS CALLED	DOGL0370
MINPACK-SUPPLIED ... DPMPAR,ENORM	DOGL0380
	DOGL0390
	DOGL0400
	DOGL0410
	DOGL0420
	DOGL0430
	DOGL0440
	DOGL0450
	DOGL0460
	DOGL0470
	DOGL0480
	DOGL0490
	DOGL0500
	DOGL0510
	DOGL0520
	DOGL0530
	DOGL0540

C		DOGL0550
C	FORTTRAN-SUPPLIED ... DABS,DMAX1,DMIN1,DSQRT	DOGL0560
C		DOGL0570
C	ARGONNE NATIONAL LABORATORY. MINPACK PROJECT. MARCH 1980.	DOGL0580
C	BURTON S. GARBOW, KENNETH E. HILLSTROM, JORGE J. MORE	DOGL0590
C		DOGL0600
C	*****	DOGL0610
	INTEGER I,J,JJ,JP1,K,L	DOGL0620
	DOUBLE PRECISION ALPHA,BNORM,EPSMCH,GNORM,ONE,QNORM,SGNORM,SUM,	DOGL0630
	* TEMP,ZERO	DOGL0640
	DOUBLE PRECISION DPMPAR,ENORM	DOGL0650
	DATA ONE,ZERO /1.0D0,0.0D0/	DOGL0660
C		DOGL0670
C	EPSMCH IS THE MACHINE PRECISION.	DOGL0680
C		DOGL0690
	EPSMCH = DPMPAR(1)	DOGL0700
C		DOGL0710
C	FIRST, CALCULATE THE GAUSS-NEWTON DIRECTION.	DOGL0720
C		DOGL0730
	JJ = (N*(N + 1))/2 + 1	DOGL0740
	DO 50 K = 1, N	DOGL0750
	J = N - K + 1	DOGL0760
	JP1 = J + 1	DOGL0770
	JJ = JJ - K	DOGL0780
	L = JJ + 1	DOGL0790
	SUM = ZERO	DOGL0800
	IF (N .LT. JP1) GO TO 20	DOGL0810
	DO 10 I = JP1, N	DOGL0820
	SUM = SUM + R(L)*X(I)	DOGL0830
	L = L + 1	DOGL0840
10	CONTINUE	DOGL0850
20	CONTINUE	DOGL0860
	TEMP = R(JJ)	DOGL0870
	IF (TEMP .NE. ZERO) GO TO 40	DOGL0880
	L = J	DOGL0890
	DO 30 I = 1, J	DOGL0900
	TEMP = DMAX1(TEMP,DABS(R(L)))	DOGL0910
	L = L + N - I	DOGL0920
30	CONTINUE	DOGL0930
	TEMP = EPSMCH*TEMP	DOGL0940
	IF (TEMP .EQ. ZERO) TEMP = EPSMCH	DOGL0950
40	CONTINUE	DOGL0960
	X(J) = (QTB(J) - SUM)/TEMP	DOGL0970
50	CONTINUE	DOGL0980
C		DOGL0990
C	TEST WHETHER THE GAUSS-NEWTON DIRECTION IS ACCEPTABLE.	DOGL1000
C		DOGL1010
	DO 60 J = 1, N	DOGL1020
	WA1(J) = ZERO	DOGL1030
	WA2(J) = DIAG(J)*X(J)	DOGL1040
60	CONTINUE	DOGL1050
	QNORM = ENORM(N,WA2)	DOGL1060
	IF (QNORM .LE. DELTA) GO TO 140	DOGL1070
C		DOGL1080

C	THE GAUSS-NEWTON DIRECTION IS NOT ACCEPTABLE.	DOGL1090
C	NEXT, CALCULATE THE SCALED GRADIENT DIRECTION.	DOGL1100
C		DOGL1110
	L = 1	DOGL1120
	DO 80 J = 1, N	DOGL1130
	TEMP = QTB(J)	DOGL1140
	DO 70 I = J, N	DOGL1150
	WA1(I) = WA1(I) + R(L)*TEMP	DOGL1160
	L = L + 1	DOGL1170
70	CONTINUE	DOGL1180
	WA1(J) = WA1(J)/DIAG(J)	DOGL1190
80	CONTINUE	DOGL1200
C		DOGL1210
C	CALCULATE THE NORM OF THE SCALED GRADIENT AND TEST FOR	DOGL1220
C	THE SPECIAL CASE IN WHICH THE SCALED GRADIENT IS ZERO.	DOGL1230
C		DOGL1240
	GNORM = ENORM(N,WA1)	DOGL1250
	SGNORM = ZERO	DOGL1260
	ALPHA = DELTA/QNORM	DOGL1270
	IF (GNORM .EQ. ZERO) GO TO 120	DOGL1280
C		DOGL1290
C	CALCULATE THE POINT ALONG THE SCALED GRADIENT	DOGL1300
C	AT WHICH THE QUADRATIC IS MINIMIZED.	DOGL1310
C		DOGL1320
	DO 90 J = 1, N	DOGL1330
	WA1(J) = (WA1(J)/GNORM)/DIAG(J)	DOGL1340
90	CONTINUE	DOGL1350
	L = 1	DOGL1360
	DO 110 J = 1, N	DOGL1370
	SUM = ZERO	DOGL1380
	DO 100 I = J, N	DOGL1390
	SUM = SUM + R(L)*WA1(I)	DOGL1400
	L = L + 1	DOGL1410
100	CONTINUE	DOGL1420
	WA2(J) = SUM	DOGL1430
110	CONTINUE	DOGL1440
	TEMP = ENORM(N,WA2)	DOGL1450
	SGNORM = (GNORM/TEMP)/TEMP	DOGL1460
C		DOGL1470
C	TEST WHETHER THE SCALED GRADIENT DIRECTION IS ACCEPTABLE.	DOGL1480
C		DOGL1490
	ALPHA = ZERO	DOGL1500
	IF (SGNORM .GE. DELTA) GO TO 120	DOGL1510
C		DOGL1520
C	THE SCALED GRADIENT DIRECTION IS NOT ACCEPTABLE.	DOGL1530
C	FINALLY, CALCULATE THE POINT ALONG THE DOGLEG	DOGL1540
C	AT WHICH THE QUADRATIC IS MINIMIZED.	DOGL1550
C		DOGL1560
	BNORM = ENORM(N,QTB)	DOGL1570
	TEMP = (BNORM/GNORM)*(BNORM/QNORM)*(SGNORM/DELTA)	DOGL1580
	TEMP = TEMP - (DELTA/QNORM)*(SGNORM/DELTA)**2	DOGL1590
*	+ DSQRT((TEMP-(DELTA/QNORM))**2	DOGL1600
*	+(ONE-(DELTA/QNORM)**2)*(ONE-(SGNORM/DELTA)**2))	DOGL1610
	ALPHA = ((DELTA/QNORM)*(ONE - (SGNORM/DELTA)**2))/TEMP	DOGL1620

120	CONTINUE	DOGL1630
C		DOGL1640
C	FORM APPROPRIATE CONVEX COMBINATION OF THE GAUSS-NEWTON	DOGL1650
C	DIRECTION AND THE SCALED GRADIENT DIRECTION.	DOGL1660
C		DOGL1670
	TEMP = (ONE - ALPHA)*DMIN1(SGNORM,DELTA)	DOGL1680
	DO 130 J = 1, N	DOGL1690
	X(J) = TEMP*WA1(J) + ALPHA*X(J)	DOGL1700
130	CONTINUE	DOGL1710
140	CONTINUE	DOGL1720
	RETURN	DOGL1730
C		DOGL1740
C	LAST CARD OF SUBROUTINE DOGLEG.	DOGL1750
C		DOGL1760
	END	DOGL1770

DOUBLE PRECISION FUNCTION ENORM(N,X)

INTEGER N

DOUBLE PRECISION X(N)

FUNCTION ENORM

GIVEN AN N-VECTOR X, THIS FUNCTION CALCULATES THE
EUCLIDEAN NORM OF X.

THE EUCLIDEAN NORM IS COMPUTED BY ACCUMULATING THE SUM OF
SQUARES IN THREE DIFFERENT SUMS. THE SUMS OF SQUARES FOR THE
SMALL AND LARGE COMPONENTS ARE SCALED SO THAT NO OVERFLOWS
OCCUR. NON-DESTRUCTIVE UNDERFLOWS ARE PERMITTED. UNDERFLOWS
AND OVERFLOWS DO NOT OCCUR IN THE COMPUTATION OF THE UNSCALED
SUM OF SQUARES FOR THE INTERMEDIATE COMPONENTS.
THE DEFINITIONS OF SMALL, INTERMEDIATE AND LARGE COMPONENTS
DEPEND ON TWO CONSTANTS, RDWARF AND RGIANT. THE MAIN
RESTRICTIONS ON THESE CONSTANTS ARE THAT RDWARF**2 NOT
UNDERFLOW AND RGIANT**2 NOT OVERFLOW. THE CONSTANTS
GIVEN HERE ARE SUITABLE FOR EVERY KNOWN COMPUTER.

THE FUNCTION STATEMENT IS

DOUBLE PRECISION FUNCTION ENORM(N,X)

WHERE

N IS A POSITIVE INTEGER INPUT VARIABLE.

X IS AN INPUT ARRAY OF LENGTH N.

SUBPROGRAMS CALLED

FORTTRAN-SUPPLIED ... DABS,DSQRT

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BURTON S. GARBOW, KENNETH E. HILLSTROM, JORGE J. MORE

INTEGER I

DOUBLE PRECISION AGIANT,FLOATN,ONE,RDWARF,RGIANT,S1,S2,S3,XABS,
* X1MAX,X3MAX,ZERO

DATA ONE,ZERO,RDWARF,RGIANT /1.0D0,0.0D0,3.834D-20,1.304D19/

S1 = ZERO

S2 = ZERO

S3 = ZERO

X1MAX = ZERO

X3MAX = ZERO

FLOATN = N

AGIANT = RGIANT/FLOATN

DO 90 I = 1, N

XABS = DABS(X(I))

IF (XABS .GT. RDWARF .AND. XABS .LT. AGIANT) GO TO 70

ENRM0010

ENRM0020

ENRM0030

ENRM0040

ENRM0050

ENRM0060

ENRM0070

ENRM0080

ENRM0090

ENRM0100

ENRM0110

ENRM0120

ENRM0130

ENRM0140

ENRM0150

ENRM0160

ENRM0170

ENRM0180

ENRM0190

ENRM0200

ENRM0210

ENRM0220

ENRM0230

ENRM0240

ENRM0250

ENRM0260

ENRM0270

ENRM0280

ENRM0290

ENRM0300

ENRM0310

ENRM0320

ENRM0330

ENRM0340

ENRM0350

ENRM0360

ENRM0370

ENRM0380

ENRM0390

ENRM0400

ENRM0410

ENRM0420

ENRM0430

ENRM0440

ENRM0450

ENRM0460

ENRM0470

ENRM0480

ENRM0490

ENRM0500

ENRM0510

ENRM0520

ENRM0530

ENRM0540

	IF (XABS .LE. RDWARF) GO TO 30	ENRM0550
C		ENRM0560
C	SUM FOR LARGE COMPONENTS.	ENRM0570
C		ENRM0580
	IF (XABS .LE. X1MAX) GO TO 10	ENRM0590
	S1 = ONE + S1*(X1MAX/XABS)**2	ENRM0600
	X1MAX = XABS	ENRM0610
	GO TO 20	ENRM0620
10	CONTINUE	ENRM0630
	S1 = S1 + (XABS/X1MAX)**2	ENRM0640
20	CONTINUE	ENRM0650
	GO TO 60	ENRM0660
30	CONTINUE	ENRM0670
C		ENRM0680
C	SUM FOR SMALL COMPONENTS.	ENRM0690
C		ENRM0700
	IF (XABS .LE. X3MAX) GO TO 40	ENRM0710
	S3 = ONE + S3*(X3MAX/XABS)**2	ENRM0720
	X3MAX = XABS	ENRM0730
	GO TO 50	ENRM0740
40	CONTINUE	ENRM0750
	IF (XABS .NE. ZERO) S3 = S3 + (XABS/X3MAX)**2	ENRM0760
50	CONTINUE	ENRM0770
60	CONTINUE	ENRM0780
	GO TO 80	ENRM0790
70	CONTINUE	ENRM0800
C		ENRM0810
C	SUM FOR INTERMEDIATE COMPONENTS.	ENRM0820
C		ENRM0830
	S2 = S2 + XABS**2	ENRM0840
80	CONTINUE	ENRM0850
90	CONTINUE	ENRM0860
C		ENRM0870
C	CALCULATION OF NORM.	ENRM0880
C		ENRM0890
	IF (S1 .EQ. ZERO) GO TO 100	ENRM0900
	ENORM = X1MAX*DSQRT(S1+(S2/X1MAX)/X1MAX)	ENRM0910
	GO TO 130	ENRM0920
100	CONTINUE	ENRM0930
	IF (S2 .EQ. ZERO) GO TO 110	ENRM0940
	IF (S2 .GE. X3MAX)	ENRM0950
*	ENORM = DSQRT(S2*(ONE+(X3MAX/S2)*(X3MAX*S3)))	ENRM0960
	IF (S2 .LT. X3MAX)	ENRM0970
*	ENORM = DSQRT(X3MAX*((S2/X3MAX)+(X3MAX*S3)))	ENRM0980
	GO TO 120	ENRM0990
110	CONTINUE	ENRM1000
	ENORM = X3MAX*DSQRT(S3)	ENRM1010
120	CONTINUE	ENRM1020
130	CONTINUE	ENRM1030
	RETURN	ENRM1040
C		ENRM1050
C	LAST CARD OF FUNCTION ENORM.	ENRM1060
C		ENRM1070
	END	ENRM1080

```

SUBROUTINE FDJAC1(FCN,N,X,FVEC,FJAC,LDFJAC,IFLAG,ML,MU,EPSFCN,
*          WA1,WA2)
INTEGER N,LDFJAC,IFLAG,ML,MU
DOUBLE PRECISION EPSFCN
DOUBLE PRECISION X(N),FVEC(N),FJAC(LDFJAC,N),WA1(N),WA2(N)
*****

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```

SUBROUTINE FDJAC1

```

```

THIS SUBROUTINE COMPUTES A FORWARD-DIFFERENCE APPROXIMATION
TO THE N BY N JACOBIAN MATRIX ASSOCIATED WITH A SPECIFIED
PROBLEM OF N FUNCTIONS IN N VARIABLES. IF THE JACOBIAN HAS
A BANDED FORM, THEN FUNCTION EVALUATIONS ARE SAVED BY ONLY
APPROXIMATING THE NONZERO TERMS.

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THE SUBROUTINE STATEMENT IS

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```

SUBROUTINE FDJAC1(FCN,N,X,FVEC,FJAC,LDFJAC,IFLAG,ML,MU,EPSFCN,
          WA1,WA2)

```

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WHERE

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```

FCN IS THE NAME OF THE USER-SUPPLIED SUBROUTINE WHICH
CALCULATES THE FUNCTIONS. FCN MUST BE DECLARED
IN AN EXTERNAL STATEMENT IN THE USER CALLING
PROGRAM, AND SHOULD BE WRITTEN AS FOLLOWS.

```

```

SUBROUTINE FCN(N,X,FVEC,IFLAG)
INTEGER N,IFLAG
DOUBLE PRECISION X(N),FVEC(N)
-----

```

```

CALCULATE THE FUNCTIONS AT X AND
RETURN THIS VECTOR IN FVEC.
-----

```

```

RETURN
END

```

```

THE VALUE OF IFLAG SHOULD NOT BE CHANGED BY FCN UNLESS
THE USER WANTS TO TERMINATE EXECUTION OF FDJAC1.
IN THIS CASE SET IFLAG TO A NEGATIVE INTEGER.

```

```

N IS A POSITIVE INTEGER INPUT VARIABLE SET TO THE NUMBER
OF FUNCTIONS AND VARIABLES.

```

```

X IS AN INPUT ARRAY OF LENGTH N.

```

```

FVEC IS AN INPUT ARRAY OF LENGTH N WHICH MUST CONTAIN THE
FUNCTIONS EVALUATED AT X.

```

```

FJAC IS AN OUTPUT N BY N ARRAY WHICH CONTAINS THE
APPROXIMATION TO THE JACOBIAN MATRIX EVALUATED AT X.

```

```

LDFJAC IS A POSITIVE INTEGER INPUT VARIABLE NOT LESS THAN N
WHICH SPECIFIES THE LEADING DIMENSION OF THE ARRAY FJAC.

```

```

FDJ10010
FDJ10020
FDJ10030
FDJ10040
FDJ10050
FDJ10060
FDJ10070
FDJ10080
FDJ10090
FDJ10100
FDJ10110
FDJ10120
FDJ10130
FDJ10140
FDJ10150
FDJ10160
FDJ10170
FDJ10180
FDJ10190
FDJ10200
FDJ10210
FDJ10220
FDJ10230
FDJ10240
FDJ10250
FDJ10260
FDJ10270
FDJ10280
FDJ10290
FDJ10300
FDJ10310
FDJ10320
FDJ10330
FDJ10340
FDJ10350
FDJ10360
FDJ10370
FDJ10380
FDJ10390
FDJ10400
FDJ10410
FDJ10420
FDJ10430
FDJ10440
FDJ10450
FDJ10460
FDJ10470
FDJ10480
FDJ10490
FDJ10500
FDJ10510
FDJ10520
FDJ10530
FDJ10540

```

C		FDJ10550
C	IFLAG IS AN INTEGER VARIABLE WHICH CAN BE USED TO TERMINATE	FDJ10560
C	THE EXECUTION OF FDJAC1. SEE DESCRIPTION OF FCN.	FDJ10570
C		FDJ10580
C	ML IS A NONNEGATIVE INTEGER INPUT VARIABLE WHICH SPECIFIES	FDJ10590
C	THE NUMBER OF SUBDIAGONALS WITHIN THE BAND OF THE	FDJ10600
C	JACOBIAN MATRIX. IF THE JACOBIAN IS NOT BANDED, SET	FDJ10610
C	ML TO AT LEAST N - 1.	FDJ10620
C		FDJ10630
C	EPSFCN IS AN INPUT VARIABLE USED IN DETERMINING A SUITABLE	FDJ10640
C	STEP LENGTH FOR THE FORWARD-DIFFERENCE APPROXIMATION. THIS	FDJ10650
C	APPROXIMATION ASSUMES THAT THE RELATIVE ERRORS IN THE	FDJ10660
C	FUNCTIONS ARE OF THE ORDER OF EPSFCN. IF EPSFCN IS LESS	FDJ10670
C	THAN THE MACHINE PRECISION, IT IS ASSUMED THAT THE RELATIVE	FDJ10680
C	ERRORS IN THE FUNCTIONS ARE OF THE ORDER OF THE MACHINE	FDJ10690
C	PRECISION.	FDJ10700
C		FDJ10710
C	MU IS A NONNEGATIVE INTEGER INPUT VARIABLE WHICH SPECIFIES	FDJ10720
C	THE NUMBER OF SUPERDIAGONALS WITHIN THE BAND OF THE	FDJ10730
C	JACOBIAN MATRIX. IF THE JACOBIAN IS NOT BANDED, SET	FDJ10740
C	MU TO AT LEAST N - 1.	FDJ10750
C		FDJ10760
C	WA1 AND WA2 ARE WORK ARRAYS OF LENGTH N. IF ML + MU + 1 IS AT	FDJ10770
C	LEAST N, THEN THE JACOBIAN IS CONSIDERED DENSE, AND WA2 IS	FDJ10780
C	NOT REFERENCED.	FDJ10790
C		FDJ10800
C	SUBPROGRAMS CALLED	FDJ10810
C		FDJ10820
C	MINPACK-SUPPLIED ... DPMPAR	FDJ10830
C		FDJ10840
C	FORTTRAN-SUPPLIED ... DABS,DMAX1,DSQRT	FDJ10850
C		FDJ10860
C	ARGONNE NATIONAL LABORATORY. MINPACK PROJECT. MARCH 1980.	FDJ10870
C	BURTON S. GARBOW, KENNETH E. HILLSTROM, JORGE J. MORE	FDJ10880
C		FDJ10890
C	*****	FDJ10900
C	INTEGER I,J,K,MSUM	FDJ10910
C	DOUBLE PRECISION EPS,EPSMCH,H,TEMP,ZERO	FDJ10920
C	DOUBLE PRECISION DPMPAR	FDJ10930
C	DATA ZERO /0.0D0/	FDJ10940
C		FDJ10950
C	EPSMCH IS THE MACHINE PRECISION.	FDJ10960
C		FDJ10970
C	EPSMCH = DPMPAR(1)	FDJ10980
C		FDJ10990
C	EPS = DSQRT(DMAX1(EPSFCN, EPSMCH))	FDJ11000
C	MSUM = ML + MU + 1	FDJ11010
C	IF (MSUM .LT. N) GO TO 40	FDJ11020
C		FDJ11030
C	COMPUTATION OF DENSE APPROXIMATE JACOBIAN.	FDJ11040
C		FDJ11050
C	DO 20 J = 1, N	FDJ11060
	TEMP = X(J)	FDJ11070
	H = EPS*DABS(TEMP)	FDJ11080

	IF (H .EQ. ZERO) H = EPS	FDJ11090
	X(J) = TEMP + H	FDJ11100
	CALL FCN(N,X,WA1,IFLAG)	FDJ11110
	IF (IFLAG .LT. 0) GO TO 30	FDJ11120
	X(J) = TEMP	FDJ11130
	DO 10 I = 1, N	FDJ11140
	FJAC(I,J) = (WA1(I) - FVEC(I))/H	FDJ11150
10	CONTINUE	FDJ11160
20	CONTINUE	FDJ11170
30	CONTINUE	FDJ11180
	GO TO 110	FDJ11190
40	CONTINUE	FDJ11200
C		FDJ11210
C	COMPUTATION OF BANDED APPROXIMATE JACOBIAN.	FDJ11220
C		FDJ11230
	DO 90 K = 1, MSUM	FDJ11240
	DO 60 J = K, N, MSUM	FDJ11250
	WA2(J) = X(J)	FDJ11260
	H = EPS*DABS(WA2(J))	FDJ11270
	IF (H .EQ. ZERO) H = EPS	FDJ11280
	X(J) = WA2(J) + H	FDJ11290
60	CONTINUE	FDJ11300
	CALL FCN(N,X,WA1,IFLAG)	FDJ11310
	IF (IFLAG .LT. 0) GO TO 100	FDJ11320
	DO 80 J = K, N, MSUM	FDJ11330
	X(J) = WA2(J)	FDJ11340
	H = EPS*DABS(WA2(J))	FDJ11350
	IF (H .EQ. ZERO) H = EPS	FDJ11360
	DO 70 I = 1, N	FDJ11370
	FJAC(I,J) = ZERO	FDJ11380
	IF (I .GE. J - MU .AND. I .LE. J + ML)	FDJ11390
	FJAC(I,J) = (WA1(I) - FVEC(I))/H	FDJ11400
	*	FDJ11410
70	CONTINUE	FDJ11420
80	CONTINUE	FDJ11430
90	CONTINUE	FDJ11440
100	CONTINUE	FDJ11450
110	CONTINUE	FDJ11460
	RETURN	FDJ11470
C		FDJ11480
C	LAST CARD OF SUBROUTINE FDJAC1.	FDJ11490
C		FDJ11500
	END	


```

SUBROUTINE FDJAC2(FCN,M,N,X,FVEC,FJAC,LDFJAC,IFLAG,EPSFCN,WA)
INTEGER M,N,LDFJAC,IFLAG
DOUBLE PRECISION EPSFCN
DOUBLE PRECISION X(N),FVEC(M),FJAC(LDFJAC,N),WA(M)
*****

```

```

SUBROUTINE FDJAC2

```

```

THIS SUBROUTINE COMPUTES A FORWARD-DIFFERENCE APPROXIMATION
TO THE M BY N JACOBIAN MATRIX ASSOCIATED WITH A SPECIFIED
PROBLEM OF M FUNCTIONS IN N VARIABLES.

```

```

THE SUBROUTINE STATEMENT IS

```

```

SUBROUTINE FDJAC2(FCN,M,N,X,FVEC,FJAC,LDFJAC,IFLAG,EPSFCN,WA)

```

```

WHERE

```

```

FCN IS THE NAME OF THE USER-SUPPLIED SUBROUTINE WHICH
CALCULATES THE FUNCTIONS. FCN MUST BE DECLARED
IN AN EXTERNAL STATEMENT IN THE USER CALLING
PROGRAM, AND SHOULD BE WRITTEN AS FOLLOWS.

```

```

SUBROUTINE FCN(M,N,X,FVEC,IFLAG)
INTEGER M,N,IFLAG
DOUBLE PRECISION X(N),FVEC(M)
-----

```

```

CALCULATE THE FUNCTIONS AT X AND
RETURN THIS VECTOR IN FVEC.
-----

```

```

RETURN
END

```

```

THE VALUE OF IFLAG SHOULD NOT BE CHANGED BY FCN UNLESS
THE USER WANTS TO TERMINATE EXECUTION OF FDJAC2.
IN THIS CASE SET IFLAG TO A NEGATIVE INTEGER.

```

```

M IS A POSITIVE INTEGER INPUT VARIABLE SET TO THE NUMBER
OF FUNCTIONS.

```

```

N IS A POSITIVE INTEGER INPUT VARIABLE SET TO THE NUMBER
OF VARIABLES. N MUST NOT EXCEED M.

```

```

X IS AN INPUT ARRAY OF LENGTH N.

```

```

FVEC IS AN INPUT ARRAY OF LENGTH M WHICH MUST CONTAIN THE
FUNCTIONS EVALUATED AT X.

```

```

FJAC IS AN OUTPUT M BY N ARRAY WHICH CONTAINS THE
APPROXIMATION TO THE JACOBIAN MATRIX EVALUATED AT X.

```

```

LDFJAC IS A POSITIVE INTEGER INPUT VARIABLE NOT LESS THAN M
WHICH SPECIFIES THE LEADING DIMENSION OF THE ARRAY FJAC.

```

```

FDJ20010
FDJ20020
FDJ20030
FDJ20040
FDJ20050
FDJ20060
FDJ20070
FDJ20080
FDJ20090
FDJ20100
FDJ20110
FDJ20120
FDJ20130
FDJ20140
FDJ20150
FDJ20160
FDJ20170
FDJ20180
FDJ20190
FDJ20200
FDJ20210
FDJ20220
FDJ20230
FDJ20240
FDJ20250
FDJ20260
FDJ20270
FDJ20280
FDJ20290
FDJ20300
FDJ20310
FDJ20320
FDJ20330
FDJ20340
FDJ20350
FDJ20360
FDJ20370
FDJ20380
FDJ20390
FDJ20400
FDJ20410
FDJ20420
FDJ20430
FDJ20440
FDJ20450
FDJ20460
FDJ20470
FDJ20480
FDJ20490
FDJ20500
FDJ20510
FDJ20520
FDJ20530
FDJ20540

```

C	IFLAG IS AN INTEGER VARIABLE WHICH CAN BE USED TO TERMINATE	FDJ20550
C	THE EXECUTION OF FDJAC2. SEE DESCRIPTION OF FCN.	FDJ20560
C		FDJ20570
C	EPSFCN IS AN INPUT VARIABLE USED IN DETERMINING A SUITABLE	FDJ20580
C	STEP LENGTH FOR THE FORWARD-DIFFERENCE APPROXIMATION. THIS	FDJ20590
C	APPROXIMATION ASSUMES THAT THE RELATIVE ERRORS IN THE	FDJ20600
C	FUNCTIONS ARE OF THE ORDER OF EPSFCN. IF EPSFCN IS LESS	FDJ20610
C	THAN THE MACHINE PRECISION, IT IS ASSUMED THAT THE RELATIVE	FDJ20620
C	ERRORS IN THE FUNCTIONS ARE OF THE ORDER OF THE MACHINE	FDJ20630
C	PRECISION.	FDJ20640
C		FDJ20650
C	WA IS A WORK ARRAY OF LENGTH M.	FDJ20660
C		FDJ20670
C	SUBPROGRAMS CALLED	FDJ20680
C		FDJ20690
C	USER-SUPPLIED FCN	FDJ20700
C		FDJ20710
C	MINPACK-SUPPLIED ... DPMPAR	FDJ20720
C		FDJ20730
C	FORTTRAN-SUPPLIED ... DABS,DMAX1,DSQRT	FDJ20740
C		FDJ20750
C	ARGONNE NATIONAL LABORATORY. MINPACK PROJECT. MARCH 1980.	FDJ20760
C	BURTON S. GARBOW, KENNETH E. HILLSTROM, JORGE J. MORE	FDJ20770
C		FDJ20780
C	*****	FDJ20790
	INTEGER I,J	FDJ20800
	DOUBLE PRECISION EPS,EPSMCH,H,TEMP,ZERO	FDJ20810
	DOUBLE PRECISION DPMPAR	FDJ20820
	DATA ZERO /0.0D0/	FDJ20830
C		FDJ20840
C	EPSMCH IS THE MACHINE PRECISION.	FDJ20850
C		FDJ20860
	EPSMCH = DPMPAR(1)	FDJ20870
C		FDJ20880
	EPS = DSQRT(DMAX1(EPSFCN,EPSMCH))	FDJ20890
	DO 20 J = 1, N	FDJ20900
	TEMP = X(J)	FDJ20910
	H = EPS*DABS(TEMP)	FDJ20920
	IF (H .EQ. ZERO) H = EPS	FDJ20930
	X(J) = TEMP + H	FDJ20940
	CALL FCN(M,N,X,WA,IFLAG)	FDJ20950
	IF (IFLAG .LT. 0) GO TO 30	FDJ20960
	X(J) = TEMP	FDJ20970
	DO 10 I = 1, M	FDJ20980
	FJAC(I,J) = (WA(I) - FVEC(I))/H	FDJ20990
10	CONTINUE	FDJ21000
20	CONTINUE	FDJ21010
30	CONTINUE	FDJ21020
	RETURN	FDJ21030
C		FDJ21040
C	LAST CARD OF SUBROUTINE FDJAC2.	FDJ21050
C		FDJ21060
	END	FDJ21070

SUBROUTINE HYBRD(FCN,N,X,FVEC,XTOL,MAXFEV,ML,MU,EPSFCN,DIAG,	HYBD0010
* MODE,FACTOR,NPRINT,INFO,NFEV,FJAC,LDFJAC,R,LR,	HYBD0020
* QTF,WA1,WA2,WA3,WA4)	HYBD0030
INTEGER N,MAXFEV,ML,MU,MODE,NPRINT,INFO,NFEV,LDFJAC,LR	HYBD0040
DOUBLE PRECISION XTOL,EPSFCN,FACTOR	HYBD0050
DOUBLE PRECISION X(N),FVEC(N),DIAG(N),FJAC(LDFJAC,N),R(LR),	HYBD0060
* QTF(N),WA1(N),WA2(N),WA3(N),WA4(N)	HYBD0070
EXTERNAL FCN	HYBD0080
*****	HYBD0090
	HYBD0100
SUBROUTINE HYBRD	HYBD0110
	HYBD0120
THE PURPOSE OF HYBRD IS TO FIND A ZERO OF A SYSTEM OF	HYBD0130
N NONLINEAR FUNCTIONS IN N VARIABLES BY A MODIFICATION	HYBD0140
OF THE POWELL HYBRID METHOD. THE USER MUST PROVIDE A	HYBD0150
SUBROUTINE WHICH CALCULATES THE FUNCTIONS. THE JACOBIAN IS	HYBD0160
THEN CALCULATED BY A FORWARD-DIFFERENCE APPROXIMATION.	HYBD0170
	HYBD0180
THE SUBROUTINE STATEMENT IS	HYBD0190
	HYBD0200
SUBROUTINE HYBRD(FCN,N,X,FVEC,XTOL,MAXFEV,ML,MU,EPSFCN,	HYBD0210
DIAG,MODE,FACTOR,NPRINT,INFO,NFEV,FJAC,	HYBD0220
LDFJAC,R,LR,QTF,WA1,WA2,WA3,WA4)	HYBD0230
	HYBD0240
WHERE	HYBD0250
	HYBD0260
FCN IS THE NAME OF THE USER-SUPPLIED SUBROUTINE WHICH	HYBD0270
CALCULATES THE FUNCTIONS. FCN MUST BE DECLARED	HYBD0280
IN AN EXTERNAL STATEMENT IN THE USER CALLING	HYBD0290
PROGRAM, AND SHOULD BE WRITTEN AS FOLLOWS.	HYBD0300
	HYBD0310
SUBROUTINE FCN(N,X,FVEC,IFLAG)	HYBD0320
INTEGER N,IFLAG	HYBD0330
DOUBLE PRECISION X(N),FVEC(N)	HYBD0340
-----	HYBD0350
CALCULATE THE FUNCTIONS AT X AND	HYBD0360
RETURN THIS VECTOR IN FVEC.	HYBD0370
-----	HYBD0380
RETURN	HYBD0390
END	HYBD0400
	HYBD0410
THE VALUE OF IFLAG SHOULD NOT BE CHANGED BY FCN UNLESS	HYBD0420
THE USER WANTS TO TERMINATE EXECUTION OF HYBRD.	HYBD0430
IN THIS CASE SET IFLAG TO A NEGATIVE INTEGER.	HYBD0440
	HYBD0450
N IS A POSITIVE INTEGER INPUT VARIABLE SET TO THE NUMBER	HYBD0460
OF FUNCTIONS AND VARIABLES.	HYBD0470
	HYBD0480
X IS AN ARRAY OF LENGTH N. ON INPUT X MUST CONTAIN	HYBD0490
AN INITIAL ESTIMATE OF THE SOLUTION VECTOR. ON OUTPUT X	HYBD0500
CONTAINS THE FINAL ESTIMATE OF THE SOLUTION VECTOR.	HYBD0510
	HYBD0520
FVEC IS AN OUTPUT ARRAY OF LENGTH N WHICH CONTAINS	HYBD0530
THE FUNCTIONS EVALUATED AT THE OUTPUT X.	HYBD0540

C		HYBD0550
C	XTOL IS A NONNEGATIVE INPUT VARIABLE. TERMINATION	HYBD0560
C	OCCURS WHEN THE RELATIVE ERROR BETWEEN TWO CONSECUTIVE	HYBD0570
C	ITERATES IS AT MOST XTOL.	HYBD0580
C		HYBD0590
C	MAXFEV IS A POSITIVE INTEGER INPUT VARIABLE. TERMINATION	HYBD0600
C	OCCURS WHEN THE NUMBER OF CALLS TO FCN IS AT LEAST MAXFEV	HYBD0610
C	BY THE END OF AN ITERATION.	HYBD0620
C		HYBD0630
C	ML IS A NONNEGATIVE INTEGER INPUT VARIABLE WHICH SPECIFIES	HYBD0640
C	THE NUMBER OF SUBDIAGONALS WITHIN THE BAND OF THE	HYBD0650
C	JACOBIAN MATRIX. IF THE JACOBIAN IS NOT BANDED, SET	HYBD0660
C	ML TO AT LEAST N - 1.	HYBD0670
C		HYBD0680
C	MU IS A NONNEGATIVE INTEGER INPUT VARIABLE WHICH SPECIFIES	HYBD0690
C	THE NUMBER OF SUPERDIAGONALS WITHIN THE BAND OF THE	HYBD0700
C	JACOBIAN MATRIX. IF THE JACOBIAN IS NOT BANDED, SET	HYBD0710
C	MU TO AT LEAST N - 1.	HYBD0720
C		HYBD0730
C	EPSFCN IS AN INPUT VARIABLE USED IN DETERMINING A SUITABLE	HYBD0740
C	STEP LENGTH FOR THE FORWARD-DIFFERENCE APPROXIMATION. THIS	HYBD0750
C	APPROXIMATION ASSUMES THAT THE RELATIVE ERRORS IN THE	HYBD0760
C	FUNCTIONS ARE OF THE ORDER OF EPSFCN. IF EPSFCN IS LESS	HYBD0770
C	THAN THE MACHINE PRECISION, IT IS ASSUMED THAT THE RELATIVE	HYBD0780
C	ERRORS IN THE FUNCTIONS ARE OF THE ORDER OF THE MACHINE	HYBD0790
C	PRECISION.	HYBD0800
C		HYBD0810
C	DIAG IS AN ARRAY OF LENGTH N. IF MODE = 1 (SEE	HYBD0820
C	BELOW), DIAG IS INTERNALLY SET. IF MODE = 2, DIAG	HYBD0830
C	MUST CONTAIN POSITIVE ENTRIES THAT SERVE AS	HYBD0840
C	MULTIPLICATIVE SCALE FACTORS FOR THE VARIABLES.	HYBD0850
C		HYBD0860
C	MODE IS AN INTEGER INPUT VARIABLE. IF MODE = 1, THE	HYBD0870
C	VARIABLES WILL BE SCALED INTERNALLY. IF MODE = 2,	HYBD0880
C	THE SCALING IS SPECIFIED BY THE INPUT DIAG. OTHER	HYBD0890
C	VALUES OF MODE ARE EQUIVALENT TO MODE = 1.	HYBD0900
C		HYBD0910
C	FACTOR IS A POSITIVE INPUT VARIABLE USED IN DETERMINING THE	HYBD0920
C	INITIAL STEP BOUND. THIS BOUND IS SET TO THE PRODUCT OF	HYBD0930
C	FACTOR AND THE EUCLIDEAN NORM OF DIAG*X IF NONZERO, OR ELSE	HYBD0940
C	TO FACTOR ITSELF. IN MOST CASES FACTOR SHOULD LIE IN THE	HYBD0950
C	INTERVAL (.1,100.). 100. IS A GENERALLY RECOMMENDED VALUE.	HYBD0960
C		HYBD0970
C	NPRINT IS AN INTEGER INPUT VARIABLE THAT ENABLES CONTROLLED	HYBD0980
C	PRINTING OF ITERATES IF IT IS POSITIVE. IN THIS CASE,	HYBD0990
C	FCN IS CALLED WITH IFLAG = 0 AT THE BEGINNING OF THE FIRST	HYBD1000
C	ITERATION AND EVERY NPRINT ITERATIONS THEREAFTER AND	HYBD1010
C	IMMEDIATELY PRIOR TO RETURN, WITH X AND FVEC AVAILABLE	HYBD1020
C	FOR PRINTING. IF NPRINT IS NOT POSITIVE, NO SPECIAL CALLS	HYBD1030
C	OF FCN WITH IFLAG = 0 ARE MADE.	HYBD1040
C		HYBD1050
C	INFO IS AN INTEGER OUTPUT VARIABLE. IF THE USER HAS	HYBD1060
C	TERMINATED EXECUTION, INFO IS SET TO THE (NEGATIVE)	HYBD1070
C	VALUE OF IFLAG. SEE DESCRIPTION OF FCN. OTHERWISE,	HYBD1080

C	INFO IS SET AS FOLLOWS.	HYBD1090
C		HYBD1100
C	INFO = 0 IMPROPER INPUT PARAMETERS.	HYBD1110
C		HYBD1120
C	INFO = 1 RELATIVE ERROR BETWEEN TWO CONSECUTIVE ITERATES	HYBD1130
C	IS AT MOST XTOL.	HYBD1140
C		HYBD1150
C	INFO = 2 NUMBER OF CALLS TO FCN HAS REACHED OR EXCEEDED	HYBD1160
C	MAXFEV.	HYBD1170
C		HYBD1180
C	INFO = 3 XTOL IS TOO SMALL. NO FURTHER IMPROVEMENT IN	HYBD1190
C	THE APPROXIMATE SOLUTION X IS POSSIBLE.	HYBD1200
C		HYBD1210
C	INFO = 4 ITERATION IS NOT MAKING GOOD PROGRESS, AS	HYBD1220
C	MEASURED BY THE IMPROVEMENT FROM THE LAST	HYBD1230
C	FIVE JACOBIAN EVALUATIONS.	HYBD1240
C		HYBD1250
C	INFO = 5 ITERATION IS NOT MAKING GOOD PROGRESS, AS	HYBD1260
C	MEASURED BY THE IMPROVEMENT FROM THE LAST	HYBD1270
C	TEN ITERATIONS.	HYBD1280
C		HYBD1290
C	NFEV IS AN INTEGER OUTPUT VARIABLE SET TO THE NUMBER OF	HYBD1300
C	CALLS TO FCN.	HYBD1310
C		HYBD1320
C	FJAC IS AN OUTPUT N BY N ARRAY WHICH CONTAINS THE	HYBD1330
C	ORTHOGONAL MATRIX Q PRODUCED BY THE QR FACTORIZATION	HYBD1340
C	OF THE FINAL APPROXIMATE JACOBIAN.	HYBD1350
C		HYBD1360
C	LDFJAC IS A POSITIVE INTEGER INPUT VARIABLE NOT LESS THAN N	HYBD1370
C	WHICH SPECIFIES THE LEADING DIMENSION OF THE ARRAY FJAC.	HYBD1380
C		HYBD1390
C	R IS AN OUTPUT ARRAY OF LENGTH LR WHICH CONTAINS THE	HYBD1400
C	UPPER TRIANGULAR MATRIX PRODUCED BY THE QR FACTORIZATION	HYBD1410
C	OF THE FINAL APPROXIMATE JACOBIAN, STORED ROWWISE.	HYBD1420
C		HYBD1430
C	LR IS A POSITIVE INTEGER INPUT VARIABLE NOT LESS THAN	HYBD1440
C	$(N*(N+1))/2$.	HYBD1450
C		HYBD1460
C	QTF IS AN OUTPUT ARRAY OF LENGTH N WHICH CONTAINS	HYBD1470
C	THE VECTOR $(Q \text{ TRANSPOSE}) * FVEC$.	HYBD1480
C		HYBD1490
C	WA1, WA2, WA3, AND WA4 ARE WORK ARRAYS OF LENGTH N.	HYBD1500
C		HYBD1510
C	SUBPROGRAMS CALLED	HYBD1520
C		HYBD1530
C	USER-SUPPLIED FCN	HYBD1540
C		HYBD1550
C	MINPACK-SUPPLIED ... DOGLEG, DPMPAR, ENORM, FDJAC1,	HYBD1560
C	QFORM, QRFAC, RIMPYQ, RIUPDT	HYBD1570
C		HYBD1580
C	FORTTRAN-SUPPLIED ... DABS, DMAX1, DMIN1, MINO, MOD	HYBD1590
C		HYBD1600
C	ARGONNE NATIONAL LABORATORY. MINPACK PROJECT. MARCH 1980.	HYBD1610
C	BURTON S. GARBOW, KENNETH E. HILLSTROM, JORGE J. MORE	HYBD1620

C		HYBD1630
C	*****	HYBD1640
	INTEGER I, IFLAG, ITER, J, JM1, L, MSUM, NCFAIL, NCSUC, NSLOW1, NSLOW2	HYBD1650
	INTEGER IWA(1)	HYBD1660
	LOGICAL JEVAL, SING	HYBD1670
	DOUBLE PRECISION ACTRED, DELTA, EPSMCH, FNORM, FNORM1, ONE, PNORM,	HYBD1680
*	PRERED, P1, P5, P001, P0001, RATIO, SUM, TEMP, XNORM,	HYBD1690
*	ZERO	HYBD1700
	DOUBLE PRECISION DPMPAR, ENORM	HYBD1710
	DATA ONE, P1, P5, P001, P0001, ZERO	HYBD1720
*	/1.0D0, 1.0D-1, 5.0D-1, 1.0D-3, 1.0D-4, 0.0D0/	HYBD1730
C		HYBD1740
C	EPSMCH IS THE MACHINE PRECISION.	HYBD1750
C		HYBD1760
	EPSMCH = DPMPAR(1)	HYBD1770
C		HYBD1780
	INFO = 0	HYBD1790
	IFLAG = 0	HYBD1800
	NFEV = 0	HYBD1810
C		HYBD1820
C	CHECK THE INPUT PARAMETERS FOR ERRORS.	HYBD1830
C		HYBD1840
	IF (N .LE. 0 .OR. XTOL .LT. ZERO .OR. MAXFEV .LE. 0	HYBD1850
*	.OR. ML .LT. 0 .OR. MU .LT. 0 .OR. FACTOR .LE. ZERO	HYBD1860
*	.OR. LDFJAC .LT. N .OR. LR .LT. (N*(N + 1))/2) GO TO 300	HYBD1870
	IF (MODE .NE. 2) GO TO 20	HYBD1880
	DO 10 J = 1, N	HYBD1890
	IF (DIAG(J) .LE. ZERO) GO TO 300	HYBD1900
10	CONTINUE	HYBD1910
20	CONTINUE	HYBD1920
C		HYBD1930
C	EVALUATE THE FUNCTION AT THE STARTING POINT	HYBD1940
C	AND CALCULATE ITS NORM.	HYBD1950
C		HYBD1960
	IFLAG = 1	HYBD1970
	CALL FCN(N, X, FVEC, IFLAG)	HYBD1980
	NFEV = 1	HYBD1990
	IF (IFLAG .LT. 0) GO TO 300	HYBD2000
	FNORM = ENORM(N, FVEC)	HYBD2010
C		HYBD2020
C	DETERMINE THE NUMBER OF CALLS TO FCN NEEDED TO COMPUTE	HYBD2030
C	THE JACOBIAN MATRIX.	HYBD2040
C		HYBD2050
	MSUM = MIN0(ML+MU+1, N)	HYBD2060
C		HYBD2070
C	INITIALIZE ITERATION COUNTER AND MONITORS.	HYBD2080
C		HYBD2090
	ITER = 1	HYBD2100
	NCSUC = 0	HYBD2110
	NCFAIL = 0	HYBD2120
	NSLOW1 = 0	HYBD2130
	NSLOW2 = 0	HYBD2140
C		HYBD2150
C	BEGINNING OF THE OUTER LOOP.	HYBD2160

C		HYBD2170
30	CONTINUE	HYBD2180
	JEVAL = .TRUE.	HYBD2190
C		HYBD2200
C	CALCULATE THE JACOBIAN MATRIX.	HYBD2210
C		HYBD2220
	IFLAG = 2	HYBD2230
	CALL FDJAC1(FCN,N,X,FVEC,FJAC,LDFJAC,IFLAG,ML,MU,EPSFCN,WA1,	HYBD2240
*	WA2)	HYBD2250
	NFEV = NFEV + MSUM	HYBD2260
	IF (IFLAG .LT. 0) GO TO 300	HYBD2270
C		HYBD2280
C	COMPUTE THE QR FACTORIZATION OF THE JACOBIAN.	HYBD2290
C		HYBD2300
	CALL QRFAC(N,N,FJAC,LDFJAC,.FALSE.,IWA,1,WA1,WA2,WA3)	HYBD2310
C		HYBD2320
C	ON THE FIRST ITERATION AND IF MODE IS 1, SCALE ACCORDING	HYBD2330
C	TO THE NORMS OF THE COLUMNS OF THE INITIAL JACOBIAN.	HYBD2340
C		HYBD2350
	IF (ITER .NE. 1) GO TO 70	HYBD2360
	IF (MODE .EQ. 2) GO TO 50	HYBD2370
	DO 40 J = 1, N	HYBD2380
	DIAG(J) = WA2(J)	HYBD2390
	IF (WA2(J) .EQ. ZERO) DIAG(J) = ONE	HYBD2400
40	CONTINUE	HYBD2410
50	CONTINUE	HYBD2420
C		HYBD2430
C	ON THE FIRST ITERATION, CALCULATE THE NORM OF THE SCALED X	HYBD2440
C	AND INITIALIZE THE STEP BOUND DELTA.	HYBD2450
C		HYBD2460
	DO 60 J = 1, N	HYBD2470
	WA3(J) = DIAG(J)*X(J)	HYBD2480
60	CONTINUE	HYBD2490
	XNORM = ENORM(N,WA3)	HYBD2500
	DELTA = FACTOR*XNORM	HYBD2510
	IF (DELTA .EQ. ZERO) DELTA = FACTOR	HYBD2520
70	CONTINUE	HYBD2530
C		HYBD2540
C	FORM (Q TRANSPOSE)*FVEC AND STORE IN QTF.	HYBD2550
C		HYBD2560
	DO 80 I = 1, N	HYBD2570
	QTF(I) = FVEC(I)	HYBD2580
80	CONTINUE	HYBD2590
	DO 120 J = 1, N	HYBD2600
	IF (FJAC(J,J) .EQ. ZERO) GO TO 110	HYBD2610
	SUM = ZERO	HYBD2620
	DO 90 I = J, N	HYBD2630
	SUM = SUM + FJAC(I,J)*QTF(I)	HYBD2640
90	CONTINUE	HYBD2650
	TEMP = -SUM/FJAC(J,J)	HYBD2660
	DO 100 I = J, N	HYBD2670
	QTF(I) = QTF(I) + FJAC(I,J)*TEMP	HYBD2680
100	CONTINUE	HYBD2690
110	CONTINUE	HYBD2700

120	CONTINUE	HYBD2710
C		HYBD2720
C	COPY THE TRIANGULAR FACTOR OF THE QR FACTORIZATION INTO R.	HYBD2730
C		HYBD2740
	SING = .FALSE.	HYBD2750
	DO 150 J = 1, N	HYBD2760
	L = J	HYBD2770
	JM1 = J - 1	HYBD2780
	IF (JM1 .LT. 1) GO TO 140	HYBD2790
	DO 130 I = 1, JM1	HYBD2800
	R(L) = FJAC(I,J)	HYBD2810
	L = L + N - I	HYBD2820
130	CONTINUE	HYBD2830
140	CONTINUE	HYBD2840
	R(L) = WA1(J)	HYBD2850
	IF (WA1(J) .EQ. ZERO) SING = .TRUE.	HYBD2860
150	CONTINUE	HYBD2870
C		HYBD2880
C	ACCUMULATE THE ORTHOGONAL FACTOR IN FJAC.	HYBD2890
C		HYBD2900
	CALL QFORM(N,N,FJAC,LDFJAC,WA1)	HYBD2910
C		HYBD2920
C	RESCALE IF NECESSARY.	HYBD2930
C		HYBD2940
	IF (MODE .EQ. 2) GO TO 170	HYBD2950
	DO 160 J = 1, N	HYBD2960
	DIAG(J) = DMAX1(DIAG(J),WA2(J))	HYBD2970
160	CONTINUE	HYBD2980
170	CONTINUE	HYBD2990
C		HYBD3000
C	BEGINNING OF THE INNER LOOP.	HYBD3010
C		HYBD3020
180	CONTINUE	HYBD3030
C		HYBD3040
C	IF REQUESTED, CALL FCN TO ENABLE PRINTING OF ITERATES.	HYBD3050
C		HYBD3060
	IF (NPRINT .LE. 0) GO TO 190	HYBD3070
	IFLAG = 0	HYBD3080
	IF (MOD(ITER-1,NPRINT) .EQ. 0) CALL FCN(N,X,FVEC,IFLAG)	HYBD3090
	IF (IFLAG .LT. 0) GO TO 300	HYBD3100
190	CONTINUE	HYBD3110
C		HYBD3120
C	DETERMINE THE DIRECTION P.	HYBD3130
C		HYBD3140
	CALL DOGLEG(N,R,LR,DIAG,QTF,DELTA,WA1,WA2,WA3)	HYBD3150
C		HYBD3160
C	STORE THE DIRECTION P AND X + P. CALCULATE THE NORM OF P.	HYBD3170
C		HYBD3180
	DO 200 J = 1, N	HYBD3190
	WA1(J) = -WA1(J)	HYBD3200
	WA2(J) = X(J) + WA1(J)	HYBD3210
	WA3(J) = DIAG(J)*WA1(J)	HYBD3220
200	CONTINUE	HYBD3230
	PNORM = ENORM(N,WA3)	HYBD3240

C		HYBD3250
C	ON THE FIRST ITERATION, ADJUST THE INITIAL STEP BOUND.	HYBD3260
C		HYBD3270
	IF (ITER .EQ. 1) DELTA = DMIN1(DELTA,PNORM)	HYBD3280
C		HYBD3290
C	EVALUATE THE FUNCTION AT X + P AND CALCULATE ITS NORM.	HYBD3300
C		HYBD3310
	IFLAG = 1	HYBD3320
	CALL FCN(N,WA2,WA4,IFLAG)	HYBD3330
	NFEV = NFEV + 1	HYBD3340
	IF (IFLAG .LT. 0) GO TO 300	HYBD3350
	FNORM1 = ENORM(N,WA4)	HYBD3360
C		HYBD3370
C	COMPUTE THE SCALED ACTUAL REDUCTION.	HYBD3380
C		HYBD3390
	ACTRED = -ONE	HYBD3400
	IF (FNORM1 .LT. FNORM) ACTRED = ONE - (FNORM1/FNORM)**2	HYBD3410
C		HYBD3420
C	COMPUTE THE SCALED PREDICTED REDUCTION.	HYBD3430
C		HYBD3440
	L = 1	HYBD3450
	DO 220 I = 1, N	HYBD3460
	SUM = ZERO	HYBD3470
	DO 210 J = I, N	HYBD3480
	SUM = SUM + R(L)*WA1(J)	HYBD3490
	L = L + 1	HYBD3500
210	CONTINUE	HYBD3510
	WA3(I) = QTF(I) + SUM	HYBD3520
220	CONTINUE	HYBD3530
	TEMP = ENORM(N,WA3)	HYBD3540
	PRERED = ZERO	HYBD3550
	IF (TEMP .LT. FNORM) PRERED = ONE - (TEMP/FNORM)**2	HYBD3560
C		HYBD3570
C	COMPUTE THE RATIO OF THE ACTUAL TO THE PREDICTED	HYBD3580
C	REDUCTION.	HYBD3590
C		HYBD3600
	RATIO = ZERO	HYBD3610
	IF (PRERED .GT. ZERO) RATIO = ACTRED/PRERED	HYBD3620
C		HYBD3630
C	UPDATE THE STEP BOUND.	HYBD3640
C		HYBD3650
	IF (RATIO .GE. P1) GO TO 230	HYBD3660
	NCSUC = 0	HYBD3670
	NCFAIL = NCFAIL + 1	HYBD3680
	DELTA = P5*DELTA	HYBD3690
	GO TO 240	HYBD3700
230	CONTINUE	HYBD3710
	NCFAIL = 0	HYBD3720
	NCSUC = NCSUC + 1	HYBD3730
	IF (RATIO .GE. P5 .OR. NCSUC .GT. 1)	HYBD3740
*	DELTA = DMAX1(DELTA,PNORM/P5)	HYBD3750
	IF (DABS(RATIO-ONE) .LE. P1) DELTA = PNORM/P5	HYBD3760
240	CONTINUE	HYBD3770
C		HYBD3780

C	TEST FOR SUCCESSFUL ITERATION.	HYBD3790
C		HYBD3800
	IF (RATIO .LT. P0001) GO TO 260	HYBD3810
C		HYBD3820
C	SUCCESSFUL ITERATION. UPDATE X, FVEC, AND THEIR NORMS.	HYBD3830
C		HYBD3840
	DO 250 J = 1, N	HYBD3850
	X(J) = WA2(J)	HYBD3860
	WA2(J) = DIAG(J)*X(J)	HYBD3870
	FVEC(J) = WA4(J)	HYBD3880
250	CONTINUE	HYBD3890
	XNORM = ENORM(N,WA2)	HYBD3900
	FNORM = FNORM1	HYBD3910
	ITER = ITER + 1	HYBD3920
260	CONTINUE	HYBD3930
C		HYBD3940
C	DETERMINE THE PROGRESS OF THE ITERATION.	HYBD3950
C		HYBD3960
	NSLOW1 = NSLOW1 + 1	HYBD3970
	IF (ACTRED .GE. P001) NSLOW1 = 0	HYBD3980
	IF (JEVAL) NSLOW2 = NSLOW2 + 1	HYBD3990
	IF (ACTRED .GE. P1) NSLOW2 = 0	HYBD4000
C		HYBD4010
C	TEST FOR CONVERGENCE.	HYBD4020
C		HYBD4030
	IF (DELTA .LE. XTOL*XNORM .OR. FNORM .EQ. ZERO) INFO = 1	HYBD4040
	IF (INFO .NE. 0) GO TO 300	HYBD4050
C		HYBD4060
C	TESTS FOR TERMINATION AND STRINGENT TOLERANCES.	HYBD4070
C		HYBD4080
	IF (NFEV .GE. MAXFEV) INFO = 2	HYBD4090
	IF (P1*DMAX1(P1*DELTA,PNORM) .LE. EPSMCH*XNORM) INFO = 3	HYBD4100
	IF (NSLOW2 .EQ. 5) INFO = 4	HYBD4110
	IF (NSLOW1 .EQ. 10) INFO = 5	HYBD4120
	IF (INFO .NE. 0) GO TO 300	HYBD4130
C		HYBD4140
C	CRITERION FOR RECALCULATING JACOBIAN APPROXIMATION	HYBD4150
C	BY FORWARD DIFFERENCES.	HYBD4160
C		HYBD4170
	IF (NCFAIL .EQ. 2) GO TO 290	HYBD4180
C		HYBD4190
C	CALCULATE THE RANK ONE MODIFICATION TO THE JACOBIAN	HYBD4200
C	AND UPDATE QTF IF NECESSARY.	HYBD4210
C		HYBD4220
	DO 280 J = 1, N	HYBD4230
	SUM = ZERO	HYBD4240
	DO 270 I = 1, N	HYBD4250
	SUM = SUM + FJAC(I,J)*WA4(I)	HYBD4260
270	CONTINUE	HYBD4270
	WA2(J) = (SUM - WA3(J))/PNORM	HYBD4280
	WA1(J) = DIAG(J)*((DIAG(J)*WA1(J))/PNORM)	HYBD4290
	IF (RATIO .GE. P0001) QTF(J) = SUM	HYBD4300
280	CONTINUE	HYBD4310
C		HYBD4320

C	COMPUTE THE QR FACTORIZATION OF THE UPDATED JACOBIAN.	HYBD4330
C		HYBD4340
	CALL R1UPDT(N,N,R,LR,WA1,WA2,WA3,SING)	HYBD4350
	CALL R1MPYQ(N,N,FJAC,LDFJAC,WA2,WA3)	HYBD4360
	CALL R1MPYQ(1,N,QTF,1,WA2,WA3)	HYBD4370
C		HYBD4380
C	END OF THE INNER LOOP.	HYBD4390
C		HYBD4400
	JEVAL = .FALSE.	HYBD4410
	GO TO 180	HYBD4420
290	CONTINUE	HYBD4430
C		HYBD4440
C	END OF THE OUTER LOOP.	HYBD4450
C		HYBD4460
	GO TO 30	HYBD4470
300	CONTINUE	HYBD4480
C		HYBD4490
C	TERMINATION, EITHER NORMAL OR USER IMPOSED.	HYBD4500
C		HYBD4510
	IF (IFLAG .LT. 0) INFO = IFLAG	HYBD4520
	IFLAG = 0	HYBD4530
	IF (NPRINT .GT. 0) CALL FCN(N,X,FVEC,IFLAG)	HYBD4540
	RETURN	HYBD4550
C		HYBD4560
C	LAST CARD OF SUBROUTINE HYBRD.	HYBD4570
C		HYBD4580
	END	HYBD4590

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SUBROUTINE HYBRD1 (FCN,N,X,FVEC,TOL,INFO,WA,LWA)
  INTEGER N,INFO,LWA
  DOUBLE PRECISION TOL
  DOUBLE PRECISION X(N),FVEC(N),WA(LWA)
  EXTERNAL FCN
  *****

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SUBROUTINE HYBRD1

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  THE PURPOSE OF HYBRD1 IS TO FIND A ZERO OF A SYSTEM OF
  N NONLINEAR FUNCTIONS IN N VARIABLES BY A MODIFICATION
  OF THE POWELL HYBRID METHOD. THIS IS DONE BY USING THE
  MORE GENERAL NONLINEAR EQUATION SOLVER HYBRD. THE USER
  MUST PROVIDE A SUBROUTINE WHICH CALCULATES THE FUNCTIONS.
  THE JACOBIAN IS THEN CALCULATED BY A FORWARD-DIFFERENCE
  APPROXIMATION.

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  THE SUBROUTINE STATEMENT IS

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    SUBROUTINE HYBRD1 (FCN,N,X,FVEC,TOL,INFO,WA,LWA)

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  WHERE

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    FCN IS THE NAME OF THE USER-SUPPLIED SUBROUTINE WHICH
    CALCULATES THE FUNCTIONS. FCN MUST BE DECLARED
    IN AN EXTERNAL STATEMENT IN THE USER CALLING
    PROGRAM, AND SHOULD BE WRITTEN AS FOLLOWS.

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    SUBROUTINE FCN(N,X,FVEC,IFLAG)
    INTEGER N,IFLAG
    DOUBLE PRECISION X(N),FVEC(N)
    -----

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    CALCULATE THE FUNCTIONS AT X AND
    RETURN THIS VECTOR IN FVEC.
    -----

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```

    RETURN
    END

```

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    THE VALUE OF IFLAG SHOULD NOT BE CHANGED BY FCN UNLESS
    THE USER WANTS TO TERMINATE EXECUTION OF HYBRD1.
    IN THIS CASE SET IFLAG TO A NEGATIVE INTEGER.

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  N IS A POSITIVE INTEGER INPUT VARIABLE SET TO THE NUMBER
  OF FUNCTIONS AND VARIABLES.

```

```

  X IS AN ARRAY OF LENGTH N. ON INPUT X MUST CONTAIN
  AN INITIAL ESTIMATE OF THE SOLUTION VECTOR. ON OUTPUT X
  CONTAINS THE FINAL ESTIMATE OF THE SOLUTION VECTOR.

```

```

  FVEC IS AN OUTPUT ARRAY OF LENGTH N WHICH CONTAINS
  THE FUNCTIONS EVALUATED AT THE OUTPUT X.

```

```

  TOL IS A NONNEGATIVE INPUT VARIABLE. TERMINATION OCCURS
  WHEN THE ALGORITHM ESTIMATES THAT THE RELATIVE ERROR

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HYD10010
HYD10020
HYD10030
HYD10040
HYD10050
HYD10060
HYD10070
HYD10080
HYD10090
HYD10100
HYD10110
HYD10120
HYD10130
HYD10140
HYD10150
HYD10160
HYD10170
HYD10180
HYD10190
HYD10200
HYD10210
HYD10220
HYD10230
HYD10240
HYD10250
HYD10260
HYD10270
HYD10280
HYD10290
HYD10300
HYD10310
HYD10320
HYD10330
HYD10340
HYD10350
HYD10360
HYD10370
HYD10380
HYD10390
HYD10400
HYD10410
HYD10420
HYD10430
HYD10440
HYD10450
HYD10460
HYD10470
HYD10480
HYD10490
HYD10500
HYD10510
HYD10520
HYD10530
HYD10540

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C	BETWEEN X AND THE SOLUTION IS AT MOST TOL.	HYD10550
C		HYD10560
C	INFO IS AN INTEGER OUTPUT VARIABLE. IF THE USER HAS	HYD10570
C	TERMINATED EXECUTION, INFO IS SET TO THE (NEGATIVE)	HYD10580
C	VALUE OF IFLAG. SEE DESCRIPTION OF FCN. OTHERWISE,	HYD10590
C	INFO IS SET AS FOLLOWS.	HYD10600
C		HYD10610
C	INFO = 0 IMPROPER INPUT PARAMETERS.	HYD10620
C		HYD10630
C	INFO = 1 ALGORITHM ESTIMATES THAT THE RELATIVE ERROR	HYD10640
C	BETWEEN X AND THE SOLUTION IS AT MOST TOL.	HYD10650
C		HYD10660
C	INFO = 2 NUMBER OF CALLS TO FCN HAS REACHED OR EXCEEDED	HYD10670
C	200*(N+1).	HYD10680
C		HYD10690
C	INFO = 3 TOL IS TOO SMALL. NO FURTHER IMPROVEMENT IN	HYD10700
C	THE APPROXIMATE SOLUTION X IS POSSIBLE.	HYD10710
C		HYD10720
C	INFO = 4 ITERATION IS NOT MAKING GOOD PROGRESS.	HYD10730
C		HYD10740
C	WA IS A WORK ARRAY OF LENGTH LWA.	HYD10750
C		HYD10760
C	LWA IS A POSITIVE INTEGER INPUT VARIABLE NOT LESS THAN	HYD10770
C	(N*(3*N+13))/2.	HYD10780
C		HYD10790
C	SUBPROGRAMS CALLED	HYD10800
C		HYD10810
C	USER-SUPPLIED FCN	HYD10820
C		HYD10830
C	MINPACK-SUPPLIED ... HYBRD	HYD10840
C		HYD10850
C	ARGONNE NATIONAL LABORATORY. MINPACK PROJECT. MARCH 1980.	HYD10860
C	BURTON S. GARBOW, KENNETH E. HILLSTROM, JORGE J. MORE	HYD10870
C		HYD10880
C	*****	HYD10890
C	INTEGER INDEX,J,LR,MAXFEV,ML,MODE,MU,NFEV,NPRINT	HYD10900
C	DOUBLE PRECISION EPSFCN,FACTOR,ONE,XTOL,ZERO	HYD10910
C	DATA FACTOR,ONE,ZERO /1.0D2,1.0D0,0.0D0/	HYD10920
C	INFO = 0	HYD10930
C		HYD10940
C	CHECK THE INPUT PARAMETERS FOR ERRORS.	HYD10950
C		HYD10960
C	IF (N .LE. 0 .OR. TOL .LT. ZERO .OR. LWA .LT. (N*(3*N + 13))/2)	HYD10970
C	* GO TO 20	HYD10980
C		HYD10990
C	CALL HYBRD.	HYD11000
C		HYD11010
C	MAXFEV = 200*(N + 1)	HYD11020
C	XTOL = TOL	HYD11030
C	ML = N - 1	HYD11040
C	MU = N - 1	HYD11050
C	EPSFCN = ZERO	HYD11060
C	MODE = 2	HYD11070
C	DO 10 J = 1, N	HYD11080

	WA(J) = ONE	HYD11090
10	CONTINUE	HYD11100
	NPRINT = 0	HYD11110
	LR = (N*(N + 1))/2	HYD11120
	INDEX = 6*N + LR	HYD11130
	CALL HYBRD(FCN,N,X,FVEC,XTOL,MAXFEV,ML,MU,EPSFCN,WA(1),MODE,	HYD11140
	* FACTOR,NPRINT,INFO,NFEV,WA(INDEX+1),N,WA(6*N+1),LR,	HYD11150
	* WA(N+1),WA(2*N+1),WA(3*N+1),WA(4*N+1),WA(5*N+1))	HYD11160
	IF (INFO .EQ. 5) INFO = 4	HYD11170
20	CONTINUE	HYD11180
	RETURN	HYD11190
C		HYD11200
C	LAST CARD OF SUBROUTINE HYBRD1.	HYD11210
C		HYD11220
	END	HYD11230

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SUBROUTINE HYBRJ(FCN,N,X,FVEC,FJAC,LDFJAC,XTOL,MAXFEV,DIAG,MODE, HYBJ0010
*          FACTOR,NPRINT,INFO,NFEV,NJEV,R,LR,QTF,WA1,WA2, HYBJ0020
*          WA3,WA4) HYBJ0030
  INTEGER N,LDFJAC,MAXFEV,MODE,NPRINT,INFO,NFEV,NJEV,LR HYBJ0040
  DOUBLE PRECISION XTOL,FACTOR HYBJ0050
  DOUBLE PRECISION X(N),FVEC(N),FJAC(LDFJAC,N),DIAG(N),R(LR), HYBJ0060
*          QTF(N),WA1(N),WA2(N),WA3(N),WA4(N) HYBJ0070
  ***** HYBJ0080
C          HYBJ0090
C          SUBROUTINE HYBRJ HYBJ0100
C          HYBJ0110
C          THE PURPOSE OF HYBRJ IS TO FIND A ZERO OF A SYSTEM OF HYBJ0120
C          N NONLINEAR FUNCTIONS IN N VARIABLES BY A MODIFICATION HYBJ0130
C          OF THE POWELL HYBRID METHOD. THE USER MUST PROVIDE A HYBJ0140
C          SUBROUTINE WHICH CALCULATES THE FUNCTIONS AND THE JACOBIAN. HYBJ0150
C          HYBJ0160
C          THE SUBROUTINE STATEMENT IS HYBJ0170
C          HYBJ0180
C          SUBROUTINE HYBRJ(FCN,N,X,FVEC,FJAC,LDFJAC,XTOL,MAXFEV,DIAG, HYBJ0190
C          MODE,FACTOR,NPRINT,INFO,NFEV,NJEV,R,LR,QTF, HYBJ0200
C          WA1,WA2,WA3,WA4) HYBJ0210
C          HYBJ0220
C          WHERE HYBJ0230
C          HYBJ0240
C          FCN IS THE NAME OF THE USER-SUPPLIED SUBROUTINE WHICH HYBJ0250
C          CALCULATES THE FUNCTIONS AND THE JACOBIAN. FCN MUST HYBJ0260
C          BE DECLARED IN AN EXTERNAL STATEMENT IN THE USER HYBJ0270
C          CALLING PROGRAM, AND SHOULD BE WRITTEN AS FOLLOWS. HYBJ0280
C          HYBJ0290
C          SUBROUTINE FCN(N,X,FVEC,FJAC,LDFJAC,IFLAG) HYBJ0300
C          INTEGER N,LDFJAC,IFLAG HYBJ0310
C          DOUBLE PRECISION X(N),FVEC(N),FJAC(LDFJAC,N) HYBJ0320
C          ----- HYBJ0330
C          IF IFLAG = 1 CALCULATE THE FUNCTIONS AT X AND HYBJ0340
C          RETURN THIS VECTOR IN FVEC. DO NOT ALTER FJAC. HYBJ0350
C          IF IFLAG = 2 CALCULATE THE JACOBIAN AT X AND HYBJ0360
C          RETURN THIS MATRIX IN FJAC. DO NOT ALTER FVEC. HYBJ0370
C          ----- HYBJ0380
C          RETURN HYBJ0390
C          END HYBJ0400
C          HYBJ0410
C          THE VALUE OF IFLAG SHOULD NOT BE CHANGED BY FCN UNLESS HYBJ0420
C          THE USER WANTS TO TERMINATE EXECUTION OF HYBRJ. HYBJ0430
C          IN THIS CASE SET IFLAG TO A NEGATIVE INTEGER. HYBJ0440
C          HYBJ0450
C          N IS A POSITIVE INTEGER INPUT VARIABLE SET TO THE NUMBER HYBJ0460
C          OF FUNCTIONS AND VARIABLES. HYBJ0470
C          HYBJ0480
C          X IS AN ARRAY OF LENGTH N. ON INPUT X MUST CONTAIN HYBJ0490
C          AN INITIAL ESTIMATE OF THE SOLUTION VECTOR. ON OUTPUT X HYBJ0500
C          CONTAINS THE FINAL ESTIMATE OF THE SOLUTION VECTOR. HYBJ0510
C          HYBJ0520
C          FVEC IS AN OUTPUT ARRAY OF LENGTH N WHICH CONTAINS HYBJ0530
C          THE FUNCTIONS EVALUATED AT THE OUTPUT X. HYBJ0540

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C		HYBJ0550
C	FJAC IS AN OUTPUT N BY N ARRAY WHICH CONTAINS THE	HYBJ0560
C	ORTHOGONAL MATRIX Q PRODUCED BY THE QR FACTORIZATION	HYBJ0570
C	OF THE FINAL APPROXIMATE JACOBIAN.	HYBJ0580
C		HYBJ0590
C	LDFJAC IS A POSITIVE INTEGER INPUT VARIABLE NOT LESS THAN N	HYBJ0600
C	WHICH SPECIFIES THE LEADING DIMENSION OF THE ARRAY FJAC.	HYBJ0610
C		HYBJ0620
C	XTOL IS A NONNEGATIVE INPUT VARIABLE. TERMINATION	HYBJ0630
C	OCCURS WHEN THE RELATIVE ERROR BETWEEN TWO CONSECUTIVE	HYBJ0640
C	ITERATES IS AT MOST XTOL.	HYBJ0650
C		HYBJ0660
C	MAXFEV IS A POSITIVE INTEGER INPUT VARIABLE. TERMINATION	HYBJ0670
C	OCCURS WHEN THE NUMBER OF CALLS TO FCN WITH IFLAG = 1	HYBJ0680
C	HAS REACHED MAXFEV.	HYBJ0690
C		HYBJ0700
C	DIAG IS AN ARRAY OF LENGTH N. IF MODE = 1 (SEE	HYBJ0710
C	BELOW), DIAG IS INTERNALLY SET. IF MODE = 2, DIAG	HYBJ0720
C	MUST CONTAIN POSITIVE ENTRIES THAT SERVE AS	HYBJ0730
C	MULTIPLICATIVE SCALE FACTORS FOR THE VARIABLES.	HYBJ0740
C		HYBJ0750
C	MODE IS AN INTEGER INPUT VARIABLE. IF MODE = 1, THE	HYBJ0760
C	VARIABLES WILL BE SCALED INTERNALLY. IF MODE = 2,	HYBJ0770
C	THE SCALING IS SPECIFIED BY THE INPUT DIAG. OTHER	HYBJ0780
C	VALUES OF MODE ARE EQUIVALENT TO MODE = 1.	HYBJ0790
C		HYBJ0800
C	FACTOR IS A POSITIVE INPUT VARIABLE USED IN DETERMINING THE	HYBJ0810
C	INITIAL STEP BOUND. THIS BOUND IS SET TO THE PRODUCT OF	HYBJ0820
C	FACTOR AND THE EUCLIDEAN NORM OF DIAG*X IF NONZERO, OR ELSE	HYBJ0830
C	TO FACTOR ITSELF. IN MOST CASES FACTOR SHOULD LIE IN THE	HYBJ0840
C	INTERVAL (.1,100.). 100. IS A GENERALLY RECOMMENDED VALUE.	HYBJ0850
C		HYBJ0860
C	NPRINT IS AN INTEGER INPUT VARIABLE THAT ENABLES CONTROLLED	HYBJ0870
C	PRINTING OF ITERATES IF IT IS POSITIVE. IN THIS CASE,	HYBJ0880
C	FCN IS CALLED WITH IFLAG = 0 AT THE BEGINNING OF THE FIRST	HYBJ0890
C	ITERATION AND EVERY NPRINT ITERATIONS THEREAFTER AND	HYBJ0900
C	IMMEDIATELY PRIOR TO RETURN, WITH X AND FVEC AVAILABLE	HYBJ0910
C	FOR PRINTING. FVEC AND FJAC SHOULD NOT BE ALTERED.	HYBJ0920
C	IF NPRINT IS NOT POSITIVE, NO SPECIAL CALLS OF FCN	HYBJ0930
C	WITH IFLAG = 0 ARE MADE.	HYBJ0940
C		HYBJ0950
C	INFO IS AN INTEGER OUTPUT VARIABLE. IF THE USER HAS	HYBJ0960
C	TERMINATED EXECUTION, INFO IS SET TO THE (NEGATIVE)	HYBJ0970
C	VALUE OF IFLAG. SEE DESCRIPTION OF FCN. OTHERWISE,	HYBJ0980
C	INFO IS SET AS FOLLOWS.	HYBJ0990
C		HYBJ1000
C	INFO = 0 IMPROPER INPUT PARAMETERS.	HYBJ1010
C		HYBJ1020
C	INFO = 1 RELATIVE ERROR BETWEEN TWO CONSECUTIVE ITERATES	HYBJ1030
C	IS AT MOST XTOL.	HYBJ1040
C		HYBJ1050
C	INFO = 2 NUMBER OF CALLS TO FCN WITH IFLAG = 1 HAS	HYBJ1060
C	REACHED MAXFEV.	HYBJ1070
C		HYBJ1080

	EPSMCH = DPMPAR(1)	HYBJ1630
C	INFO = 0	HYBJ1640
	IFLAG = 0	HYBJ1650
	NFEV = 0	HYBJ1660
	NJEV = 0	HYBJ1670
C		HYBJ1680
C	CHECK THE INPUT PARAMETERS FOR ERRORS.	HYBJ1690
C		HYBJ1700
	IF (N .LE. 0 .OR. LDFJAC .LT. N .OR. XTOL .LT. ZERO	HYBJ1710
	* .OR. MAXFEV .LE. 0 .OR. FACTOR .LE. ZERO	HYBJ1720
	* .OR. LR .LT. (N*(N + 1))/2) GO TO 300	HYBJ1730
	IF (MODE .NE. 2) GO TO 20	HYBJ1740
	DO 10 J = 1, N	HYBJ1750
	IF (DIAG(J) .LE. ZERO) GO TO 300	HYBJ1760
10	CONTINUE	HYBJ1770
20	CONTINUE	HYBJ1780
C		HYBJ1790
C	EVALUATE THE FUNCTION AT THE STARTING POINT	HYBJ1800
C	AND CALCULATE ITS NORM.	HYBJ1810
C		HYBJ1820
	IFLAG = 1	HYBJ1830
	CALL FCN(N,X,FVEC,FJAC,LDFJAC,IFLAG)	HYBJ1840
	NFEV = 1	HYBJ1850
	IF (IFLAG .LT. 0) GO TO 300	HYBJ1860
	FNORM = ENORM(N,FVEC)	HYBJ1870
C		HYBJ1880
C	INITIALIZE ITERATION COUNTER AND MONITORS.	HYBJ1890
C		HYBJ1900
	ITER = 1	HYBJ1910
	NCSUC = 0	HYBJ1920
	NCFAIL = 0	HYBJ1930
	NSLOW1 = 0	HYBJ1940
	NSLOW2 = 0	HYBJ1950
C		HYBJ1960
C	BEGINNING OF THE OUTER LOOP.	HYBJ1970
C		HYBJ1980
	30 CONTINUE	HYBJ1990
	JEVAL = .TRUE.	HYBJ2000
C		HYBJ2010
C	CALCULATE THE JACOBIAN MATRIX.	HYBJ2020
C		HYBJ2030
	IFLAG = 2	HYBJ2040
	CALL FCN(N,X,FVEC,FJAC,LDFJAC,IFLAG)	HYBJ2050
	NJEV = NJEV + 1	HYBJ2060
	IF (IFLAG .LT. 0) GO TO 300	HYBJ2070
C		HYBJ2080
C	COMPUTE THE QR FACTORIZATION OF THE JACOBIAN.	HYBJ2090
C		HYBJ2100
	CALL QRFAC(N,N,FJAC,LDFJAC,.FALSE.,IWA,1,WA1,WA2,WA3)	HYBJ2110
C		HYBJ2120
C	ON THE FIRST ITERATION AND IF MODE IS 1, SCALE ACCORDING	HYBJ2130
C	TO THE NORMS OF THE COLUMNS OF THE INITIAL JACOBIAN.	HYBJ2140
C		HYBJ2150
C		HYBJ2160

	IF (ITER .NE. 1) GO TO 70	HYBJ2170
	IF (MODE .EQ. 2) GO TO 50	HYBJ2180
	DO 40 J = 1, N	HYBJ2190
	DIAG(J) = WA2(J)	HYBJ2200
	IF (WA2(J) .EQ. ZERO) DIAG(J) = ONE	HYBJ2210
40	CONTINUE	HYBJ2220
50	CONTINUE	HYBJ2230
C		HYBJ2240
C	ON THE FIRST ITERATION, CALCULATE THE NORM OF THE SCALED X	HYBJ2250
C	AND INITIALIZE THE STEP BOUND DELTA.	HYBJ2260
C		HYBJ2270
	DO 60 J = 1, N	HYBJ2280
	WA3(J) = DIAG(J)*X(J)	HYBJ2290
60	CONTINUE	HYBJ2300
	XNORM = ENORM(N,WA3)	HYBJ2310
	DELTA = FACTOR*XNORM	HYBJ2320
	IF (DELTA .EQ. ZERO) DELTA = FACTOR	HYBJ2330
70	CONTINUE	HYBJ2340
C		HYBJ2350
C	FORM (Q TRANSPOSE)*FVEC AND STORE IN QTF.	HYBJ2360
C		HYBJ2370
	DO 80 I = 1, N	HYBJ2380
	QTF(I) = FVEC(I)	HYBJ2390
80	CONTINUE	HYBJ2400
	DO 120 J = 1, N	HYBJ2410
	IF (FJAC(J,J) .EQ. ZERO) GO TO 110	HYBJ2420
	SUM = ZERO	HYBJ2430
	DO 90 I = J, N	HYBJ2440
	SUM = SUM + FJAC(I,J)*QTF(I)	HYBJ2450
90	CONTINUE	HYBJ2460
	TEMP = -SUM/FJAC(J,J)	HYBJ2470
	DO 100 I = J, N	HYBJ2480
	QTF(I) = QTF(I) + FJAC(I,J)*TEMP	HYBJ2490
100	CONTINUE	HYBJ2500
110	CONTINUE	HYBJ2510
120	CONTINUE	HYBJ2520
C		HYBJ2530
C	COPY THE TRIANGULAR FACTOR OF THE QR FACTORIZATION INTO R.	HYBJ2540
C		HYBJ2550
	SING = .FALSE.	HYBJ2560
	DO 150 J = 1, N	HYBJ2570
	L = J	HYBJ2580
	JM1 = J - 1	HYBJ2590
	IF (JM1 .LT. 1) GO TO 140	HYBJ2600
	DO 130 I = 1, JM1	HYBJ2610
	R(L) = FJAC(I,J)	HYBJ2620
	L = L + N - I	HYBJ2630
130	CONTINUE	HYBJ2640
140	CONTINUE	HYBJ2650
	R(L) = WA1(J)	HYBJ2660
	IF (WA1(J) .EQ. ZERO) SING = .TRUE.	HYBJ2670
150	CONTINUE	HYBJ2680
C		HYBJ2690
C	ACCUMULATE THE ORTHOGONAL FACTOR IN FJAC.	HYBJ2700

C	CALL QFORM(N,N,FJAC,LDFJAC,WA1)	HYBJ2710
C		HYBJ2720
C	RESCALE IF NECESSARY.	HYBJ2730
C		HYBJ2740
	IF (MODE .EQ. 2) GO TO 170	HYBJ2750
	DO 160 J = 1, N	HYBJ2760
	DIAG(J) = DMAX1(DIAG(J),WA2(J))	HYBJ2770
160	CONTINUE	HYBJ2780
170	CONTINUE	HYBJ2790
C		HYBJ2800
C	BEGINNING OF THE INNER LOOP.	HYBJ2810
C		HYBJ2820
C		HYBJ2830
180	CONTINUE	HYBJ2840
C		HYBJ2850
C	IF REQUESTED, CALL FCN TO ENABLE PRINTING OF ITERATES.	HYBJ2860
C		HYBJ2870
	IF (NPRINT .LE. 0) GO TO 190	HYBJ2880
	IFLAG = 0	HYBJ2890
	IF (MOD(ITER-1,NPRINT) .EQ. 0)	HYBJ2900
*	CALL FCN(N,X,FVEC,FJAC,LDFJAC,IFLAG)	HYBJ2910
	IF (IFLAG .LT. 0) GO TO 300	HYBJ2920
190	CONTINUE	HYBJ2930
C		HYBJ2940
C	DETERMINE THE DIRECTION P.	HYBJ2950
C		HYBJ2960
	CALL DOGLEG(N,R,LR,DIAG,QTF,DELTA,WA1,WA2,WA3)	HYBJ2970
C		HYBJ2980
C	STORE THE DIRECTION P AND X + P. CALCULATE THE NORM OF P.	HYBJ2990
C		HYBJ3000
	DO 200 J = 1, N	HYBJ3010
	WA1(J) = -WA1(J)	HYBJ3020
	WA2(J) = X(J) + WA1(J)	HYBJ3030
	WA3(J) = DIAG(J)*WA1(J)	HYBJ3040
200	CONTINUE	HYBJ3050
	PNORM = ENORM(N,WA3)	HYBJ3060
C		HYBJ3070
C	ON THE FIRST ITERATION, ADJUST THE INITIAL STEP BOUND.	HYBJ3080
C		HYBJ3090
	IF (ITER .EQ. 1) DELTA = DMIN1(DELTA,PNORM)	HYBJ3100
C		HYBJ3110
C	EVALUATE THE FUNCTION AT X + P AND CALCULATE ITS NORM.	HYBJ3120
C		HYBJ3130
	IFLAG = 1	HYBJ3140
	CALL FCN(N,WA2,WA4,FJAC,LDFJAC,IFLAG)	HYBJ3150
	NFEV = NFEV + 1	HYBJ3160
	IF (IFLAG .LT. 0) GO TO 300	HYBJ3170
	FNORM1 = ENORM(N,WA4)	HYBJ3180
C		HYBJ3190
C	COMPUTE THE SCALED ACTUAL REDUCTION.	HYBJ3200
C		HYBJ3210
	ACTRED = -ONE	HYBJ3220
	IF (FNORM1 .LT. FNORM) ACTRED = ONE - (FNORM1/FNORM)**2	HYBJ3230
C		HYBJ3240

C	COMPUTE THE SCALED PREDICTED REDUCTION.	HYBJ3250
C		HYBJ3260
	L = 1	HYBJ3270
	DO 220 I = 1, N	HYBJ3280
	SUM = ZERO	HYBJ3290
	DO 210 J = 1, N	HYBJ3300
	SUM = SUM + R(L)*WA1(J)	HYBJ3310
	L = L + 1	HYBJ3320
210	CONTINUE	HYBJ3330
	WA3(I) = QTF(I) + SUM	HYBJ3340
220	CONTINUE	HYBJ3350
	TEMP = ENORM(N,WA3)	HYBJ3360
	PRERED = ZERO	HYBJ3370
	IF (TEMP .LT. FNORM) PRERED = ONE - (TEMP/FNORM)**2	HYBJ3380
C		HYBJ3390
C	COMPUTE THE RATIO OF THE ACTUAL TO THE PREDICTED	HYBJ3400
C	REDUCTION.	HYBJ3410
C		HYBJ3420
	RATIO = ZERO	HYBJ3430
	IF (PRERED .GT. ZERO) RATIO = ACTRED/PRERED	HYBJ3440
C		HYBJ3450
C	UPDATE THE STEP BOUND.	HYBJ3460
C		HYBJ3470
	IF (RATIO .GE. P1) GO TO 230	HYBJ3480
	NCSUC = 0	HYBJ3490
	NCFAIL = NCFAIL + 1	HYBJ3500
	DELTA = P5*DELTA	HYBJ3510
	GO TO 240	HYBJ3520
230	CONTINUE	HYBJ3530
	NCFAIL = 0	HYBJ3540
	NCSUC = NCSUC + 1	HYBJ3550
	IF (RATIO .GE. P5 .OR. NCSUC .GT. 1)	HYBJ3560
*	DELTA = DMAX1(DELTA,PNORM/P5)	HYBJ3570
	IF (DABS(RATIO-ONE) .LE. P1) DELTA = PNORM/P5	HYBJ3580
240	CONTINUE	HYBJ3590
C		HYBJ3600
C	TEST FOR SUCCESSFUL ITERATION.	HYBJ3610
C		HYBJ3620
	IF (RATIO .LT. P0001) GO TO 260	HYBJ3630
C		HYBJ3640
C	SUCCESSFUL ITERATION. UPDATE X, FVEC, AND THEIR NORMS.	HYBJ3650
C		HYBJ3660
	DO 250 J = 1, N	HYBJ3670
	X(J) = WA2(J)	HYBJ3680
	WA2(J) = DIAG(J)*X(J)	HYBJ3690
	FVEC(J) = WA4(J)	HYBJ3700
250	CONTINUE	HYBJ3710
	XNORM = ENORM(N,WA2)	HYBJ3720
	FNORM = FNORM1	HYBJ3730
	ITER = ITER + 1	HYBJ3740
260	CONTINUE	HYBJ3750
C		HYBJ3760
C	DETERMINE THE PROGRESS OF THE ITERATION.	HYBJ3770
C		HYBJ3780

	NSLOW1 = NSLOW1 + 1	HYBJ3790
	IF (ACTRED .GE. P001) NSLOW1 = 0	HYBJ3800
	IF (JEVAL) NSLOW2 = NSLOW2 + 1	HYBJ3810
	IF (ACTRED .GE. P1) NSLOW2 = 0	HYBJ3820
C		HYBJ3830
C	TEST FOR CONVERGENCE.	HYBJ3840
C		HYBJ3850
	IF (DELTA .LE. XTOL*XNORM .OR. FNORM .EQ. ZERO) INFO = 1	HYBJ3860
	IF (INFO .NE. 0) GO TO 300	HYBJ3870
C		HYBJ3880
C	TESTS FOR TERMINATION AND STRINGENT TOLERANCES.	HYBJ3890
C		HYBJ3900
	IF (NFEV .GE. MAXFEV) INFO = 2	HYBJ3910
	IF (P1*DMAX1(P1*DELTA,PNORM) .LE. EPSMCH*XNORM) INFO = 3	HYBJ3920
	IF (NSLOW2 .EQ. 5) INFO = 4	HYBJ3930
	IF (NSLOW1 .EQ. 10) INFO = 5	HYBJ3940
	IF (INFO .NE. 0) GO TO 300	HYBJ3950
C		HYBJ3960
C	CRITERION FOR RECALCULATING JACOBIAN.	HYBJ3970
C		HYBJ3980
	IF (NCFAIL .EQ. 2) GO TO 290	HYBJ3990
C		HYBJ4000
C	CALCULATE THE RANK ONE MODIFICATION TO THE JACOBIAN	HYBJ4010
C	AND UPDATE QTF IF NECESSARY.	HYBJ4020
C		HYBJ4030
	DO 280 J = 1, N	HYBJ4040
	SUM = ZERO	HYBJ4050
	DO 270 I = 1, N	HYBJ4060
	SUM = SUM + FJAC(I,J)*WA4(I)	HYBJ4070
270	CONTINUE	HYBJ4080
	WA2(J) = (SUM - WA3(J))/PNORM	HYBJ4090
	WA1(J) = DIAG(J)*((DIAG(J)*WA1(J))/PNORM)	HYBJ4100
	IF (RATIO .GE. P0001) QTF(J) = SUM	HYBJ4110
280	CONTINUE	HYBJ4120
C		HYBJ4130
C	COMPUTE THE QR FACTORIZATION OF THE UPDATED JACOBIAN.	HYBJ4140
C		HYBJ4150
	CALL RIUPDT(N,N,R,LR,WA1,WA2,WA3,SING)	HYBJ4160
	CALL RIMPYQ(N,N,FJAC,LDFJAC,WA2,WA3)	HYBJ4170
	CALL RIMPYQ(1,N,QTF,1,WA2,WA3)	HYBJ4180
C		HYBJ4190
C	END OF THE INNER LOOP.	HYBJ4200
C		HYBJ4210
	JEVAL = .FALSE.	HYBJ4220
	GO TO 180	HYBJ4230
290	CONTINUE	HYBJ4240
C		HYBJ4250
C	END OF THE OUTER LOOP.	HYBJ4260
C		HYBJ4270
	GO TO 30	HYBJ4280
300	CONTINUE	HYBJ4290
C		HYBJ4300
C	TERMINATION, EITHER NORMAL OR USER IMPOSED.	HYBJ4310
C		HYBJ4320


```
IF (IFLAG .LT. 0) INFO = IFLAG  
IFLAG = 0  
IF (NPRINT .GT. 0) CALL FCN(N,X,FVEC,FJAC,LDFJAC,IFLAG)  
RETURN
```

C
C
C

LAST CARD OF SUBROUTINE HYBRJ.

END

HYBJ4330
HYBJ4340
HYBJ4350
HYBJ4360
HYBJ4370
HYBJ4380
HYBJ4390
HYBJ4400

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SUBROUTINE HYBRJ1(FCN,N,X,FVEC,FJAC,LDFJAC,TOL,INFO,WA,LWA)
  INTEGER N,LDFJAC,INFO,LWA
  DOUBLE PRECISION TOL
  DOUBLE PRECISION X(N),FVEC(N),FJAC(LDFJAC,N),WA(LWA)
  EXTERNAL FCN

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SUBROUTINE HYBRJ1

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  THE PURPOSE OF HYBRJ1 IS TO FIND A ZERO OF A SYSTEM OF
  N NONLINEAR FUNCTIONS IN N VARIABLES BY A MODIFICATION
  OF THE POWELL HYBRID METHOD. THIS IS DONE BY USING THE
  MORE GENERAL NONLINEAR EQUATION SOLVER HYBRJ. THE USER
  MUST PROVIDE A SUBROUTINE WHICH CALCULATES THE FUNCTIONS
  AND THE JACOBIAN.

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  THE SUBROUTINE STATEMENT IS

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    SUBROUTINE HYBRJ1(FCN,N,X,FVEC,FJAC,LDFJAC,TOL,INFO,WA,LWA)

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  WHERE

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    FCN IS THE NAME OF THE USER-SUPPLIED SUBROUTINE WHICH
    CALCULATES THE FUNCTIONS AND THE JACOBIAN. FCN MUST
    BE DECLARED IN AN EXTERNAL STATEMENT IN THE USER
    CALLING PROGRAM, AND SHOULD BE WRITTEN AS FOLLOWS.

```

```

    SUBROUTINE FCN(N,X,FVEC,FJAC,LDFJAC,IFLAG)
    INTEGER N,LDFJAC,IFLAG
    DOUBLE PRECISION X(N),FVEC(N),FJAC(LDFJAC,N)
    -----

```

```

    IF IFLAG = 1 CALCULATE THE FUNCTIONS AT X AND
    RETURN THIS VECTOR IN FVEC. DO NOT ALTER FJAC.
    IF IFLAG = 2 CALCULATE THE JACOBIAN AT X AND
    RETURN THIS MATRIX IN FJAC. DO NOT ALTER FVEC.
    -----

```

```

    RETURN
    END

```

```

    THE VALUE OF IFLAG SHOULD NOT BE CHANGED BY FCN UNLESS
    THE USER WANTS TO TERMINATE EXECUTION OF HYBRJ1.
    IN THIS CASE SET IFLAG TO A NEGATIVE INTEGER.

```

```

  N IS A POSITIVE INTEGER INPUT VARIABLE SET TO THE NUMBER
  OF FUNCTIONS AND VARIABLES.

```

```

  X IS AN ARRAY OF LENGTH N. ON INPUT X MUST CONTAIN
  AN INITIAL ESTIMATE OF THE SOLUTION VECTOR. ON OUTPUT X
  CONTAINS THE FINAL ESTIMATE OF THE SOLUTION VECTOR.

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```

  FVEC IS AN OUTPUT ARRAY OF LENGTH N WHICH CONTAINS
  THE FUNCTIONS EVALUATED AT THE OUTPUT X.

```

```

  FJAC IS AN OUTPUT N BY N ARRAY WHICH CONTAINS THE

```

```

HYJ10010
HYJ10020
HYJ10030
HYJ10040
HYJ10050
HYJ10060
HYJ10070
HYJ10080
HYJ10090
HYJ10100
HYJ10110
HYJ10120
HYJ10130
HYJ10140
HYJ10150
HYJ10160
HYJ10170
HYJ10180
HYJ10190
HYJ10200
HYJ10210
HYJ10220
HYJ10230
HYJ10240
HYJ10250
HYJ10260
HYJ10270
HYJ10280
HYJ10290
HYJ10300
HYJ10310
HYJ10320
HYJ10330
HYJ10340
HYJ10350
HYJ10360
HYJ10370
HYJ10380
HYJ10390
HYJ10400
HYJ10410
HYJ10420
HYJ10430
HYJ10440
HYJ10450
HYJ10460
HYJ10470
HYJ10480
HYJ10490
HYJ10500
HYJ10510
HYJ10520
HYJ10530
HYJ10540

```

ORTHOGONAL MATRIX Q PRODUCED BY THE QR FACTORIZATION
OF THE FINAL APPROXIMATE JACOBIAN.

LDFJAC IS A POSITIVE INTEGER INPUT VARIABLE NOT LESS THAN N
WHICH SPECIFIES THE LEADING DIMENSION OF THE ARRAY FJAC.

TOL IS A NONNEGATIVE INPUT VARIABLE. TERMINATION OCCURS
WHEN THE ALGORITHM ESTIMATES THAT THE RELATIVE ERROR
BETWEEN X AND THE SOLUTION IS AT MOST TOL.

INFO IS AN INTEGER OUTPUT VARIABLE. IF THE USER HAS
TERMINATED EXECUTION, INFO IS SET TO THE (NEGATIVE)
VALUE OF IFLAG. SEE DESCRIPTION OF FCN. OTHERWISE,
INFO IS SET AS FOLLOWS.

INFO = 0 IMPROPER INPUT PARAMETERS.

INFO = 1 ALGORITHM ESTIMATES THAT THE RELATIVE ERROR
BETWEEN X AND THE SOLUTION IS AT MOST TOL.

INFO = 2 NUMBER OF CALLS TO FCN WITH IFLAG = 1 HAS
REACHED $100 \cdot (N+1)$.

INFO = 3 TOL IS TOO SMALL. NO FURTHER IMPROVEMENT IN
THE APPROXIMATE SOLUTION X IS POSSIBLE.

INFO = 4 ITERATION IS NOT MAKING GOOD PROGRESS.

WA IS A WORK ARRAY OF LENGTH LWA.

LWA IS A POSITIVE INTEGER INPUT VARIABLE NOT LESS THAN
 $(N \cdot (N+13))/2$.

SUBPROGRAMS CALLED

USER-SUPPLIED FCN

MINPACK-SUPPLIED ... HYBRJ

ARGONNE NATIONAL LABORATORY. MINPACK PROJECT. MARCH 1980.
BURTON S. GARBOW, KENNETH E. HILLSTROM, JORGE J. MORE

INTEGER J,LR,MAXFEV,MODE,NFEV,NJEV,NPRINT
DOUBLE PRECISION FACTOR,ONE,XTOL,ZERO
DATA FACTOR,ONE,ZERO /1.0D2,1.0D0,0.0D0/
INFO = 0

CHECK THE INPUT PARAMETERS FOR ERRORS.

IF (N .LE. 0 .OR. LDFJAC .LT. N .OR. TOL .LT. ZERO
* .OR. LWA .LT. $(N \cdot (N + 13))/2$) GO TO 20

CALL HYBRJ.

HYJ10550
HYJ10560
HYJ10570
HYJ10580
HYJ10590
HYJ10600
HYJ10610
HYJ10620
HYJ10630
HYJ10640
HYJ10650
HYJ10660
HYJ10670
HYJ10680
HYJ10690
HYJ10700
HYJ10710
HYJ10720
HYJ10730
HYJ10740
HYJ10750
HYJ10760
HYJ10770
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HYJ10790
HYJ10800
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HYJ10890
HYJ10900
HYJ10910
HYJ10920
HYJ10930
HYJ10940
HYJ10950
HYJ10960
HYJ10970
HYJ10980
HYJ10990
HYJ11000
HYJ11010
HYJ11020
HYJ11030
HYJ11040
HYJ11050
HYJ11060
HYJ11070
HYJ11080

C		HYJ11090
	MAXFEV = 100*(N + 1)	HYJ11100
	XTOL = TOL	HYJ11110
	MODE = 2	HYJ11120
	DO 10 J = 1, N	HYJ11130
	WA(J) = ONE	HYJ11140
10	CONTINUE	HYJ11150
	NPRINT = 0	HYJ11160
	LR = (N*(N + 1))/2	HYJ11170
	CALL HYBRJ(FCN,N,X,FVEC,FJAC,LDFJAC,XTOL,MAXFEV,WA(1),MODE,	HYJ11180
	* FACTOR,NPRINT,INFO,NFEV,NJEV,WA(6*N+1),LR,WA(N+1),	HYJ11190
	* WA(2*N+1),WA(3*N+1),WA(4*N+1),WA(5*N+1))	HYJ11200
	IF (INFO .EQ. 5) INFO = 4	HYJ11210
20	CONTINUE	HYJ11220
	RETURN	HYJ11230
C		HYJ11240
C	LAST CARD OF SUBROUTINE HYBRJ1.	HYJ11250
C		HYJ11260
	END	HYJ11270

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SUBROUTINE LMDER(FCN,M,N,X,FVEC,FJAC,LDFJAC,FTOL,XTOL,GTOL,      LMDR0010
*          MAXFEV,DIAG,MODE,FACTOR,NPRINT,INFO,NFEV,NJEV,      LMDR0020
*          IPVT,QTF,WA1,WA2,WA3,WA4)                            LMDR0030
INTEGER M,N,LDFJAC,MAXFEV,MODE,NPRINT,INFO,NFEV,NJEV          LMDR0040
INTEGER IPVT(N)                                                LMDR0050
DOUBLE PRECISION FTOL,XTOL,GTOL,FACTOR                        LMDR0060
DOUBLE PRECISION X(N),FVEC(M),FJAC(LDFJAC,N),DIAG(N),QTF(N),  LMDR0070
*          WA1(N),WA2(N),WA3(N),WA4(M)                        LMDR0080
*****                                                        LMDR0090
C                                                                LMDR0100
C                                                                LMDR0110
C          SUBROUTINE LMDER                                    LMDR0120
C                                                                LMDR0130
C          THE PURPOSE OF LMDER IS TO MINIMIZE THE SUM OF THE SQUARES OF      LMDR0140
C          M NONLINEAR FUNCTIONS IN N VARIABLES BY A MODIFICATION OF          LMDR0150
C          THE LEVENBERG-MARQUARDT ALGORITHM. THE USER MUST PROVIDE A        LMDR0160
C          SUBROUTINE WHICH CALCULATES THE FUNCTIONS AND THE JACOBIAN.        LMDR0170
C                                                                LMDR0180
C          THE SUBROUTINE STATEMENT IS                                       LMDR0190
C                                                                LMDR0200
C          SUBROUTINE LMDER(FCN,M,N,X,FVEC,FJAC,LDFJAC,FTOL,XTOL,GTOL,      LMDR0210
C          MAXFEV,DIAG,MODE,FACTOR,NPRINT,INFO,NFEV,            LMDR0220
C          NJEV,IPVT,QTF,WA1,WA2,WA3,WA4)                                LMDR0230
C                                                                LMDR0240
C          WHERE                                                            LMDR0250
C                                                                LMDR0260
C          FCN IS THE NAME OF THE USER-SUPPLIED SUBROUTINE WHICH            LMDR0270
C          CALCULATES THE FUNCTIONS AND THE JACOBIAN. FCN MUST              LMDR0280
C          BE DECLARED IN AN EXTERNAL STATEMENT IN THE USER                LMDR0290
C          CALLING PROGRAM, AND SHOULD BE WRITTEN AS FOLLOWS.              LMDR0300
C                                                                LMDR0310
C          SUBROUTINE FCN(M,N,X,FVEC,FJAC,LDFJAC,IFLAG)                  LMDR0320
C          INTEGER M,N,LDFJAC,IFLAG                                       LMDR0330
C          DOUBLE PRECISION X(N),FVEC(M),FJAC(LDFJAC,N)                LMDR0340
C          -----                                                        LMDR0350
C          IF IFLAG = 1 CALCULATE THE FUNCTIONS AT X AND                  LMDR0360
C          RETURN THIS VECTOR IN FVEC. DO NOT ALTER FJAC.                 LMDR0370
C          IF IFLAG = 2 CALCULATE THE JACOBIAN AT X AND                    LMDR0380
C          RETURN THIS MATRIX IN FJAC. DO NOT ALTER FVEC.                 LMDR0390
C          -----                                                        LMDR0400
C          RETURN                                                            LMDR0410
C          END                                                              LMDR0420
C                                                                LMDR0430
C          THE VALUE OF IFLAG SHOULD NOT BE CHANGED BY FCN UNLESS          LMDR0440
C          THE USER WANTS TO TERMINATE EXECUTION OF LMDER.                LMDR0450
C          IN THIS CASE SET IFLAG TO A NEGATIVE INTEGER.                  LMDR0460
C                                                                LMDR0470
C          M IS A POSITIVE INTEGER INPUT VARIABLE SET TO THE NUMBER          LMDR0480
C          OF FUNCTIONS.                                                    LMDR0490
C                                                                LMDR0500
C          N IS A POSITIVE INTEGER INPUT VARIABLE SET TO THE NUMBER          LMDR0510
C          OF VARIABLES. N MUST NOT EXCEED M.                             LMDR0520
C                                                                LMDR0530
C          X IS AN ARRAY OF LENGTH N. ON INPUT X MUST CONTAIN              LMDR0540
C          AN INITIAL ESTIMATE OF THE SOLUTION VECTOR. ON OUTPUT X

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C	CONTAINS THE FINAL ESTIMATE OF THE SOLUTION VECTOR.	LMDR0550
C		LMDR0560
C	FVEC IS AN OUTPUT ARRAY OF LENGTH M WHICH CONTAINS	LMDR0570
C	THE FUNCTIONS EVALUATED AT THE OUTPUT X.	LMDR0580
C		LMDR0590
C	FJAC IS AN OUTPUT M BY N ARRAY. THE UPPER N BY N SUBMATRIX	LMDR0600
C	OF FJAC CONTAINS AN UPPER TRIANGULAR MATRIX R WITH	LMDR0610
C	DIAGONAL ELEMENTS OF NONINCREASING MAGNITUDE SUCH THAT	LMDR0620
C		LMDR0630
C	$P^T (JAC^T * JAC) P = R^T R,$	LMDR0640
C		LMDR0650
C		LMDR0660
C	WHERE P IS A PERMUTATION MATRIX AND JAC IS THE FINAL	LMDR0670
C	CALCULATED JACOBIAN. COLUMN J OF P IS COLUMN IPVT(J)	LMDR0680
C	(SEE BELOW) OF THE IDENTITY MATRIX. THE LOWER TRAPEZOIDAL	LMDR0690
C	PART OF FJAC CONTAINS INFORMATION GENERATED DURING	LMDR0700
C	THE COMPUTATION OF R.	LMDR0710
C		LMDR0720
C	LDFJAC IS A POSITIVE INTEGER INPUT VARIABLE NOT LESS THAN M	LMDR0730
C	WHICH SPECIFIES THE LEADING DIMENSION OF THE ARRAY FJAC.	LMDR0740
C		LMDR0750
C	FTOL IS A NONNEGATIVE INPUT VARIABLE. TERMINATION	LMDR0760
C	OCCURS WHEN BOTH THE ACTUAL AND PREDICTED RELATIVE	LMDR0770
C	REDUCTIONS IN THE SUM OF SQUARES ARE AT MOST FTOL.	LMDR0780
C	THEREFORE, FTOL MEASURES THE RELATIVE ERROR DESIRED	LMDR0790
C	IN THE SUM OF SQUARES.	LMDR0800
C		LMDR0810
C	XTOL IS A NONNEGATIVE INPUT VARIABLE. TERMINATION	LMDR0820
C	OCCURS WHEN THE RELATIVE ERROR BETWEEN TWO CONSECUTIVE	LMDR0830
C	ITERATES IS AT MOST XTOL. THEREFORE, XTOL MEASURES THE	LMDR0840
C	RELATIVE ERROR DESIRED IN THE APPROXIMATE SOLUTION.	LMDR0850
C		LMDR0860
C	GTOL IS A NONNEGATIVE INPUT VARIABLE. TERMINATION	LMDR0870
C	OCCURS WHEN THE COSINE OF THE ANGLE BETWEEN FVEC AND	LMDR0880
C	ANY COLUMN OF THE JACOBIAN IS AT MOST GTOL IN ABSOLUTE	LMDR0890
C	VALUE. THEREFORE, GTOL MEASURES THE ORTHOGONALITY	LMDR0900
C	DESIRED BETWEEN THE FUNCTION VECTOR AND THE COLUMNS	LMDR0910
C	OF THE JACOBIAN.	LMDR0920
C		LMDR0930
C	MAXFEV IS A POSITIVE INTEGER INPUT VARIABLE. TERMINATION	LMDR0940
C	OCCURS WHEN THE NUMBER OF CALLS TO FCN WITH IFLAG = 1	LMDR0950
C	HAS REACHED MAXFEV.	LMDR0960
C		LMDR0970
C	DIAG IS AN ARRAY OF LENGTH N. IF MODE = 1 (SEE	LMDR0980
C	BELOW), DIAG IS INTERNALLY SET. IF MODE = 2, DIAG	LMDR0990
C	MUST CONTAIN POSITIVE ENTRIES THAT SERVE AS	LMDR1000
C	MULTIPLICATIVE SCALE FACTORS FOR THE VARIABLES.	LMDR1010
C		LMDR1020
C	MODE IS AN INTEGER INPUT VARIABLE. IF MODE = 1, THE	LMDR1030
C	VARIABLES WILL BE SCALED INTERNALLY. IF MODE = 2,	LMDR1040
C	THE SCALING IS SPECIFIED BY THE INPUT DIAG. OTHER	LMDR1050
C	VALUES OF MODE ARE EQUIVALENT TO MODE = 1.	LMDR1060
C		LMDR1070
C	FACTOR IS A POSITIVE INPUT VARIABLE USED IN DETERMINING THE	LMDR1080

C	INITIAL STEP BOUND. THIS BOUND IS SET TO THE PRODUCT OF	LMDR1090
C	FACTOR AND THE EUCLIDEAN NORM OF DIAG^*X IF NONZERO, OR ELSE	LMDR1100
C	TO FACTOR ITSELF. IN MOST CASES FACTOR SHOULD LIE IN THE	LMDR1110
C	INTERVAL $(.1, 100.)$. 100. IS A GENERALLY RECOMMENDED VALUE.	LMDR1120
C		LMDR1130
C	NPRINT IS AN INTEGER INPUT VARIABLE THAT ENABLES CONTROLLED	LMDR1140
C	PRINTING OF ITERATES IF IT IS POSITIVE. IN THIS CASE,	LMDR1150
C	FCN IS CALLED WITH IFLAG = 0 AT THE BEGINNING OF THE FIRST	LMDR1160
C	ITERATION AND EVERY NPRINT ITERATIONS THEREAFTER AND	LMDR1170
C	IMMEDIATELY PRIOR TO RETURN, WITH X, FVEC, AND FJAC	LMDR1180
C	AVAILABLE FOR PRINTING. FVEC AND FJAC SHOULD NOT BE	LMDR1190
C	ALTERED. IF NPRINT IS NOT POSITIVE, NO SPECIAL CALLS	LMDR1200
C	OF FCN WITH IFLAG = 0 ARE MADE.	LMDR1210
C		LMDR1220
C	INFO IS AN INTEGER OUTPUT VARIABLE. IF THE USER HAS	LMDR1230
C	TERMINATED EXECUTION, INFO IS SET TO THE (NEGATIVE)	LMDR1240
C	VALUE OF IFLAG. SEE DESCRIPTION OF FCN. OTHERWISE,	LMDR1250
C	INFO IS SET AS FOLLOWS.	LMDR1260
C		LMDR1270
C	INFO = 0 IMPROPER INPUT PARAMETERS.	LMDR1280
C		LMDR1290
C	INFO = 1 BOTH ACTUAL AND PREDICTED RELATIVE REDUCTIONS	LMDR1300
C	IN THE SUM OF SQUARES ARE AT MOST FTOL.	LMDR1310
C		LMDR1320
C	INFO = 2 RELATIVE ERROR BETWEEN TWO CONSECUTIVE ITERATES	LMDR1330
C	IS AT MOST XTOL.	LMDR1340
C		LMDR1350
C	INFO = 3 CONDITIONS FOR INFO = 1 AND INFO = 2 BOTH HOLD.	LMDR1360
C		LMDR1370
C	INFO = 4 THE COSINE OF THE ANGLE BETWEEN FVEC AND ANY	LMDR1380
C	COLUMN OF THE JACOBIAN IS AT MOST GTOL IN	LMDR1390
C	ABSOLUTE VALUE.	LMDR1400
C		LMDR1410
C	INFO = 5 NUMBER OF CALLS TO FCN WITH IFLAG = 1 HAS	LMDR1420
C	REACHED MAXFEV.	LMDR1430
C		LMDR1440
C	INFO = 6 FTOL IS TOO SMALL. NO FURTHER REDUCTION IN	LMDR1450
C	THE SUM OF SQUARES IS POSSIBLE.	LMDR1460
C		LMDR1470
C	INFO = 7 XTOL IS TOO SMALL. NO FURTHER IMPROVEMENT IN	LMDR1480
C	THE APPROXIMATE SOLUTION X IS POSSIBLE.	LMDR1490
C		LMDR1500
C	INFO = 8 GTOL IS TOO SMALL. FVEC IS ORTHOGONAL TO THE	LMDR1510
C	COLUMNS OF THE JACOBIAN TO MACHINE PRECISION.	LMDR1520
C		LMDR1530
C	NFEV IS AN INTEGER OUTPUT VARIABLE SET TO THE NUMBER OF	LMDR1540
C	CALLS TO FCN WITH IFLAG = 1.	LMDR1550
C		LMDR1560
C	NJEV IS AN INTEGER OUTPUT VARIABLE SET TO THE NUMBER OF	LMDR1570
C	CALLS TO FCN WITH IFLAG = 2.	LMDR1580
C		LMDR1590
C	IPVT IS AN INTEGER OUTPUT ARRAY OF LENGTH N. IPVT	LMDR1600
C	DEFINES A PERMUTATION MATRIX P SUCH THAT $\text{JAC}^*P = Q^*R$,	LMDR1610
C	WHERE JAC IS THE FINAL CALCULATED JACOBIAN, Q IS	LMDR1620

C	ORTHOGONAL (NOT STORED), AND R IS UPPER TRIANGULAR	LMDR1630
C	WITH DIAGONAL ELEMENTS OF NONINCREASING MAGNITUDE.	LMDR1640
C	COLUMN J OF P IS COLUMN IPVT(J) OF THE IDENTITY MATRIX.	LMDR1650
C		LMDR1660
C	QTF IS AN OUTPUT ARRAY OF LENGTH N WHICH CONTAINS	LMDR1670
C	THE FIRST N ELEMENTS OF THE VECTOR (Q TRANSPOSE)*FVEC.	LMDR1680
C		LMDR1690
C	WA1, WA2, AND WA3 ARE WORK ARRAYS OF LENGTH N.	LMDR1700
C		LMDR1710
C	WA4 IS A WORK ARRAY OF LENGTH M.	LMDR1720
C		LMDR1730
C	SUBPROGRAMS CALLED	LMDR1740
C		LMDR1750
C	USER-SUPPLIED FCN	LMDR1760
C		LMDR1770
C	MINPACK-SUPPLIED ... DPMPAR,ENORM,LMPAR,QRFAC	LMDR1780
C		LMDR1790
C	FORTTRAN-SUPPLIED ... DABS,DMAX1,DMIN1,DSQRT,MOD	LMDR1800
C		LMDR1810
C	ARGONNE NATIONAL LABORATORY. MINPACK PROJECT. MARCH 1980.	LMDR1820
C	BURTON S. GARBOW, KENNETH E. HILLSTROM, JORGE J. MORE	LMDR1830
C		LMDR1840
C	*****	LMDR1850
	INTEGER I,IFLAG,ITER,J,L	LMDR1860
	DOUBLE PRECISION ACTRED,DELTA,DIRDER,EPSMCH,FNORM,FNORM1,GNORM,	LMDR1870
*	ONE,PAR,PNORM,PRERED,P1,P5,P25,P75,P0001,RATIO,	LMDR1880
*	SUM,TEMP,TEMP1,TEMP2,XNORM,ZERO	LMDR1890
	DOUBLE PRECISION DPMPAR,ENORM	LMDR1900
	DATA ONE,P1,P5,P25,P75,P0001,ZERO	LMDR1910
*	/1.0D0,1.0D-1,5.0D-1,2.5D-1,7.5D-1,1.0D-4,0.0D0/	LMDR1920
C		LMDR1930
C	EPSMCH IS THE MACHINE PRECISION.	LMDR1940
C		LMDR1950
	EPSMCH = DPMPAR(1)	LMDR1960
C		LMDR1970
	INFO = 0	LMDR1980
	IFLAG = 0	LMDR1990
	NFEV = 0	LMDR2000
	NJEV = 0	LMDR2010
C		LMDR2020
C	CHECK THE INPUT PARAMETERS FOR ERRORS.	LMDR2030
C		LMDR2040
	IF (N .LE. 0 .OR. M .LT. N .OR. LDFJAC .LT. M	LMDR2050
*	.OR. FTOL .LT. ZERO .OR. XTOL .LT. ZERO .OR. GTOL .LT. ZERO	LMDR2060
*	.OR. MAXFEV .LE. 0 .OR. FACTOR .LE. ZERO) GO TO 300	LMDR2070
	IF (MODE .NE. 2) GO TO 20	LMDR2080
	DO 10 J = 1, N	LMDR2090
	IF (DIAG(J) .LE. ZERO) GO TO 300	LMDR2100
10	CONTINUE	LMDR2110
20	CONTINUE	LMDR2120
C		LMDR2130
C	EVALUATE THE FUNCTION AT THE STARTING POINT	LMDR2140
C	AND CALCULATE ITS NORM.	LMDR2150
C		LMDR2160

	IFLAG = 1	LMDR2170
	CALL FCN(M,N,X,FVEC,FJAC,LDFJAC,IFLAG)	LMDR2180
	NFEV = 1	LMDR2190
	IF (IFLAG .LT. 0) GO TO 300	LMDR2200
	FNORM = ENORM(M,FVEC)	LMDR2210
C		LMDR2220
C	INITIALIZE LEVENBERG-MARQUARDT PARAMETER AND ITERATION COUNTER.	LMDR2230
C		LMDR2240
	PAR = ZERO	LMDR2250
	ITER = 1	LMDR2260
C		LMDR2270
C	BEGINNING OF THE OUTER LOOP.	LMDR2280
C		LMDR2290
	30 CONTINUE	LMDR2300
C		LMDR2310
C	CALCULATE THE JACOBIAN MATRIX.	LMDR2320
C		LMDR2330
	IFLAG = 2	LMDR2340
	CALL FCN(M,N,X,FVEC,FJAC,LDFJAC,IFLAG)	LMDR2350
	NJEV = NJEV + 1	LMDR2360
	IF (IFLAG .LT. 0) GO TO 300	LMDR2370
C		LMDR2380
C	IF REQUESTED, CALL FCN TO ENABLE PRINTING OF ITERATES.	LMDR2390
C		LMDR2400
	IF (NPRINT .LE. 0) GO TO 40	LMDR2410
	IFLAG = 0	LMDR2420
	IF (MOD(ITER-1,NPRINT) .EQ. 0)	LMDR2430
	* CALL FCN(M,N,X,FVEC,FJAC,LDFJAC,IFLAG)	LMDR2440
	IF (IFLAG .LT. 0) GO TO 300	LMDR2450
	40 CONTINUE	LMDR2460
C		LMDR2470
C	COMPUTE THE QR FACTORIZATION OF THE JACOBIAN.	LMDR2480
C		LMDR2490
	CALL QRFAC(M,N,FJAC,LDFJAC,.TRUE.,IPVT,N,WA1,WA2,WA3)	LMDR2500
C		LMDR2510
C	ON THE FIRST ITERATION AND IF MODE IS 1, SCALE ACCORDING	LMDR2520
C	TO THE NORMS OF THE COLUMNS OF THE INITIAL JACOBIAN.	LMDR2530
C		LMDR2540
	IF (ITER .NE. 1) GO TO 80	LMDR2550
	IF (MODE .EQ. 2) GO TO 60	LMDR2560
	DO 50 J = 1, N	LMDR2570
	DIAG(J) = WA2(J)	LMDR2580
	IF (WA2(J) .EQ. ZERO) DIAG(J) = ONE	LMDR2590
50	CONTINUE	LMDR2600
60	CONTINUE	LMDR2610
C		LMDR2620
C	ON THE FIRST ITERATION, CALCULATE THE NORM OF THE SCALED X	LMDR2630
C	AND INITIALIZE THE STEP BOUND DELTA.	LMDR2640
C		LMDR2650
	DO 70 J = 1, N	LMDR2660
	WA3(J) = DIAG(J)*X(J)	LMDR2670
70	CONTINUE	LMDR2680
	XNORM = ENORM(N,WA3)	LMDR2690
	DELTA = FACTOR*XNORM	LMDR2700

	IF (DELTA .EQ. ZERO) DELTA = FACTOR	LMDR2710
80	CONTINUE	LMDR2720
C		LMDR2730
C	FORM (Q TRANSPOSE)*FVEC AND STORE THE FIRST N COMPONENTS IN	LMDR2740
C	QTF.	LMDR2750
C		LMDR2760
	DO 90 I = 1, M	LMDR2770
	WA4(I) = FVEC(I)	LMDR2780
90	CONTINUE	LMDR2790
	DO 130 J = 1, N	LMDR2800
	IF (FJAC(J,J) .EQ. ZERO) GO TO 120	LMDR2810
	SUM = ZERO	LMDR2820
	DO 100 I = J, M	LMDR2830
	SUM = SUM + FJAC(I,J)*WA4(I)	LMDR2840
100	CONTINUE	LMDR2850
	TEMP = -SUM/FJAC(J,J)	LMDR2860
	DO 110 I = J, M	LMDR2870
	WA4(I) = WA4(I) + FJAC(I,J)*TEMP	LMDR2880
110	CONTINUE	LMDR2890
120	CONTINUE	LMDR2900
	FJAC(J,J) = WA1(J)	LMDR2910
	QTF(J) = WA4(J)	LMDR2920
130	CONTINUE	LMDR2930
C		LMDR2940
C	COMPUTE THE NORM OF THE SCALED GRADIENT.	LMDR2950
C		LMDR2960
	GNORM = ZERO	LMDR2970
	IF (FNORM .EQ. ZERO) GO TO 170	LMDR2980
	DO 160 J = 1, N	LMDR2990
	L = IPV1(J)	LMDR3000
	IF (WA2(L) .EQ. ZERO) GO TO 150	LMDR3010
	SUM = ZERO	LMDR3020
	DO 140 I = 1, J	LMDR3030
	SUM = SUM + FJAC(I,J)*(QTF(I)/FNORM)	LMDR3040
140	CONTINUE	LMDR3050
	GNORM = DMAX1(GNORM,DABS(SUM/WA2(L)))	LMDR3060
150	CONTINUE	LMDR3070
160	CONTINUE	LMDR3080
170	CONTINUE	LMDR3090
C		LMDR3100
C	TEST FOR CONVERGENCE OF THE GRADIENT NORM.	LMDR3110
C		LMDR3120
	IF (GNORM .LE. GTOL) INFO = 4	LMDR3130
	IF (INFO .NE. 0) GO TO 300	LMDR3140
C		LMDR3150
C	RESCALE IF NECESSARY.	LMDR3160
C		LMDR3170
	IF (MODE .EQ. 2) GO TO 190	LMDR3180
	DO 180 J = 1, N	LMDR3190
	DIAG(J) = DMAX1(DIAG(J),WA2(J))	LMDR3200
180	CONTINUE	LMDR3210
190	CONTINUE	LMDR3220
C		LMDR3230
C	BEGINNING OF THE INNER LOOP.	LMDR3240

C			LMDR3250
200	CONTINUE		LMDR3260
C			LMDR3270
C	DETERMINE THE LEVENBERG-MARQUARDT PARAMETER.		LMDR3280
C			LMDR3290
	CALL LMPAR(N,FJAC,LDFJAC,IPVT,DIAG,QTF,DELTA,PAR,WA1,WA2,		LMDR3300
*	WA3,WA4)		LMDR3310
C			LMDR3320
C	STORE THE DIRECTION P AND X + P. CALCULATE THE NORM OF P.		LMDR3330
C			LMDR3340
	DO 210 J = 1, N		LMDR3350
	WA1(J) = -WA1(J)		LMDR3360
	WA2(J) = X(J) + WA1(J)		LMDR3370
	WA3(J) = DIAG(J)*WA1(J)		LMDR3380
210	CONTINUE		LMDR3390
	PNORM = ENORM(N,WA3)		LMDR3400
C			LMDR3410
C	ON THE FIRST ITERATION, ADJUST THE INITIAL STEP BOUND.		LMDR3420
C			LMDR3430
	IF (ITER .EQ. 1) DELTA = DMIN1(DELTA,PNORM)		LMDR3440
C			LMDR3450
C	EVALUATE THE FUNCTION AT X + P AND CALCULATE ITS NORM.		LMDR3460
C			LMDR3470
	IFLAG = 1		LMDR3480
	CALL FCN(M,N,WA2,WA4,FJAC,LDFJAC,IFLAG)		LMDR3490
	NFEV = NFEV + 1		LMDR3500
	IF (IFLAG .LT. 0) GO TO 300		LMDR3510
	FNORM1 = ENORM(M,WA4)		LMDR3520
C			LMDR3530
C	COMPUTE THE SCALED ACTUAL REDUCTION.		LMDR3540
C			LMDR3550
	ACTRED = -ONE		LMDR3560
	IF (P1*FNORM1 .LT. FNORM) ACTRED = ONE - (FNORM1/FNORM)**2		LMDR3570
C			LMDR3580
C	COMPUTE THE SCALED PREDICTED REDUCTION AND		LMDR3590
C	THE SCALED DIRECTIONAL DERIVATIVE.		LMDR3600
C			LMDR3610
	DO 230 J = 1, N		LMDR3620
	WA3(J) = ZERO		LMDR3630
	L = IPVT(J)		LMDR3640
	TEMP = WA1(L)		LMDR3650
	DO 220 I = 1, J		LMDR3660
	WA3(I) = WA3(I) + FJAC(I,J)*TEMP		LMDR3670
220	CONTINUE		LMDR3680
230	CONTINUE		LMDR3690
	TEMP1 = ENORM(N,WA3)/FNORM		LMDR3700
	TEMP2 = (DSQRT(PAR)*PNORM)/FNORM		LMDR3710
	PRERED = TEMP1**2 + TEMP2**2/P5		LMDR3720
	DIRDER = -(TEMP1**2 + TEMP2**2)		LMDR3730
C			LMDR3740
C	COMPUTE THE RATIO OF THE ACTUAL TO THE PREDICTED		LMDR3750
C	REDUCTION.		LMDR3760
C			LMDR3770
	RATIO = ZERO		LMDR3780

	IF (PRERED .NE. ZERO) RATIO = ACTRED/PRERED	LMDR3790
C		LMDR3800
C	UPDATE THE STEP BOUND.	LMDR3810
C		LMDR3820
	IF (RATIO .GT. P25) GO TO 240	LMDR3830
	IF (ACTRED .GE. ZERO) TEMP = P5	LMDR3840
	IF (ACTRED .LT. ZERO)	LMDR3850
*	TEMP = P5*DIRDER/(DIRDER + P5*ACTRED)	LMDR3860
	IF (P1*FNORM1 .GE. FNORM .OR. TEMP .LT. P1) TEMP = P1	LMDR3870
	DELTA = TEMP*DMIN1(DELTA,PNORM/P1)	LMDR3880
	PAR = PAR/TEMP	LMDR3890
	GO TO 260	LMDR3900
240	CONTINUE	LMDR3910
	IF (PAR .NE. ZERO .AND. RATIO .LT. P75) GO TO 250	LMDR3920
	DELTA = PNORM/P5	LMDR3930
	PAR = P5*PAR	LMDR3940
250	CONTINUE	LMDR3950
260	CONTINUE	LMDR3960
C		LMDR3970
C	TEST FOR SUCCESSFUL ITERATION.	LMDR3980
C		LMDR3990
	IF (RATIO .LT. P0001) GO TO 290	LMDR4000
C		LMDR4010
C	SUCCESSFUL ITERATION. UPDATE X, FVEC, AND THEIR NORMS.	LMDR4020
C		LMDR4030
	DO 270 J = 1, N	LMDR4040
	X(J) = WA2(J)	LMDR4050
	WA2(J) = DIAG(J)*X(J)	LMDR4060
270	CONTINUE	LMDR4070
	DO 280 I = 1, M	LMDR4080
	FVEC(I) = WA4(I)	LMDR4090
280	CONTINUE	LMDR4100
	XNORM = ENORM(N,WA2)	LMDR4110
	FNORM = FNORM1	LMDR4120
	ITER = ITER + 1	LMDR4130
290	CONTINUE	LMDR4140
C		LMDR4150
C	TESTS FOR CONVERGENCE.	LMDR4160
C		LMDR4170
	IF (DABS(ACTRED) .LE. FTOL .AND. PRERED .LE. FTOL	LMDR4180
*	.AND. P5*RATIO .LE. ONE) INFO = 1	LMDR4190
	IF (DELTA .LE. XTOL*XNORM) INFO = 2	LMDR4200
	IF (DABS(ACTRED) .LE. FTOL .AND. PRERED .LE. FTOL	LMDR4210
*	.AND. P5*RATIO .LE. ONE .AND. INFO .EQ. 2) INFO = 3	LMDR4220
	IF (INFO .NE. 0) GO TO 300	LMDR4230
C		LMDR4240
C	TESTS FOR TERMINATION AND STRINGENT TOLERANCES.	LMDR4250
C		LMDR4260
	IF (NFEV .GE. MAXFEV) INFO = 5	LMDR4270
	IF (DABS(ACTRED) .LE. EPSMCH .AND. PRERED .LE. EPSMCH	LMDR4280
*	.AND. P5*RATIO .LE. ONE) INFO = 6	LMDR4290
	IF (DELTA .LE. EPSMCH*XNORM) INFO = 7	LMDR4300
	IF (GNORM .LE. EPSMCH) INFO = 8	LMDR4310
	IF (INFO .NE. 0) GO TO 300	LMDR4320

C		LMDR4330
C	END OF THE INNER LOOP. REPEAT IF ITERATION UNSUCCESSFUL.	LMDR4340
C		LMDR4350
C	IF (RATIO .LT. P0001) GO TO 200	LMDR4360
C		LMDR4370
C	END OF THE OUTER LOOP.	LMDR4380
C		LMDR4390
	GO TO 30	LMDR4400
300	CONTINUE	LMDR4410
C		LMDR4420
C	TERMINATION, EITHER NORMAL OR USER IMPOSED.	LMDR4430
C		LMDR4440
	IF (IFLAG .LT. 0) INFO = IFLAG	LMDR4450
	IFLAG = 0	LMDR4460
	IF (NPRINT .GT. 0) CALL FCN(M,N,X,FVEC,FJAC,LDFJAC,IFLAG).	LMDR4470
	RETURN	LMDR4480
C		LMDR4490
C	LAST CARD OF SUBROUTINE LMDER.	LMDR4500
C		LMDR4510
	END	LMDR4520

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SUBROUTINE LMDER1(FCN,M,N,X,FVEC,FJAC,LDFJAC,TOL,INFO,IPVT,WA,
* LWA)

INTEGER M,N,LDFJAC,INFO,LWA

INTEGER IPVT(N)

DOUBLE PRECISION TOL

DOUBLE PRECISION X(N),FVEC(M),FJAC(LDFJAC,N),WA(LWA)

EXTERNAL FCN

SUBROUTINE LMDER1

THE PURPOSE OF LMDER1 IS TO MINIMIZE THE SUM OF THE SQUARES OF
M NONLINEAR FUNCTIONS IN N VARIABLES BY A MODIFICATION OF THE
LEVENBERG-MARQUARDT ALGORITHM. THIS IS DONE BY USING THE MORE
GENERAL LEAST-SQUARES SOLVER LMDER. THE USER MUST PROVIDE A
SUBROUTINE WHICH CALCULATES THE FUNCTIONS AND THE JACOBIAN.

THE SUBROUTINE STATEMENT IS

SUBROUTINE LMDER1(FCN,M,N,X,FVEC,FJAC,LDFJAC,TOL,INFO,
IPVT,WA,LWA)

WHERE

FCN IS THE NAME OF THE USER-SUPPLIED SUBROUTINE WHICH
CALCULATES THE FUNCTIONS AND THE JACOBIAN. FCN MUST
BE DECLARED IN AN EXTERNAL STATEMENT IN THE USER
CALLING PROGRAM, AND SHOULD BE WRITTEN AS FOLLOWS.

SUBROUTINE FCN(M,N,X,FVEC,FJAC,LDFJAC,IFLAG)

INTEGER M,N,LDFJAC,IFLAG

DOUBLE PRECISION X(N),FVEC(M),FJAC(LDFJAC,N)

IF IFLAG = 1 CALCULATE THE FUNCTIONS AT X AND
RETURN THIS VECTOR IN FVEC. DO NOT ALTER FJAC.

IF IFLAG = 2 CALCULATE THE JACOBIAN AT X AND
RETURN THIS MATRIX IN FJAC. DO NOT ALTER FVEC.

RETURN

END

THE VALUE OF IFLAG SHOULD NOT BE CHANGED BY FCN UNLESS
THE USER WANTS TO TERMINATE EXECUTION OF LMDER1.
IN THIS CASE SET IFLAG TO A NEGATIVE INTEGER.

M IS A POSITIVE INTEGER INPUT VARIABLE SET TO THE NUMBER
OF FUNCTIONS.

N IS A POSITIVE INTEGER INPUT VARIABLE SET TO THE NUMBER
OF VARIABLES. N MUST NOT EXCEED M.

X IS AN ARRAY OF LENGTH N. ON INPUT X MUST CONTAIN
AN INITIAL ESTIMATE OF THE SOLUTION VECTOR. ON OUTPUT X
CONTAINS THE FINAL ESTIMATE OF THE SOLUTION VECTOR.

LMR10010
LMR10020
LMR10030
LMR10040
LMR10050
LMR10060
LMR10070
LMR10080
LMR10090
LMR10100
LMR10110
LMR10120
LMR10130
LMR10140
LMR10150
LMR10160
LMR10170
LMR10180
LMR10190
LMR10200
LMR10210
LMR10220
LMR10230
LMR10240
LMR10250
LMR10260
LMR10270
LMR10280
LMR10290
LMR10300
LMR10310
LMR10320
LMR10330
LMR10340
LMR10350
LMR10360
LMR10370
LMR10380
LMR10390
LMR10400
LMR10410
LMR10420
LMR10430
LMR10440
LMR10450
LMR10460
LMR10470
LMR10480
LMR10490
LMR10500
LMR10510
LMR10520
LMR10530
LMR10540

FVEC IS AN OUTPUT ARRAY OF LENGTH M WHICH CONTAINS
THE FUNCTIONS EVALUATED AT THE OUTPUT X.

FJAC IS AN OUTPUT M BY N ARRAY. THE UPPER N BY N SUBMATRIX
OF FJAC CONTAINS AN UPPER TRIANGULAR MATRIX R WITH
DIAGONAL ELEMENTS OF NONINCREASING MAGNITUDE SUCH THAT

$$P^T (JAC^T JAC) P = R^T R,$$

WHERE P IS A PERMUTATION MATRIX AND JAC IS THE FINAL
CALCULATED JACOBIAN. COLUMN J OF P IS COLUMN IPV T(J)
(SEE BELOW) OF THE IDENTITY MATRIX. THE LOWER TRAPEZOIDAL
PART OF FJAC CONTAINS INFORMATION GENERATED DURING
THE COMPUTATION OF R.

LDFJAC IS A POSITIVE INTEGER INPUT VARIABLE NOT LESS THAN M
WHICH SPECIFIES THE LEADING DIMENSION OF THE ARRAY FJAC.

TOL IS A NONNEGATIVE INPUT VARIABLE. TERMINATION OCCURS
WHEN THE ALGORITHM ESTIMATES EITHER THAT THE RELATIVE
ERROR IN THE SUM OF SQUARES IS AT MOST TOL OR THAT
THE RELATIVE ERROR BETWEEN X AND THE SOLUTION IS AT
MOST TOL.

INFO IS AN INTEGER OUTPUT VARIABLE. IF THE USER HAS
TERMINATED EXECUTION, INFO IS SET TO THE (NEGATIVE)
VALUE OF IFLAG. SEE DESCRIPTION OF FCN. OTHERWISE,
INFO IS SET AS FOLLOWS.

INFO = 0 IMPROPER INPUT PARAMETERS.

INFO = 1 ALGORITHM ESTIMATES THAT THE RELATIVE ERROR
IN THE SUM OF SQUARES IS AT MOST TOL.

INFO = 2 ALGORITHM ESTIMATES THAT THE RELATIVE ERROR
BETWEEN X AND THE SOLUTION IS AT MOST TOL.

INFO = 3 CONDITIONS FOR INFO = 1 AND INFO = 2 BOTH HOLD.

INFO = 4 FVEC IS ORTHOGONAL TO THE COLUMNS OF THE
JACOBIAN TO MACHINE PRECISION.

INFO = 5 NUMBER OF CALLS TO FCN WITH IFLAG = 1 HAS
REACHED 100*(N+1).

INFO = 6 TOL IS TOO SMALL. NO FURTHER REDUCTION IN
THE SUM OF SQUARES IS POSSIBLE.

INFO = 7 TOL IS TOO SMALL. NO FURTHER IMPROVEMENT IN
THE APPROXIMATE SOLUTION X IS POSSIBLE.

IPVT IS AN INTEGER OUTPUT ARRAY OF LENGTH N. IPV T

LMR10550
LMR10560
LMR10570
LMR10580
LMR10590
LMR10600
LMR10610
LMR10620
LMR10630
LMR10640
LMR10650
LMR10660
LMR10670
LMR10680
LMR10690
LMR10700
LMR10710
LMR10720
LMR10730
LMR10740
LMR10750
LMR10760
LMR10770
LMR10780
LMR10790
LMR10800
LMR10810
LMR10820
LMR10830
LMR10840
LMR10850
LMR10860
LMR10870
LMR10880
LMR10890
LMR10900
LMR10910
LMR10920
LMR10930
LMR10940
LMR10950
LMR10960
LMR10970
LMR10980
LMR10990
LMR11000
LMR11010
LMR11020
LMR11030
LMR11040
LMR11050
LMR11060
LMR11070
LMR11080

C	DEFINES A PERMUTATION MATRIX P SUCH THAT $JAC * P = Q * R$,	LMR11090
C	WHERE JAC IS THE FINAL CALCULATED JACOBIAN, Q IS	LMR11100
C	ORTHOGONAL (NOT STORED), AND R IS UPPER TRIANGULAR	LMR11110
C	WITH DIAGONAL ELEMENTS OF NONINCREASING MAGNITUDE.	LMR11120
C	COLUMN J OF P IS COLUMN IPV T(J) OF THE IDENTITY MATRIX.	LMR11130
C		LMR11140
C	WA IS A WORK ARRAY OF LENGTH LWA.	LMR11150
C		LMR11160
C	LWA IS A POSITIVE INTEGER INPUT VARIABLE NOT LESS THAN $5 * N + M$.	LMR11170
C		LMR11180
C	SUBPROGRAMS CALLED	LMR11190
C		LMR11200
C	USER-SUPPLIED FCN	LMR11210
C		LMR11220
C	MINPACK-SUPPLIED ... LMDER	LMR11230
C		LMR11240
C	ARGONNE NATIONAL LABORATORY. MINPACK PROJECT. MARCH 1980.	LMR11250
C	BURTON S. GARBOW, KENNETH E. HILLSTROM, JORGE J. MORE	LMR11260
C		LMR11270
C	*****	LMR11280
	INTEGER MAXFEV, MODE, NFEV, NJEV, NPRINT	LMR11290
	DOUBLE PRECISION FACTOR, FTOL, GTOL, XTOL, ZERO	LMR11300
	DATA FACTOR, ZERO /1.0D2, 0.0D0/	LMR11310
	INFO = 0	LMR11320
C		LMR11330
C	CHECK THE INPUT PARAMETERS FOR ERRORS.	LMR11340
C		LMR11350
	IF (N .LE. 0 .OR. M .LT. N .OR. LDFJAC .LT. M .OR. TOL .LT. ZERO	LMR11360
	* .OR. LWA .LT. $5 * N + M$) GO TO 10	LMR11370
C		LMR11380
C	CALL LMDER.	LMR11390
C		LMR11400
	MAXFEV = $100 * (N + 1)$	LMR11410
	FTOL = TOL	LMR11420
	XTOL = TOL	LMR11430
	GTOL = ZERO	LMR11440
	MODE = 1	LMR11450
	NPRINT = 0	LMR11460
	CALL LMDER(FCN, M, N, X, FVEC, FJAC, LDFJAC, FTOL, XTOL, GTOL, MAXFEV,	LMR11470
	* WA(1), MODE, FACTOR, NPRINT, INFO, NFEV, NJEV, IPV T, WA(N+1),	LMR11480
	* WA(2*N+1), WA(3*N+1), WA(4*N+1), WA(5*N+1))	LMR11490
	IF (INFO .EQ. 8) INFO = 4	LMR11500
10	CONTINUE	LMR11510
	RETURN	LMR11520
C		LMR11530
C	LAST CARD OF SUBROUTINE LMDER1.	LMR11540
C		LMR11550
	END	LMR11560

```

SUBROUTINE LMDIF(FCN,M,N,X,FVEC,FTOL,XTOL,GTOL,MAXFEV,EPSFCN,
*          DIAG,MODE,FACTOR,NPRINT,INFO,NFEV,FJAC,LDFJAC,
*          IPVT,QTF,WA1,WA2,WA3,WA4)
  INTEGER M,N,MAXFEV,MODE,NPRINT,INFO,NFEV,LDFJAC
  INTEGER IPVT(N)
  DOUBLE PRECISION FTOL,XTOL,GTOL,EPSFCN,FACTOR
  DOUBLE PRECISION X(N),FVEC(M),DIAG(N),FJAC(LDFJAC,N),QTF(N),
*          WA1(N),WA2(N),WA3(N),WA4(M)
  EXTERNAL FCN
  *****

SUBROUTINE LMDIF

  THE PURPOSE OF LMDIF IS TO MINIMIZE THE SUM OF THE SQUARES OF
  M NONLINEAR FUNCTIONS IN N VARIABLES BY A MODIFICATION OF
  THE LEVENBERG-MARQUARDT ALGORITHM. THE USER MUST PROVIDE A
  SUBROUTINE WHICH CALCULATES THE FUNCTIONS. THE JACOBIAN IS
  THEN CALCULATED BY A FORWARD-DIFFERENCE APPROXIMATION.

  THE SUBROUTINE STATEMENT IS

    SUBROUTINE LMDIF(FCN,M,N,X,FVEC,FTOL,XTOL,GTOL,MAXFEV,EPSFCN,
      DIAG,MODE,FACTOR,NPRINT,INFO,NFEV,FJAC,
      LDFJAC,IPVT,QTF,WA1,WA2,WA3,WA4)

  WHERE

    FCN IS THE NAME OF THE USER-SUPPLIED SUBROUTINE WHICH
    CALCULATES THE FUNCTIONS. FCN MUST BE DECLARED
    IN AN EXTERNAL STATEMENT IN THE USER CALLING
    PROGRAM, AND SHOULD BE WRITTEN AS FOLLOWS.

    SUBROUTINE FCN(M,N,X,FVEC,IFLAG)
      INTEGER M,N,IFLAG
      DOUBLE PRECISION X(N),FVEC(M)
      -----
      CALCULATE THE FUNCTIONS AT X AND
      RETURN THIS VECTOR IN FVEC.
      -----
      RETURN
      END

    THE VALUE OF IFLAG SHOULD NOT BE CHANGED BY FCN UNLESS
    THE USER WANTS TO TERMINATE EXECUTION OF LMDIF.
    IN THIS CASE SET IFLAG TO A NEGATIVE INTEGER.

    M IS A POSITIVE INTEGER INPUT VARIABLE SET TO THE NUMBER
    OF FUNCTIONS.

    N IS A POSITIVE INTEGER INPUT VARIABLE SET TO THE NUMBER
    OF VARIABLES. N MUST NOT EXCEED M.

    X IS AN ARRAY OF LENGTH N. ON INPUT X MUST CONTAIN
    AN INITIAL ESTIMATE OF THE SOLUTION VECTOR. ON OUTPUT X

```

LMDF0010
 LMDF0020
 LMDF0030
 LMDF0040
 LMDF0050
 LMDF0060
 LMDF0070
 LMDF0080
 LMDF0090
 LMDF0100
 LMDF0110
 LMDF0120
 LMDF0130
 LMDF0140
 LMDF0150
 LMDF0160
 LMDF0170
 LMDF0180
 LMDF0190
 LMDF0200
 LMDF0210
 LMDF0220
 LMDF0230
 LMDF0240
 LMDF0250
 LMDF0260
 LMDF0270
 LMDF0280
 LMDF0290
 LMDF0300
 LMDF0310
 LMDF0320
 LMDF0330
 LMDF0340
 LMDF0350
 LMDF0360
 LMDF0370
 LMDF0380
 LMDF0390
 LMDF0400
 LMDF0410
 LMDF0420
 LMDF0430
 LMDF0440
 LMDF0450
 LMDF0460
 LMDF0470
 LMDF0480
 LMDF0490
 LMDF0500
 LMDF0510
 LMDF0520
 LMDF0530
 LMDF0540

C	CONTAINS THE FINAL ESTIMATE OF THE SOLUTION VECTOR.	LMDF0550
C		LMDF0560
C	FVEC IS AN OUTPUT ARRAY OF LENGTH M WHICH CONTAINS	LMDF0570
C	THE FUNCTIONS EVALUATED AT THE OUTPUT X.	LMDF0580
C		LMDF0590
C	FTOL IS A NONNEGATIVE INPUT VARIABLE. TERMINATION	LMDF0600
C	OCCURS WHEN BOTH THE ACTUAL AND PREDICTED RELATIVE	LMDF0610
C	REDUCTIONS IN THE SUM OF SQUARES ARE AT MOST FTOL.	LMDF0620
C	THEREFORE, FTOL MEASURES THE RELATIVE ERROR DESIRED	LMDF0630
C	IN THE SUM OF SQUARES.	LMDF0640
C		LMDF0650
C	XTOL IS A NONNEGATIVE INPUT VARIABLE. TERMINATION	LMDF0660
C	OCCURS WHEN THE RELATIVE ERROR BETWEEN TWO CONSECUTIVE	LMDF0670
C	ITERATES IS AT MOST XTOL. THEREFORE, XTOL MEASURES THE	LMDF0680
C	RELATIVE ERROR DESIRED IN THE APPROXIMATE SOLUTION.	LMDF0690
C		LMDF0700
C	GTOL IS A NONNEGATIVE INPUT VARIABLE. TERMINATION	LMDF0710
C	OCCURS WHEN THE COSINE OF THE ANGLE BETWEEN FVEC AND	LMDF0720
C	ANY COLUMN OF THE JACOBIAN IS AT MOST GTOL IN ABSOLUTE	LMDF0730
C	VALUE. THEREFORE, GTOL MEASURES THE ORTHOGONALITY	LMDF0740
C	DESIRED BETWEEN THE FUNCTION VECTOR AND THE COLUMNS	LMDF0750
C	OF THE JACOBIAN.	LMDF0760
C		LMDF0770
C	MAXFEV IS A POSITIVE INTEGER INPUT VARIABLE. TERMINATION	LMDF0780
C	OCCURS WHEN THE NUMBER OF CALLS TO FCN IS AT LEAST	LMDF0790
C	MAXFEV BY THE END OF AN ITERATION.	LMDF0800
C		LMDF0810
C	EPSFCN IS AN INPUT VARIABLE USED IN DETERMINING A SUITABLE	LMDF0820
C	STEP LENGTH FOR THE FORWARD-DIFFERENCE APPROXIMATION. THIS	LMDF0830
C	APPROXIMATION ASSUMES THAT THE RELATIVE ERRORS IN THE	LMDF0840
C	FUNCTIONS ARE OF THE ORDER OF EPSFCN. IF EPSFCN IS LESS	LMDF0850
C	THAN THE MACHINE PRECISION, IT IS ASSUMED THAT THE RELATIVE	LMDF0860
C	ERRORS IN THE FUNCTIONS ARE OF THE ORDER OF THE MACHINE	LMDF0870
C	PRECISION.	LMDF0880
C		LMDF0890
C	DIAG IS AN ARRAY OF LENGTH N. IF MODE = 1 (SEE	LMDF0900
C	BELOW), DIAG IS INTERNALLY SET. IF MODE = 2, DIAG	LMDF0910
C	MUST CONTAIN POSITIVE ENTRIES THAT SERVE AS	LMDF0920
C	MULTIPLICATIVE SCALE FACTORS FOR THE VARIABLES.	LMDF0930
C		LMDF0940
C	MODE IS AN INTEGER INPUT VARIABLE. IF MODE = 1, THE	LMDF0950
C	VARIABLES WILL BE SCALED INTERNALLY. IF MODE = 2,	LMDF0960
C	THE SCALING IS SPECIFIED BY THE INPUT DIAG. OTHER	LMDF0970
C	VALUES OF MODE ARE EQUIVALENT TO MODE = 1.	LMDF0980
C		LMDF0990
C	FACTOR IS A POSITIVE INPUT VARIABLE USED IN DETERMINING THE	LMDF1000
C	INITIAL STEP BOUND. THIS BOUND IS SET TO THE PRODUCT OF	LMDF1010
C	FACTOR AND THE EUCLIDEAN NORM OF DIAG*X IF NONZERO, OR ELSE	LMDF1020
C	TO FACTOR ITSELF. IN MOST CASES FACTOR SHOULD LIE IN THE	LMDF1030
C	INTERVAL (.1,100.). 100. IS A GENERALLY RECOMMENDED VALUE.	LMDF1040
C		LMDF1050
C	NPRINT IS AN INTEGER INPUT VARIABLE THAT ENABLES CONTROLLED	LMDF1060
C	PRINTING OF ITERATES IF IT IS POSITIVE. IN THIS CASE,	LMDF1070
C	FCN IS CALLED WITH IFLAG = 0 AT THE BEGINNING OF THE FIRST	LMDF1080

C	ITERATION AND EVERY NPRINT ITERATIONS THEREAFTER AND	LMDF1090
C	IMMEDIATELY PRIOR TO RETURN, WITH X AND FVEC AVAILABLE	LMDF1100
C	FOR PRINTING. IF NPRINT IS NOT POSITIVE, NO SPECIAL CALLS	LMDF1110
C	OF FCN WITH IFLAG = 0 ARE MADE.	LMDF1120
C		LMDF1130
C	INFO IS AN INTEGER OUTPUT VARIABLE. IF THE USER HAS	LMDF1140
C	TERMINATED EXECUTION, INFO IS SET TO THE (NEGATIVE)	LMDF1150
C	VALUE OF IFLAG. SEE DESCRIPTION OF FCN. OTHERWISE,	LMDF1160
C	INFO IS SET AS FOLLOWS.	LMDF1170
C		LMDF1180
C	INFO = 0 IMPROPER INPUT PARAMETERS.	LMDF1190
C		LMDF1200
C	INFO = 1 BOTH ACTUAL AND PREDICTED RELATIVE REDUCTIONS	LMDF1210
C	IN THE SUM OF SQUARES ARE AT MOST FTOL.	LMDF1220
C		LMDF1230
C	INFO = 2 RELATIVE ERROR BETWEEN TWO CONSECUTIVE ITERATES	LMDF1240
C	IS AT MOST XTOL.	LMDF1250
C		LMDF1260
C	INFO = 3 CONDITIONS FOR INFO = 1 AND INFO = 2 BOTH HOLD.	LMDF1270
C		LMDF1280
C	INFO = 4 THE COSINE OF THE ANGLE BETWEEN FVEC AND ANY	LMDF1290
C	COLUMN OF THE JACOBIAN IS AT MOST GTOL IN	LMDF1300
C	ABSOLUTE VALUE.	LMDF1310
C		LMDF1320
C	INFO = 5 NUMBER OF CALLS TO FCN HAS REACHED OR	LMDF1330
C	EXCEEDED MAXFEV.	LMDF1340
C		LMDF1350
C	INFO = 6 FTOL IS TOO SMALL. NO FURTHER REDUCTION IN	LMDF1360
C	THE SUM OF SQUARES IS POSSIBLE.	LMDF1370
C		LMDF1380
C	INFO = 7 XTOL IS TOO SMALL. NO FURTHER IMPROVEMENT IN	LMDF1390
C	THE APPROXIMATE SOLUTION X IS POSSIBLE.	LMDF1400
C		LMDF1410
C	INFO = 8 GTOL IS TOO SMALL. FVEC IS ORTHOGONAL TO THE	LMDF1420
C	COLUMNS OF THE JACOBIAN TO MACHINE PRECISION.	LMDF1430
C		LMDF1440
C	NFEV IS AN INTEGER OUTPUT VARIABLE SET TO THE NUMBER OF	LMDF1450
C	CALLS TO FCN.	LMDF1460
C		LMDF1470
C	FJAC IS AN OUTPUT M BY N ARRAY. THE UPPER N BY N SUBMATRIX	LMDF1480
C	OF FJAC CONTAINS AN UPPER TRIANGULAR MATRIX R WITH	LMDF1490
C	DIAGONAL ELEMENTS OF NONINCREASING MAGNITUDE SUCH THAT	LMDF1500
C		LMDF1510
C		LMDF1520
C	$P^T (JAC^T JAC) P = R^T R,$	LMDF1530
C		LMDF1540
C	WHERE P IS A PERMUTATION MATRIX AND JAC IS THE FINAL	LMDF1550
C	CALCULATED JACOBIAN. COLUMN J OF P IS COLUMN IPVT(J)	LMDF1560
C	(SEE BELOW) OF THE IDENTITY MATRIX. THE LOWER TRAPEZOIDAL	LMDF1570
C	PART OF FJAC CONTAINS INFORMATION GENERATED DURING	LMDF1580
C	THE COMPUTATION OF R.	LMDF1590
C		LMDF1600
C	LDJFAC IS A POSITIVE INTEGER INPUT VARIABLE NOT LESS THAN M	LMDF1610
C	WHICH SPECIFIES THE LEADING DIMENSION OF THE ARRAY FJAC.	LMDF1620

C		LMDF1630
C	IPVT IS AN INTEGER OUTPUT ARRAY OF LENGTH N. IPVT	LMDF1640
C	DEFINES A PERMUTATION MATRIX P SUCH THAT $JAC * P = Q * R$,	LMDF1650
C	WHERE JAC IS THE FINAL CALCULATED JACOBIAN, Q IS	LMDF1660
C	ORTHOGONAL (NOT STORED), AND R IS UPPER TRIANGULAR	LMDF1670
C	WITH DIAGONAL ELEMENTS OF NONINCREASING MAGNITUDE.	LMDF1680
C	COLUMN J OF P IS COLUMN IPVT(J) OF THE IDENTITY MATRIX.	LMDF1690
C		LMDF1700
C	QTF IS AN OUTPUT ARRAY OF LENGTH N WHICH CONTAINS	LMDF1710
C	THE FIRST N ELEMENTS OF THE VECTOR (Q TRANSPOSE)*FVEC.	LMDF1720
C		LMDF1730
C	WA1, WA2, AND WA3 ARE WORK ARRAYS OF LENGTH N.	LMDF1740
C		LMDF1750
C	WA4 IS A WORK ARRAY OF LENGTH M.	LMDF1760
C		LMDF1770
C	SUBPROGRAMS CALLED	LMDF1780
C		LMDF1790
C	USER-SUPPLIED FCN	LMDF1800
C		LMDF1810
C	MINPACK-SUPPLIED ... DPMPAR,ENORM,FDJAC2,LMPAR,QRFAC	LMDF1820
C		LMDF1830
C	FORTTRAN-SUPPLIED ... DABS,DMAX1,DMIN1,DSQRT,MOD	LMDF1840
C		LMDF1850
C	ARGONNE NATIONAL LABORATORY. MINPACK PROJECT. MARCH 1980.	LMDF1860
C	BURTON S. GARBOW, KENNETH E. HILLSTROM, JORGE J. MORE	LMDF1870
C		LMDF1880
C	*****	LMDF1890
C	INTEGER I,IFLAG,ITER,J,L	LMDF1900
C	DOUBLE PRECISION ACTRED,DELTA,DORDER,EPSMCH,FNORM,FNORM1,GNORM,	LMDF1910
C	* ONE,PAR,PNORM,PRERED,P1,P5,P25,P75,P0001,RATIO,	LMDF1920
C	* SUM,TEMP,TEMP1,TEMP2,XNORM,ZERO	LMDF1930
C	DOUBLE PRECISION DPMPAR,ENORM	LMDF1940
C	DATA ONE,P1,P5,P25,P75,P0001,ZERO	LMDF1950
C	* /1.0D0,1.0D-1,5.0D-1,2.5D-1,7.5D-1,1.0D-4,...0D0/	LMDF1960
C		LMDF1970
C	EPSMCH IS THE MACHINE PRECISION.	LMDF1980
C		LMDF1990
C	EPSMCH = DPMPAR(1)	LMDF2000
C		LMDF2010
C	INFO = 0	LMDF2020
C	IFLAG = 0	LMDF2030
C	NFEV = 0	LMDF2040
C		LMDF2050
C	CHECK THE INPUT PARAMETERS FOR ERRORS.	LMDF2060
C		LMDF2070
C	IF (N .LE. 0 .OR. M .LT. N .OR. LDFJAC .LT. M	LMDF2080
C	* .OR. FTOL .LT. ZERO .OR. XTOL .LT. ZERO .OR. GTOL .LT. ZERO	LMDF2090
C	* .OR. MAXFEV .LE. 0 .OR. FACTOR .LE. ZERO) GO TO 300	LMDF2100
C	IF (MODE .NE. 2) GO TO 20	LMDF2110
C	DO 10 J = 1, N	LMDF2120
C	IF (DIAG(J) .LE. ZERO) GO TO 300	LMDF2130
C	10 CONTINUE	LMDF2140
C	20 CONTINUE	LMDF2150
C		LMDF2160

C	EVALUATE THE FUNCTION AT THE STARTING POINT	LMDF2170
C	AND CALCULATE ITS NORM.	LMDF2180
C		LMDF2190
	IFLAG = 1	LMDF2200
	CALL FCN(M,N,X,FVEC,IFLAG)	LMDF2210
	NFEV = 1	LMDF2220
	IF (IFLAG .LT. 0) GO TO 300	LMDF2230
	FNORM = ENORM(M,FVEC)	LMDF2240
C		LMDF2250
C	INITIALIZE LEVENBERG-MARQUARDT PARAMETER AND ITERATION COUNTER.	LMDF2260
C		LMDF2270
	PAR = ZERO	LMDF2280
	ITER = 1	LMDF2290
C		LMDF2300
C	BEGINNING OF THE OUTER LOOP.	LMDF2310
C		LMDF2320
	30 CONTINUE	LMDF2330
C		LMDF2340
C	CALCULATE THE JACOBIAN MATRIX.	LMDF2350
C		LMDF2360
	IFLAG = 2	LMDF2370
	CALL FDJAC2(FCN,M,N,X,FVEC,FJAC,LDFJAC,IFLAG,EPSFCN,WA4)	LMDF2380
	NFEV = NFEV + N	LMDF2390
	IF (IFLAG .LT. 0) GO TO 300	LMDF2400
C		LMDF2410
C	IF REQUESTED, CALL FCN TO ENABLE PRINTING OF ITERATES.	LMDF2420
C		LMDF2430
	IF (NPRINT .LE. 0) GO TO 40	LMDF2440
	IFLAG = 0	LMDF2450
	IF (MOD(ITER-1,NPRINT) .EQ. 0) CALL FCN(M,N,X,FVEC,IFLAG)	LMDF2460
	IF (IFLAG .LT. 0) GO TO 300	LMDF2470
	40 CONTINUE	LMDF2480
C		LMDF2490
C	COMPUTE THE QR FACTORIZATION OF THE JACOBIAN.	LMDF2500
C		LMDF2510
	CALL QRFAC(M,N,FJAC,LDFJAC,.TRUE.,IPVT,N,WA1,WA2,WA3)	LMDF2520
C		LMDF2530
C	ON THE FIRST ITERATION AND IF MODE IS 1, SCALE ACCORDING	LMDF2540
C	TO THE NORMS OF THE COLUMNS OF THE INITIAL JACOBIAN.	LMDF2550
C		LMDF2560
	IF (ITER .NE. 1) GO TO 80	LMDF2570
	IF (MODE .EQ. 2) GO TO 60	LMDF2580
	DO 50 J = 1, N	LMDF2590
	DIAG(J) = WA2(J)	LMDF2600
	IF (WA2(J) .EQ. ZERO) DIAG(J) = ONE	LMDF2610
50	CONTINUE	LMDF2620
60	CONTINUE	LMDF2630
C		LMDF2640
C	ON THE FIRST ITERATION, CALCULATE THE NORM OF THE SCALED X	LMDF2650
C	AND INITIALIZE THE STEP BOUND DELTA.	LMDF2660
C		LMDF2670
	DO 70 J = 1, N	LMDF2680
	WA3(J) = DIAG(J)*X(J)	LMDF2690
70	CONTINUE	LMDF2700

	XNORM = ENORM(N,WA3)	LMDF2710
	DELTA = FACTOR*XNORM	LMDF2720
	IF (DELTA .EQ. ZERO) DELTA = FACTOR	LMDF2730
80	CONTINUE	LMDF2740
C		LMDF2750
C	FORM (Q TRANSPOSE)*FVEC AND STORE THE FIRST N COMPONENTS IN	LMDF2760
C	QTF.	LMDF2770
C		LMDF2780
	DO 90 I = 1, M	LMDF2790
	WA4(I) = FVEC(I)	LMDF2800
90	CONTINUE	LMDF2810
	DO 130 J = 1, N	LMDF2820
	IF (FJAC(J,J) .EQ. ZERO) GO TO 120	LMDF2830
	SUM = ZERO	LMDF2840
	DO 100 I = J, M	LMDF2850
	SUM = SUM + FJAC(I,J)*WA4(I)	LMDF2860
100	CONTINUE	LMDF2870
	TEMP = -SUM/FJAC(J,J)	LMDF2880
	DO 110 I = J, M	LMDF2890
	WA4(I) = WA4(I) + FJAC(I,J)*TEMP	LMDF2900
110	CONTINUE	LMDF2910
120	CONTINUE	LMDF2920
	FJAC(J,J) = WA1(J)	LMDF2930
	QTF(J) = WA4(J)	LMDF2940
130	CONTINUE	LMDF2950
C		LMDF2960
C	COMPUTE THE NORM OF THE SCALED GRADIENT.	LMDF2970
C		LMDF2980
	GNORM = ZERO	LMDF2990
	IF (FNORM .EQ. ZERO) GO TO 170	LMDF3000
	DO 160 J = 1, N	LMDF3010
	L = IPVT(J)	LMDF3020
	IF (WA2(L) .EQ. ZERO) GO TO 150	LMDF3030
	SUM = ZERO	LMDF3040
	DO 140 I = 1, J	LMDF3050
	SUM = SUM + FJAC(I,J)*(QTF(I)/FNORM)	LMDF3060
140	CONTINUE	LMDF3070
	GNORM = DMAX1(GNORM,DABS(SUM/WA2(L)))	LMDF3080
150	CONTINUE	LMDF3090
160	CONTINUE	LMDF3100
170	CONTINUE	LMDF3110
C		LMDF3120
C	TEST FOR CONVERGENCE OF THE GRADIENT NORM.	LMDF3130
C		LMDF3140
	IF (GNORM .LE. GTOL) INFO = 4	LMDF3150
	IF (INFO .NE. 0) GO TO 300	LMDF3160
C		LMDF3170
C	RESCALE IF NECESSARY.	LMDF3180
C		LMDF3190
	IF (MODE .EQ. 2) GO TO 190	LMDF3200
	DO 180 J = 1, N	LMDF3210
	DIAG(J) = DMAX1(DIAG(J),WA2(J))	LMDF3220
180	CONTINUE	LMDF3230
190	CONTINUE	LMDF3240

C		LMDF3250
C	BEGINNING OF THE INNER LOOP.	LMDF3260
C		LMDF3270
200	CONTINUE	LMDF3280
C		LMDF3290
C	DETERMINE THE LEVENBERG-MARQUARDT PARAMETER.	LMDF3300
C		LMDF3310
	CALL LMPAR(N,FJAC,LDFJAC,IPVT,DIAG,QTF,DELTA,PAR,WA1,WA2,	LMDF3320
*	WA3,WA4)	LMDF3330
C		LMDF3340
C	STORE THE DIRECTION P AND X + P. CALCULATE THE NORM OF P.	LMDF3350
C		LMDF3360
	DO 210 J = 1, N	LMDF3370
	WA1(J) = -WA1(J)	LMDF3380
	WA2(J) = X(J) + WA1(J)	LMDF3390
	WA3(J) = DIAG(J)*WA1(J)	LMDF3400
210	CONTINUE	LMDF3410
	PNORM = ENORM(N,WA3)	LMDF3420
C		LMDF3430
C	ON THE FIRST ITERATION, ADJUST THE INITIAL STEP BOUND.	LMDF3440
C		LMDF3450
	IF (ITER .EQ. 1) DELTA = DMIN1(DELTA,PNORM)	LMDF3460
C		LMDF3470
C	EVALUATE THE FUNCTION AT X + P AND CALCULATE ITS NORM.	LMDF3480
C		LMDF3490
	IFLAG = 1	LMDF3500
	CALL FCN(M,N,WA2,WA4,IFLAG)	LMDF3510
	NFEV = NFEV + 1	LMDF3520
	IF (IFLAG .LT. 0) GO TO 300	LMDF3530
	FNORM1 = ENORM(M,WA4)	LMDF3540
C		LMDF3550
C	COMPUTE THE SCALED ACTUAL REDUCTION.	LMDF3560
C		LMDF3570
	ACTRED = -ONE	LMDF3580
	IF (P1*FNORM1 .LT. FNORM) ACTRED = ONE - (FNORM1/FNORM)**2	LMDF3590
C		LMDF3600
C	COMPUTE THE SCALED PREDICTED REDUCTION AND	LMDF3610
C	THE SCALED DIRECTIONAL DERIVATIVE.	LMDF3620
C		LMDF3630
	DO 230 J = 1, N	LMDF3640
	WA3(J) = ZERO	LMDF3650
	L = IPVT(J)	LMDF3660
	TEMP = WA1(L)	LMDF3670
	DO 220 I = 1, J	LMDF3680
	WA3(I) = WA3(I) + FJAC(I,J)*TEMP	LMDF3690
220	CONTINUE	LMDF3700
230	CONTINUE	LMDF3710
	TEMP1 = ENORM(N,WA3)/FNORM	LMDF3720
	TEMP2 = (DSQRT(PAR)*PNORM)/FNORM	LMDF3730
	PRERED = TEMP1**2 + TEMP2**2/P5	LMDF3740
	DIRDER = -(TEMP1**2 + TEMP2**2)	LMDF3750
C		LMDF3760
C	COMPUTE THE RATIO OF THE ACTUAL TO THE PREDICTED	LMDF3770
C	REDUCTION.	LMDF3780

C	RATIO = ZERO	LMDF3790
	IF (PRERED .NE. ZERO) RATIO = ACTRED/PRERED	LMDF3800
C		LMDF3810
C	UPDATE THE STEP BOUND.	LMDF3820
C		LMDF3830
	IF (RATIO .GT. P25) GO TO 240	LMDF3840
	IF (ACTRED .GE. ZERO) TEMP = P5	LMDF3850
	IF (ACTRED .LT. ZERO)	LMDF3860
*	TEMP = P5*DIRDER/(DIRDER + P5*ACTRED)	LMDF3870
	IF (P1*FNORM1 .GE. FNORM .OR. TEMP .LT. P1) TEMP = P1	LMDF3880
	DELTA = TEMP*DMIN1(DELTA,PNORM/P1)	LMDF3890
	PAR = PAR/TEMP	LMDF3900
	GO TO 260	LMDF3910
240	CONTINUE	LMDF3920
	IF (PAR .NE. ZERO .AND. RATIO .LT. P75) GO TO 250	LMDF3930
	DELTA = PNORM/P5	LMDF3940
	PAR = P5*PAR	LMDF3950
250	CONTINUE	LMDF3960
260	CONTINUE	LMDF3970
C		LMDF3980
C	TEST FOR SUCCESSFUL ITERATION.	LMDF3990
C		LMDF4000
	IF (RATIO .LT. P0001) GO TO 290	LMDF4010
C		LMDF4020
C	SUCCESSFUL ITERATION. UPDATE X, FVEC, AND THEIR NORMS.	LMDF4030
C		LMDF4040
	DO 270 J = 1, N	LMDF4050
	X(J) = WA2(J)	LMDF4060
	WA2(J) = DIAG(J)*X(J)	LMDF4070
270	CONTINUE	LMDF4080
	DO 280 I = 1, M	LMDF4090
	FVEC(I) = WA4(I)	LMDF4100
280	CONTINUE	LMDF4110
	XNORM = ENORM(N,WA2)	LMDF4120
	FNORM = FNORM1	LMDF4130
	ITER = ITER + 1	LMDF4140
290	CONTINUE	LMDF4150
C		LMDF4160
C	TESTS FOR CONVERGENCE.	LMDF4170
C		LMDF4180
	IF (DABS(ACTRED) .LE. FTOL .AND. PRERED .LE. FTOL	LMDF4190
*	.AND. P5*RATIO .LE. ONE) INFO = 1	LMDF4200
	IF (DELTA .LE. XTOL*XNORM) INFO = 2	LMDF4210
	IF (DABS(ACTRED) .LE. FTOL .AND. PRERED .LE. FTOL	LMDF4220
*	.AND. P5*RATIO .LE. ONE .AND. INFO .EQ. 2) INFO = 3	LMDF4230
	IF (INFO .NE. 0) GO TO 300	LMDF4240
C		LMDF4250
C	TESTS FOR TERMINATION AND STRINGENT TOLERANCES.	LMDF4260
C		LMDF4270
	IF (NFEV .GE. MAXFEV) INFO = 5	LMDF4280
	IF (DABS(ACTRED) .LE. EPSMCH .AND. PRERED .LE. EPSMCH	LMDF4290
*	.AND. P5*RATIO .LE. ONE) INFO = 6	LMDF4300
	IF (DELTA .LE. EPSMCH*XNORM) INFO = 7	LMDF4310
		LMDF4320

	IF (GNORM .LE. EPSMCH) INFO = 8	LMDF4330
	IF (INFO .NE. 0) GO TO 300	LMDF4340
C		LMDF4350
C	END OF THE INNER LOOP. REPEAT IF ITERATION UNSUCCESSFUL.	LMDF4360
C		LMDF4370
	IF (RATIO .LT. P0001) GO TO 200	LMDF4380
C		LMDF4390
C	END OF THE OUTER LOOP.	LMDF4400
C		LMDF4410
	GO TO 30	LMDF4420
	300 CONTINUE	LMDF4430
C		LMDF4440
C	TERMINATION, EITHER NORMAL OR USER IMPOSED.	LMDF4450
C		LMDF4460
	IF (IFLAG .LT. 0) INFO = IFLAG	LMDF4470
	IFLAG = 0	LMDF4480
	IF (NPRINT .GT. 0) CALL FCN(M,N,X,FVEC,IFLAG)	LMDF4490
	RETURN	LMDF4500
C		LMDF4510
C	LAST CARD OF SUBROUTINE LMDIF.	LMDF4520
C		LMDF4530
	END	LMDF4540

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SUBROUTINE LMDIF1(FCN,M,N,X,FVEC,TOL,INFO,IWA,WA,LWA)
INTEGER M,N,INFO,LWA
INTEGER IWA(N)
DOUBLE PRECISION TOL
DOUBLE PRECISION X(N),FVEC(M),WA(LWA)
EXTERNAL FCN

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*****

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```

SUBROUTINE LMDIF1

```

```

THE PURPOSE OF LMDIF1 IS TO MINIMIZE THE SUM OF THE SQUARES OF
M NONLINEAR FUNCTIONS IN N VARIABLES BY A MODIFICATION OF THE
LEVENBERG-MARQUARDT ALGORITHM. THIS IS DONE BY USING THE MORE
GENERAL LEAST-SQUARES SOLVER LMDIF. THE USER MUST PROVIDE A
SUBROUTINE WHICH CALCULATES THE FUNCTIONS. THE JACOBIAN IS
THEN CALCULATED BY A FORWARD-DIFFERENCE APPROXIMATION.

```

```

THE SUBROUTINE STATEMENT IS

```

```

SUBROUTINE LMDIF1(FCN,M,N,X,FVEC,TOL,INFO,IWA,WA,LWA)

```

```

WHERE

```

```

FCN IS THE NAME OF THE USER-SUPPLIED SUBROUTINE WHICH
CALCULATES THE FUNCTIONS. FCN MUST BE DECLARED
IN AN EXTERNAL STATEMENT IN THE USER CALLING
PROGRAM, AND SHOULD BE WRITTEN AS FOLLOWS.

```

```

SUBROUTINE FCN(M,N,X,FVEC,IFLAG)
INTEGER M,N,IFLAG
DOUBLE PRECISION X(N),FVEC(M)

```

```

-----
CALCULATE THE FUNCTIONS AT X AND
RETURN THIS VECTOR IN FVEC.

```

```

-----
RETURN
END

```

```

THE VALUE OF IFLAG SHOULD NOT BE CHANGED BY FCN UNLESS
THE USER WANTS TO TERMINATE EXECUTION OF LMDIF1.
IN THIS CASE SET IFLAG TO A NEGATIVE INTEGER.

```

```

M IS A POSITIVE INTEGER INPUT VARIABLE SET TO THE NUMBER
OF FUNCTIONS.

```

```

N IS A POSITIVE INTEGER INPUT VARIABLE SET TO THE NUMBER
OF VARIABLES. N MUST NOT EXCEED M.

```

```

X IS AN ARRAY OF LENGTH N. ON INPUT X MUST CONTAIN
AN INITIAL ESTIMATE OF THE SOLUTION VECTOR. ON OUTPUT X
CONTAINS THE FINAL ESTIMATE OF THE SOLUTION VECTOR.

```

```

FVEC IS AN OUTPUT ARRAY OF LENGTH M WHICH CONTAINS
THE FUNCTIONS EVALUATED AT THE OUTPUT X.

```

```

LMF10010
LMF10020
LMF10030
LMF10040
LMF10050
LMF10060
LMF10070
LMF10080
LMF10090
LMF10100
LMF10110
LMF10120
LMF10130
LMF10140
LMF10150
LMF10160
LMF10170
LMF10180
LMF10190
LMF10200
LMF10210
LMF10220
LMF10230
LMF10240
LMF10250
LMF10260
LMF10270
LMF10280
LMF10290
LMF10300
LMF10310
LMF10320
LMF10330
LMF10340
LMF10350
LMF10360
LMF10370
LMF10380
LMF10390
LMF10400
LMF10410
LMF10420
LMF10430
LMF10440
LMF10450
LMF10460
LMF10470
LMF10480
LMF10490
LMF10500
LMF10510
LMF10520
LMF10530
LMF10540

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C		LMF10550
C	TOL IS A NONNEGATIVE INPUT VARIABLE. TERMINATION OCCURS	LMF10560
C	WHEN THE ALGORITHM ESTIMATES EITHER THAT THE RELATIVE	LMF10570
C	ERROR IN THE SUM OF SQUARES IS AT MOST TOL OR THAT	LMF10580
C	THE RELATIVE ERROR BETWEEN X AND THE SOLUTION IS AT	LMF10590
C	MOST TOL.	LMF10600
C		LMF10610
C	INFO IS AN INTEGER OUTPUT VARIABLE. IF THE USER HAS	LMF10620
C	TERMINATED EXECUTION, INFO IS SET TO THE (NEGATIVE)	LMF10630
C	VALUE OF IFLAG. SEE DESCRIPTION OF FCN. OTHERWISE,	LMF10640
C	INFO IS SET AS FOLLOWS.	LMF10650
C		LMF10660
C	INFO = 0 IMPROPER INPUT PARAMETERS.	LMF10670
C		LMF10680
C	INFO = 1 ALGORITHM ESTIMATES THAT THE RELATIVE ERROR	LMF10690
C	IN THE SUM OF SQUARES IS AT MOST TOL.	LMF10700
C		LMF10710
C	INFO = 2 ALGORITHM ESTIMATES THAT THE RELATIVE ERROR	LMF10720
C	BETWEEN X AND THE SOLUTION IS AT MOST TOL.	LMF10730
C		LMF10740
C	INFO = 3 CONDITIONS FOR INFO = 1 AND INFO = 2 BOTH HOLD.	LMF10750
C		LMF10760
C	INFO = 4 FVEC IS ORTHOGONAL TO THE COLUMNS OF THE	LMF10770
C	JACOBIAN TO MACHINE PRECISION.	LMF10780
C		LMF10790
C	INFO = 5 NUMBER OF CALLS TO FCN HAS REACHED OR	LMF10800
C	EXCEEDED 200*(N+1).	LMF10810
C		LMF10820
C	INFO = 6 TOL IS TOO SMALL. NO FURTHER REDUCTION IN	LMF10830
C	THE SUM OF SQUARES IS POSSIBLE.	LMF10840
C		LMF10850
C	INFO = 7 TOL IS TOO SMALL. NO FURTHER IMPROVEMENT IN	LMF10860
C	THE APPROXIMATE SOLUTION X IS POSSIBLE.	LMF10870
C		LMF10880
C	IWA IS AN INTEGER WORK ARRAY OF LENGTH N.	LMF10890
C		LMF10900
C	WA IS A WORK ARRAY OF LENGTH LWA.	LMF10910
C		LMF10920
C	LWA IS A POSITIVE INTEGER INPUT VARIABLE NOT LESS THAN	LMF10930
C	$M*N+5*N+M$.	LMF10940
C		LMF10950
C	SUBPROGRAMS CALLED	LMF10960
C		LMF10970
C	USER-SUPPLIED FCN	LMF10980
C		LMF10990
C	MINPACK-SUPPLIED ... LMDIF	LMF11000
C		LMF11010
C	ARGONNE NATIONAL LABORATORY. MINPACK PROJECT. MARCH 1980.	LMF11020
C	BURTON S. GARBOW, KENNETH E. HILLSTROM, JORGE J. MORE	LMF11030
C		LMF11040
C	*****	LMF11050
C	INTEGER MAXFEV,MODE,MP5N,NFEV,NPRINT	LMF11060
C	DOUBLE PRECISION EPSFCN,FACTOR,FTOL,GTOL,XTOL,ZERO	LMF11070
C	DATA FACTOR,ZERO /1.0D2,0.0D0/	LMF11080

	INFO = 0	LMF11090
C		LMF11100
C	CHECK THE INPUT PARAMETERS FOR ERRORS.	LMF11110
C		LMF11120
	IF (N .LE. 0 .OR. M .LT. N .OR. TOL .LT. ZERO	LMF11130
	* .OR. LWA .LT. M*N + 5*N + M) GO TO 10	LMF11140
C		LMF11150
C	CALL LMDIF.	LMF11160
C		LMF11170
	MAXFEV = 200*(N + 1)	LMF11180
	FTOL = TOL	LMF11190
	XTOL = TOL	LMF11200
	GTOL = ZERO	LMF11210
	EPSFCN = ZERO	LMF11220
	MODE = 1	LMF11230
	NPRINT = 0	LMF11240
	MP5N = M + 5*N	LMF11250
	CALL LMDIF(FCN,M,N,X,FVEC,FTOL,XTOL,GTOL,MAXFEV,EPSFCN,WA(1),	LMF11260
	* MODE,FACTOR,NPRINT,INFO,NFEV,WA(MP5N+1),M,IWA,	LMF11270
	* WA(N+1),WA(2*N+1),WA(3*N+1),WA(4*N+1),WA(5*N+1))	LMF11280
	IF (INFO .EQ. 8) INFO = 4	LMF11290
10	CONTINUE	LMF11300
	RETURN	LMF11310
C		LMF11320
C	LAST CARD OF SUBROUTINE LMDIF1.	LMF11330
C		LMF11340
	END	LMF11350

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SUBROUTINE LMPAR(N,R,LDR,IPVT,DIAG,QTB,DELTA,PAR,X,SDIAG,WA1,
*          WA2)
  INTEGER N,LDR
  INTEGER IPVT(N)
  DOUBLE PRECISION DELTA,PAR
  DOUBLE PRECISION R(LDR,N),DIAG(N),QTB(N),X(N),SDIAG(N),WA1(N),
*          WA2(N)

```

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*****

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```

SUBROUTINE LMPAR

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```

  GIVEN AN M BY N MATRIX A, AN N BY N NONSINGULAR DIAGONAL
  MATRIX D, AN M-VECTOR B, AND A POSITIVE NUMBER DELTA,
  THE PROBLEM IS TO DETERMINE A VALUE FOR THE PARAMETER
  PAR SUCH THAT IF X SOLVES THE SYSTEM

```

$$A * X = B, \quad \text{SQRT}(PAR) * D * X = 0,$$

```

  IN THE LEAST SQUARES SENSE, AND DXNORM IS THE EUCLIDEAN
  NORM OF D*X, THEN EITHER PAR IS ZERO AND

```

$$(DXNORM - DELTA) \leq 0.1 * DELTA,$$

```

  OR PAR IS POSITIVE AND

```

$$ABS(DXNORM - DELTA) \leq 0.1 * DELTA.$$

```

  THIS SUBROUTINE COMPLETES THE SOLUTION OF THE PROBLEM
  IF IT IS PROVIDED WITH THE NECESSARY INFORMATION FROM THE
  QR FACTORIZATION, WITH COLUMN PIVOTING, OF A. THAT IS, IF
  A * P = Q * R, WHERE P IS A PERMUTATION MATRIX, Q HAS ORTHOGONAL
  COLUMNS, AND R IS AN UPPER TRIANGULAR MATRIX WITH DIAGONAL
  ELEMENTS OF NONINCREASING MAGNITUDE, THEN LMPAR EXPECTS
  THE FULL UPPER TRIANGLE OF R, THE PERMUTATION MATRIX P,
  AND THE FIRST N COMPONENTS OF (Q TRANSPOSE) * B. ON OUTPUT
  LMPAR ALSO PROVIDES AN UPPER TRIANGULAR MATRIX S SUCH THAT

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$$P^T * (A^T * A + PAR * D^T * D) * P = S^T * S.$$

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  S IS EMPLOYED WITHIN LMPAR AND MAY BE OF SEPARATE INTEREST.

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  ONLY A FEW ITERATIONS ARE GENERALLY NEEDED FOR CONVERGENCE
  OF THE ALGORITHM. IF, HOWEVER, THE LIMIT OF 10 ITERATIONS
  IS REACHED, THEN THE OUTPUT PAR WILL CONTAIN THE BEST
  VALUE OBTAINED SO FAR.

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  THE SUBROUTINE STATEMENT IS

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  SUBROUTINE LMPAR(N,R,LDR,IPVT,DIAG,QTB,DELTA,PAR,X,SDIAG,
          WA1,WA2)

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```

  WHERE

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LMPR0010
LMPR0020
LMPR0030
LMPR0040
LMPR0050
LMPR0060
LMPR0070
LMPR0080
LMPR0090
LMPR0100
LMPR0110
LMPR0120
LMPR0130
LMPR0140
LMPR0150
LMPR0160
LMPR0170
LMPR0180
LMPR0190
LMPR0200
LMPR0210
LMPR0220
LMPR0230
LMPR0240
LMPR0250
LMPR0260
LMPR0270
LMPR0280
LMPR0290
LMPR0300
LMPR0310
LMPR0320
LMPR0330
LMPR0340
LMPR0350
LMPR0360
LMPR0370
LMPR0380
LMPR0390
LMPR0400
LMPR0410
LMPR0420
LMPR0430
LMPR0440
LMPR0450
LMPR0460
LMPR0470
LMPR0480
LMPR0490
LMPR0500
LMPR0510
LMPR0520
LMPR0530
LMPR0540

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C	N IS A POSITIVE INTEGER INPUT VARIABLE SET TO THE ORDER OF R.	LMPR0550
C		LMPR0560
C	R IS AN N BY N ARRAY. ON INPUT THE FULL UPPER TRIANGLE	LMPR0570
C	MUST CONTAIN THE FULL UPPER TRIANGLE OF THE MATRIX R.	LMPR0580
C	ON OUTPUT THE FULL UPPER TRIANGLE IS UNALTERED, AND THE	LMPR0590
C	STRICT LOWER TRIANGLE CONTAINS THE STRICT UPPER TRIANGLE	LMPR0600
C	(TRANPOSED) OF THE UPPER TRIANGULAR MATRIX S.	LMPR0610
C		LMPR0620
C	LDR IS A POSITIVE INTEGER INPUT VARIABLE NOT LESS THAN N	LMPR0630
C	WHICH SPECIFIES THE LEADING DIMENSION OF THE ARRAY R.	LMPR0640
C		LMPR0650
C	IPVT IS AN INTEGER INPUT ARRAY OF LENGTH N WHICH DEFINES THE	LMPR0660
C	PERMUTATION MATRIX P SUCH THAT $A \cdot P = Q \cdot R$. COLUMN J OF P	LMPR0670
C	IS COLUMN IPVT(J) OF THE IDENTITY MATRIX.	LMPR0680
C		LMPR0690
C	DIAG IS AN INPUT ARRAY OF LENGTH N WHICH MUST CONTAIN THE	LMPR0700
C	DIAGONAL ELEMENTS OF THE MATRIX D.	LMPR0710
C		LMPR0720
C	QTB IS AN INPUT ARRAY OF LENGTH N WHICH MUST CONTAIN THE FIRST	LMPR0730
C	N ELEMENTS OF THE VECTOR $(Q \text{ TRANSPOSE}) \cdot B$.	LMPR0740
C		LMPR0750
C	DELTA IS A POSITIVE INPUT VARIABLE WHICH SPECIFIES AN UPPER	LMPR0760
C	BOUND ON THE EUCLIDEAN NORM OF $D \cdot X$.	LMPR0770
C		LMPR0780
C	PAR IS A NONNEGATIVE VARIABLE. ON INPUT PAR CONTAINS AN	LMPR0790
C	INITIAL ESTIMATE OF THE LEVENBERG-MARQUARDT PARAMETER.	LMPR0800
C	ON OUTPUT PAR CONTAINS THE FINAL ESTIMATE.	LMPR0810
C		LMPR0820
C	X IS AN OUTPUT ARRAY OF LENGTH N WHICH CONTAINS THE LEAST	LMPR0830
C	SQUARES SOLUTION OF THE SYSTEM $A \cdot X = B$, $\text{SQRT}(\text{PAR}) \cdot D \cdot X = 0$,	LMPR0840
C	FOR THE OUTPUT PAR.	LMPR0850
C		LMPR0860
C	SDIAG IS AN OUTPUT ARRAY OF LENGTH N WHICH CONTAINS THE	LMPR0870
C	DIAGONAL ELEMENTS OF THE UPPER TRIANGULAR MATRIX S.	LMPR0880
C		LMPR0890
C	WA1 AND WA2 ARE WORK ARRAYS OF LENGTH N.	LMPR0900
C		LMPR0910
C	SUBPROGRAMS CALLED	LMPR0920
C		LMPR0930
C	MINPACK-SUPPLIED ... DPMPAR, ENORM, QRSOLV	LMPR0940
C		LMPR0950
C	FORTRAN-SUPPLIED ... DABS, DMAX1, DMIN1, DSQRT	LMPR0960
C		LMPR0970
C	ARGONNE NATIONAL LABORATORY. MINPACK PROJECT. MARCH 1980.	LMPR0980
C	BURTON S. GARBOW, KENNETH E. HILLSTROM, JORGE J. MORE	LMPR0990
C		LMPR1000
C	*****	LMPR1010
C	INTEGER I, ITER, J, JM1, JP1, K, L, NSING	LMPR1020
C	DOUBLE PRECISION DXNORM, DWARF, FP, GNORM, PARC, PARL, PARU, P1, P001,	LMPR1030
C	* SUM, TEMP, ZERO	LMPR1040
C	DOUBLE PRECISION DPMPAR, ENORM	LMPR1050
C	DATA P1, P001, ZERO /1.0D-1, 1.0D-3, 0.0D0/	LMPR1060
C		LMPR1070
C	DWARF IS THE SMALLEST POSITIVE MAGNITUDE.	LMPR1080

C		LMPR1090
	DWARF = DPMPAR(2)	LMPR1100
C		LMPR1110
C	COMPUTE AND STORE IN X THE GAUSS-NEWTON DIRECTION. IF THE	LMPR1120
C	JACOBIAN IS RANK-DEFICIENT, OBTAIN A LEAST SQUARES SOLUTION.	LMPR1130
C		LMPR1140
	NSING = N	LMPR1150
	DO 10 J = 1, N	LMPR1160
	WA1(J) = QTB(J)	LMPR1170
	IF (R(J,J) .EQ. ZERO .AND. NSING .EQ. N) NSING = J - 1	LMPR1180
	IF (NSING .LT. N) WA1(J) = ZERO	LMPR1190
10	CONTINUE	LMPR1200
	IF (NSING .LT. 1) GO TO 50	LMPR1210
	DO 40 K = 1, NSING	LMPR1220
	J = NSING - K + 1	LMPR1230
	WA1(J) = WA1(J)/R(J,J)	LMPR1240
	TEMP = WA1(J)	LMPR1250
	JM1 = J - 1	LMPR1260
	IF (JM1 .LT. 1) GO TO 30	LMPR1270
	DO 20 I = 1, JM1	LMPR1280
	WA1(I) = WA1(I) - R(I,J)*TEMP	LMPR1290
20	CONTINUE	LMPR1300
30	CONTINUE	LMPR1310
40	CONTINUE	LMPR1320
50	CONTINUE	LMPR1330
	DO 60 J = 1, N	LMPR1340
	L = IPVT(J)	LMPR1350
	X(L) = WA1(J)	LMPR1360
60	CONTINUE	LMPR1370
C		LMPR1380
C	INITIALIZE THE ITERATION COUNTER.	LMPR1390
C	EVALUATE THE FUNCTION AT THE ORIGIN, AND TEST	LMPR1400
C	FOR ACCEPTANCE OF THE GAUSS-NEWTON DIRECTION.	LMPR1410
C		LMPR1420
	ITER = 0	LMPR1430
	DO 70 J = 1, N	LMPR1440
	WA2(J) = DIAG(J)*X(J)	LMPR1450
70	CONTINUE	LMPR1460
	DXNORM = ENORM(N,WA2)	LMPR1470
	FP = DXNORM - DELTA	LMPR1480
	IF (FP .LE. P1*DELTA) GO TO 220	LMPR1490
C		LMPR1500
C	IF THE JACOBIAN IS NOT RANK DEFICIENT, THE NEWTON	LMPR1510
C	STEP PROVIDES A LOWER BOUND, PARL, FOR THE ZERO OF	LMPR1520
C	THE FUNCTION. OTHERWISE SET THIS BOUND TO ZERO.	LMPR1530
C		LMPR1540
	PARL = ZERO	LMPR1550
	IF (NSING .LT. N) GO TO 120	LMPR1560
	DO 80 J = 1, N	LMPR1570
	L = IPVT(J)	LMPR1580
	WA1(J) = DIAG(L)*(WA2(L)/DXNORM)	LMPR1590
80	CONTINUE	LMPR1600
	DO 110 J = 1, N	LMPR1610
	SUM = ZERO	LMPR1620

	JM1 = J - 1	LMPR1630
	IF (JM1 .LT. 1) GO TO 100	LMPR1640
	DO 90 I = 1, JM1	LMPR1650
	SUM = SUM + R(I,J)*WA1(I)	LMPR1660
90	CONTINUE	LMPR1670
100	CONTINUE	LMPR1680
	WA1(J) = (WA1(J) - SUM)/R(J,J)	LMPR1690
110	CONTINUE	LMPR1700
	TEMP = ENORM(N,WA1)	LMPR1710
	PARL = ((FP/DELTA)/TEMP)/TEMP	LMPR1720
120	CONTINUE	LMPR1730
C		LMPR1740
C	CALCULATE AN UPPER BOUND, PARU, FOR THE ZERO OF THE FUNCTION.	LMPR1750
C		LMPR1760
	DO 140 J = 1, N	LMPR1770
	SUM = ZERO	LMPR1780
	DO 130 I = 1, J	LMPR1790
	SUM = SUM + R(I,J)*QTB(I)	LMPR1800
130	CONTINUE	LMPR1810
	L = IPVT(J)	LMPR1820
	WA1(J) = SUM/DIAG(L)	LMPR1830
140	CONTINUE	LMPR1840
	GNORM = ENORM(N,WA1)	LMPR1850
	PARU = GNORM/DELTA	LMPR1860
	IF (PARU .EQ. ZERO) PARU = DWARF/DMIN1(DELTA,P1)	LMPR1870
C		LMPR1880
C	IF THE INPUT PAR LIES OUTSIDE OF THE INTERVAL (PARL,PARU),	LMPR1890
C	SET PAR TO THE CLOSER ENDPOINT.	LMPR1900
C		LMPR1910
	PAR = DMAX1(PAR,PARL)	LMPR1920
	PAR = DMIN1(PAR,PARU)	LMPR1930
	IF (PAR .EQ. ZERO) PAR = GNORM/DXNORM	LMPR1940
C		LMPR1950
C	BEGINNING OF AN ITERATION.	LMPR1960
C		LMPR1970
150	CONTINUE	LMPR1980
	ITER = ITER + 1	LMPR1990
C		LMPR2000
C	EVALUATE THE FUNCTION AT THE CURRENT VALUE OF PAR.	LMPR2010
C		LMPR2020
	IF (PAR .EQ. ZERO) PAR = DMAX1(DWARF,P001*PARU)	LMPR2030
	TEMP = DSQRT(PAR)	LMPR2040
	DO 160 J = 1, N	LMPR2050
	WA1(J) = TEMP*DIAG(J)	LMPR2060
160	CONTINUE	LMPR2070
	CALL QRSOLV(N,R,LDR,IPVT,WA1,QTB,X,SDIAG,WA2)	LMPR2080
	DO 170 J = 1, N	LMPR2090
	WA2(J) = DIAG(J)*X(J)	LMPR2100
170	CONTINUE	LMPR2110
	DXNORM = ENORM(N,WA2)	LMPR2120
	TEMP = FP	LMPR2130
	FP = DXNORM - DELTA	LMPR2140
C		LMPR2150
C	IF THE FUNCTION IS SMALL ENOUGH, ACCEPT THE CURRENT VALUE	LMPR2160

C	OF PAR. ALSO TEST FOR THE EXCEPTIONAL CASES WHERE PARL	LMPR2170
C	IS ZERO OR THE NUMBER OF ITERATIONS HAS REACHED 10.	LMPR2180
C		LMPR2190
	IF (DABS(FP) .LE. P1*DELTA	LMPR2200
*	.OR. PARL .EQ. ZERO .AND. FP .LE. TEMP	LMPR2210
*	.AND. TEMP .LT. ZERO .OR. ITER .EQ. 10) GO TO 220	LMPR2220
C		LMPR2230
C	COMPUTE THE NEWTON CORRECTION.	LMPR2240
C		LMPR2250
	DO 180 J = 1, N	LMPR2260
	L = IPVT(J)	LMPR2270
	WA1(J) = DIAG(L)*(WA2(L)/DXNORM)	LMPR2280
180	CONTINUE	LMPR2290
	DO 210 J = 1, N	LMPR2300
	WA1(J) = WA1(J)/SDIAG(J)	LMPR2310
	TEMP = WA1(J)	LMPR2320
	JP1 = J + 1	LMPR2330
	IF (N .LT. JP1) GO TO 200	LMPR2340
	DO 190 I = JP1, N	LMPR2350
	WA1(I) = WA1(I) - R(I,J)*TEMP	LMPR2360
190	CONTINUE	LMPR2370
200	CONTINUE	LMPR2380
210	CONTINUE	LMPR2390
	TEMP = ENORM(N,WA1)	LMPR2400
	PARC = ((FP/DELTA)/TEMP)/TEMP	LMPR2410
C		LMPR2420
C	DEPENDING ON THE SIGN OF THE FUNCTION, UPDATE PARL OR PARU.	LMPR2430
C		LMPR2440
	IF (FP .GT. ZERO) PARL = DMAX1(PARL,PAR)	LMPR2450
	IF (FP .LT. ZERO) PARU = DMIN1(PARU,PAR)	LMPR2460
C		LMPR2470
C	COMPUTE AN IMPROVED ESTIMATE FOR PAR.	LMPR2480
C		LMPR2490
	PAR = DMAX1(PARL,PAR+PARC)	LMPR2500
C		LMPR2510
C	END OF AN ITERATION.	LMPR2520
C		LMPR2530
	GO TO 150	LMPR2540
220	CONTINUE	LMPR2550
C		LMPR2560
C	TERMINATION.	LMPR2570
C		LMPR2580
	IF (ITER .EQ. 0) PAR = ZERO	LMPR2590
	RETURN	LMPR2600
C		LMPR2610
C	LAST CARD OF SUBROUTINE LMPAR.	LMPR2620
C		LMPR2630
	END	LMPR2640

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SUBROUTINE LMSTR(FCN,M,N,X,FVEC,FJAC,LDFJAC,FTOL,XTOL,GTOL,	LMSR0010
* MAXFEV,DIAG,MODE,FACTOR,NPRINT,INFO,NFEV,NJEV,	LMSR0020
* IPVT,QTF,WA1,WA2,WA3,WA4)	LMSR0030
INTEGER M,N,LDFJAC,MAXFEV,MODE,NPRINT,INFO,NFEV,NJEV	LMSR0040
INTEGER IPVT(N)	LMSR0050
LOGICAL SING	LMSR0060
DOUBLE PRECISION FTOL,XTOL,GTOL,FACTOR	LMSR0070
DOUBLE PRECISION X(N),FVEC(M),FJAC(LDFJAC,N),DIAG(N),QTF(N),	LMSR0080
* WA1(N),WA2(N),WA3(N),WA4(M)	LMSR0090
*****	LMSR0100
	LMSR0110
SUBROUTINE LMSTR	LMSR0120
	LMSR0130
THE PURPOSE OF LMSTR IS TO MINIMIZE THE SUM OF THE SQUARES OF	LMSR0140
M NONLINEAR FUNCTIONS IN N VARIABLES BY A MODIFICATION OF	LMSR0150
THE LEVENBERG-MARQUARDT ALGORITHM WHICH USES MINIMAL STORAGE.	LMSR0160
THE USER MUST PROVIDE A SUBROUTINE WHICH CALCULATES THE	LMSR0170
FUNCTIONS AND THE ROWS OF THE JACOBIAN.	LMSR0180
	LMSR0190
THE SUBROUTINE STATEMENT IS	LMSR0200
	LMSR0210
SUBROUTINE LMSTR(FCN,M,N,X,FVEC,FJAC,LDFJAC,FTOL,XTOL,GTOL,	LMSR0220
MAXFEV,DIAG,MODE,FACTOR,NPRINT,INFO,NFEV,	LMSR0230
NJEV,IPVT,QTF,WA1,WA2,WA3,WA4)	LMSR0240
	LMSR0250
WHERE	LMSR0260
	LMSR0270
FCN IS THE NAME OF THE USER-SUPPLIED SUBROUTINE WHICH	LMSR0280
CALCULATES THE FUNCTIONS AND THE ROWS OF THE JACOBIAN.	LMSR0290
FCN MUST BE DECLARED IN AN EXTERNAL STATEMENT IN THE	LMSR0300
USER CALLING PROGRAM, AND SHOULD BE WRITTEN AS FOLLOWS.	LMSR0310
	LMSR0320
SUBROUTINE FCN(M,N,X,FVEC,FJROW,IFLAG)	LMSR0330
INTEGER M,N,IFLAG	LMSR0340
DOUBLE PRECISION X(N),FVEC(M),FJROW(N)	LMSR0350
-----	LMSR0360
IF IFLAG = 1 CALCULATE THE FUNCTIONS AT X AND	LMSR0370
RETURN THIS VECTOR IN FVEC.	LMSR0380
IF IFLAG = I CALCULATE THE (I-1)-ST ROW OF THE	LMSR0390
JACOBIAN AT X AND RETURN THIS VECTOR IN FJROW.	LMSR0400
-----	LMSR0410
RETURN	LMSR0420
END	LMSR0430
	LMSR0440
THE VALUE OF IFLAG SHOULD NOT BE CHANGED BY FCN UNLESS	LMSR0450
THE USER WANTS TO TERMINATE EXECUTION OF LMSTR.	LMSR0460
IN THIS CASE SET IFLAG TO A NEGATIVE INTEGER.	LMSR0470
	LMSR0480
M IS A POSITIVE INTEGER INPUT VARIABLE SET TO THE NUMBER	LMSR0490
OF FUNCTIONS.	LMSR0500
	LMSR0510
N IS A POSITIVE INTEGER INPUT VARIABLE SET TO THE NUMBER	LMSR0520
OF VARIABLES. N MUST NOT EXCEED M.	LMSR0530
	LMSR0540

X IS AN ARRAY OF LENGTH N. ON INPUT X MUST CONTAIN
AN INITIAL ESTIMATE OF THE SOLUTION VECTOR. ON OUTPUT X
CONTAINS THE FINAL ESTIMATE OF THE SOLUTION VECTOR.

FVEC IS AN OUTPUT ARRAY OF LENGTH M WHICH CONTAINS
THE FUNCTIONS EVALUATED AT THE OUTPUT X.

FJAC IS AN OUTPUT N BY N ARRAY. THE UPPER TRIANGLE OF FJAC
CONTAINS AN UPPER TRIANGULAR MATRIX R SUCH THAT

$$P^T (JAC^T JAC)^T P = R^T R,$$

WHERE P IS A PERMUTATION MATRIX AND JAC IS THE FINAL
CALCULATED JACOBIAN. COLUMN J OF P IS COLUMN IPVT(J)
(SEE BELOW) OF THE IDENTITY MATRIX. THE LOWER TRIANGULAR
PART OF FJAC CONTAINS INFORMATION GENERATED DURING
THE COMPUTATION OF R.

LDFJAC IS A POSITIVE INTEGER INPUT VARIABLE NOT LESS THAN N
WHICH SPECIFIES THE LEADING DIMENSION OF THE ARRAY FJAC.

FTOL IS A NONNEGATIVE INPUT VARIABLE. TERMINATION
OCCURS WHEN BOTH THE ACTUAL AND PREDICTED RELATIVE
REDUCTIONS IN THE SUM OF SQUARES ARE AT MOST FTOL.
THEREFORE, FTOL MEASURES THE RELATIVE ERROR DESIRED
IN THE SUM OF SQUARES.

XTOL IS A NONNEGATIVE INPUT VARIABLE. TERMINATION
OCCURS WHEN THE RELATIVE ERROR BETWEEN TWO CONSECUTIVE
ITERATES IS AT MOST XTOL. THEREFORE, XTOL MEASURES THE
RELATIVE ERROR DESIRED IN THE APPROXIMATE SOLUTION.

GTOL IS A NONNEGATIVE INPUT VARIABLE. TERMINATION
OCCURS WHEN THE COSINE OF THE ANGLE BETWEEN FVEC AND
ANY COLUMN OF THE JACOBIAN IS AT MOST GTOL IN ABSOLUTE
VALUE. THEREFORE, GTOL MEASURES THE ORTHOGONALITY
DESIRED BETWEEN THE FUNCTION VECTOR AND THE COLUMNS
OF THE JACOBIAN.

MAXFEV IS A POSITIVE INTEGER INPUT VARIABLE. TERMINATION
OCCURS WHEN THE NUMBER OF CALLS TO FCN WITH IFLAG = 1
HAS REACHED MAXFEV.

DIAG IS AN ARRAY OF LENGTH N. IF MODE = 1 (SEE
BELOW), DIAG IS INTERNALLY SET. IF MODE = 2, DIAG
MUST CONTAIN POSITIVE ENTRIES THAT SERVE AS
MULTIPLICATIVE SCALE FACTORS FOR THE VARIABLES.

MODE IS AN INTEGER INPUT VARIABLE. IF MODE = 1, THE
VARIABLES WILL BE SCALED INTERNALLY. IF MODE = 2,
THE SCALING IS SPECIFIED BY THE INPUT DIAG. OTHER
VALUES OF MODE ARE EQUIVALENT TO MODE = 1.

LMSR0550
LMSR0560
LMSR0570
LMSR0580
LMSR0590
LMSR0600
LMSR0610
LMSR0620
LMSR0630
LMSR0640
LMSR0650
LMSR0660
LMSR0670
LMSR0680
LMSR0690
LMSR0700
LMSR0710
LMSR0720
LMSR0730
LMSR0740
LMSR0750
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LMSR0770
LMSR0780
LMSR0790
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LMSR0910
LMSR0920
LMSR0930
LMSR0940
LMSR0950
LMSR0960
LMSR0970
LMSR0980
LMSR0990
LMSR1000
LMSR1010
LMSR1020
LMSR1030
LMSR1040
LMSR1050
LMSR1060
LMSR1070
LMSR1080

C	FACTOR IS A POSITIVE INPUT VARIABLE USED IN DETERMINING THE	LMSR1090
C	INITIAL STEP BOUND. THIS BOUND IS SET TO THE PRODUCT OF	LMSR1100
C	FACTOR AND THE EUCLIDEAN NORM OF $\text{DIAG} \cdot X$ IF NONZERO, OR ELSE	LMSR1110
C	TO FACTOR ITSELF. IN MOST CASES FACTOR SHOULD LIE IN THE	LMSR1120
C	INTERVAL (.1,100.). 100. IS A GENERALLY RECOMMENDED VALUE.	LMSR1130
C		LMSR1140
C	NPRINT IS AN INTEGER INPUT VARIABLE THAT ENABLES CONTROLLED	LMSR1150
C	PRINTING OF ITERATES IF IT IS POSITIVE. IN THIS CASE,	LMSR1160
C	FCN IS CALLED WITH IFLAG = 0 AT THE BEGINNING OF THE FIRST	LMSR1170
C	ITERATION AND EVERY NPRINT ITERATIONS THEREAFTER AND	LMSR1180
C	IMMEDIATELY PRIOR TO RETURN, WITH X AND FVEC AVAILABLE	LMSR1190
C	FOR PRINTING. IF NPRINT IS NOT POSITIVE, NO SPECIAL CALLS	LMSR1200
C	OF FCN WITH IFLAG = 0 ARE MADE.	LMSR1210
C		LMSR1220
C	INFO IS AN INTEGER OUTPUT VARIABLE. IF THE USER HAS	LMSR1230
C	TERMINATED EXECUTION, INFO IS SET TO THE (NEGATIVE)	LMSR1240
C	VALUE OF IFLAG. SEE DESCRIPTION OF FCN. OTHERWISE,	LMSR1250
C	INFO IS SET AS FOLLOWS.	LMSR1260
C		LMSR1270
C	INFO = 0 IMPROPER INPUT PARAMETERS.	LMSR1280
C		LMSR1290
C	INFO = 1 BOTH ACTUAL AND PREDICTED RELATIVE REDUCTIONS	LMSR1300
C	IN THE SUM OF SQUARES ARE AT MOST FTOL.	LMSR1310
C		LMSR1320
C	INFO = 2 RELATIVE ERROR BETWEEN TWO CONSECUTIVE ITERATES	LMSR1330
C	IS AT MOST XTOL.	LMSR1340
C		LMSR1350
C	INFO = 3 CONDITIONS FOR INFO = 1 AND INFO = 2 BOTH HOLD.	LMSR1360
C		LMSR1370
C	INFO = 4 THE COSINE OF THE ANGLE BETWEEN FVEC AND ANY	LMSR1380
C	COLUMN OF THE JACOBIAN IS AT MOST GTOL IN	LMSR1390
C	ABSOLUTE VALUE.	LMSR1400
C		LMSR1410
C	INFO = 5 NUMBER OF CALLS TO FCN WITH IFLAG = 1 HAS	LMSR1420
C	REACHED MAXFEV.	LMSR1430
C		LMSR1440
C	INFO = 6 FTOL IS TOO SMALL. NO FURTHER REDUCTION IN	LMSR1450
C	THE SUM OF SQUARES IS POSSIBLE.	LMSR1460
C		LMSR1470
C	INFO = 7 XTOL IS TOO SMALL. NO FURTHER IMPROVEMENT IN	LMSR1480
C	THE APPROXIMATE SOLUTION X IS POSSIBLE.	LMSR1490
C		LMSR1500
C	INFO = 8 GTOL IS TOO SMALL. FVEC IS ORTHOGONAL TO THE	LMSR1510
C	COLUMNS OF THE JACOBIAN TO MACHINE PRECISION.	LMSR1520
C		LMSR1530
C	NFEV IS AN INTEGER OUTPUT VARIABLE SET TO THE NUMBER OF	LMSR1540
C	CALLS TO FCN WITH IFLAG = 1.	LMSR1550
C		LMSR1560
C	NJEV IS AN INTEGER OUTPUT VARIABLE SET TO THE NUMBER OF	LMSR1570
C	CALLS TO FCN WITH IFLAG = 2.	LMSR1580
C		LMSR1590
C	IPVT IS AN INTEGER OUTPUT ARRAY OF LENGTH N. IPVT	LMSR1600
C	DEFINES A PERMUTATION MATRIX P SUCH THAT $\text{JAC} \cdot P = Q \cdot R$,	LMSR1610
C	WHERE JAC IS THE FINAL CALCULATED JACOBIAN, Q IS	LMSR1620

C	ORTHOGONAL (NOT STORED), AND R IS UPPER TRIANGULAR.	LMSR1630
C	COLUMN J OF P IS COLUMN IPVT(J) OF THE IDENTITY MATRIX.	LMSR1640
C		LMSR1650
C	QTF IS AN OUTPUT ARRAY OF LENGTH N WHICH CONTAINS	LMSR1660
C	THE FIRST N ELEMENTS OF THE VECTOR (Q TRANSPOSE)*FVEC.	LMSR1670
C		LMSR1680
C	WA1, WA2, AND WA3 ARE WORK ARRAYS OF LENGTH N.	LMSR1690
C		LMSR1700
C	WA4 IS A WORK ARRAY OF LENGTH M.	LMSR1710
C		LMSR1720
C	SUBPROGRAMS CALLED	LMSR1730
C		LMSR1740
C	USER-SUPPLIED FCN	LMSR1750
C		LMSR1760
C	MINPACK-SUPPLIED ... DPMPAR,ENORM,LMPAR,QRFAC,RWUPDT	LMSR1770
C		LMSR1780
C	FORTTRAN-SUPPLIED ... DABS,DMAX1,DMIN1,DSQRT,MOD	LMSR1790
C		LMSR1800
C	ARGONNE NATIONAL LABORATORY. MINPACK PROJECT. MARCH 1980.	LMSR1810
C	BURTON S. GARBOW, DUDLEY V. GOETSCHER, KENNETH E. HILLSTROM,	LMSR1820
C	JORGE J. MORE	LMSR1830
C		LMSR1840
C	*****	LMSR1850
	INTEGER I,IFLAG,ITER,J,L	LMSR1860
	DOUBLE PRECISION ACTRED,DELTA,DIRDER,EPSMCH,FNORM,GNORM,	LMSR1870
*	ONE,PAR,PNORM,PRERED,P1,P5,P25,P75,P0001,RATIO,	LMSR1880
*	SUM,TEMP,TEMP1,TEMP2,XNORM,ZERO	LMSR1890
	DOUBLE PRECISION DPMPAR,ENORM	LMSR1900
	DATA ONE,P1,P5,P25,P75,P0001,ZERO	LMSR1910
*	/1.0D0,1.0D-1,5.0D-1,2.5D-1,7.5D-1,1.0D-4,0.0D0/	LMSR1920
C		LMSR1930
C	EPSMCH IS THE MACHINE PRECISION.	LMSR1940
C		LMSR1950
	EPSMCH = DPMPAR(1)	LMSR1960
C		LMSR1970
	INFO = 0	LMSR1980
	IFLAG = 0	LMSR1990
	NFEV = 0	LMSR2000
	NJEV = 0	LMSR2010
C		LMSR2020
C	CHECK THE INPUT PARAMETERS FOR ERRORS.	LMSR2030
C		LMSR2040
	IF (N .LE. 0 .OR. M .LT. N .OR. LDFJAC .LT. N	LMSR2050
*	.OR. FTOL .LT. ZERO .OR. XTOL .LT. ZERO .OR. GTOL .LT. ZERO	LMSR2060
*	.OR. MAXFEV .LE. 0 .OR. FACTOR .LE. ZERO) GO TO 340	LMSR2070
	IF (MODE .NE. 2) GO TO 20	LMSR2080
	DO 10 J = 1, N	LMSR2090
	IF (DIAG(J) .LE. ZERO) GO TO 340	LMSR2100
10	CONTINUE	LMSR2110
20	CONTINUE	LMSR2120
C		LMSR2130
C	EVALUATE THE FUNCTION AT THE STARTING POINT	LMSR2140
C	AND CALCULATE ITS NORM.	LMSR2150
C		LMSR2160

	IFLAG = 1	LMSR2170
	CALL FCN(M,N,X,FVEC,WA3,IFLAG)	LMSR2180
	NFEV = 1	LMSR2190
	IF (IFLAG .LT. 0) GO TO 340	LMSR2200
	FNORM = ENORM(M,FVEC)	LMSR2210
C		LMSR2220
C	INITIALIZE LEVENBERG-MARQUARDT PARAMETER AND ITERATION COUNTER.	LMSR2230
C		LMSR2240
	PAR = ZERO	LMSR2250
	ITER = 1	LMSR2260
C		LMSR2270
C	BEGINNING OF THE OUTER LOOP.	LMSR2280
C		LMSR2290
	30 CONTINUE	LMSR2300
C		LMSR2310
C	IF REQUESTED, CALL FCN TO ENABLE PRINTING OF ITERATES.	LMSR2320
C		LMSR2330
	IF (NPRINT .LE. 0) GO TO 40	LMSR2340
	IFLAG = 0	LMSR2350
	IF (MOD(ITER-1,NPRINT) .EQ. 0) CALL FCN(M,N,X,FVEC,WA3,IFLAG)	LMSR2360
	IF (IFLAG .LT. 0) GO TO 340	LMSR2370
	40 CONTINUE	LMSR2380
C		LMSR2390
C	COMPUTE THE QR FACTORIZATION OF THE JACOBIAN MATRIX	LMSR2400
C	CALCULATED ONE ROW AT A TIME, WHILE SIMULTANEOUSLY	LMSR2410
C	FORMING (Q TRANSPOSE)*FVEC AND STORING THE FIRST	LMSR2420
C	N COMPONENTS IN QTF.	LMSR2430
C		LMSR2440
	DO 60 J = 1, N	LMSR2450
	QTF(J) = ZERO	LMSR2460
	DO 50 I = 1, N	LMSR2470
	FJAC(I,J) = ZERO	LMSR2480
50	CONTINUE	LMSR2490
60	CONTINUE	LMSR2500
	IFLAG = 2	LMSR2510
	DO 70 I = 1, M	LMSR2520
	CALL FCN(M,N,X,FVEC,WA3,IFLAG)	LMSR2530
	IF (IFLAG .LT. 0) GO TO 340	LMSR2540
	TEMP = FVEC(I)	LMSR2550
	CALL RWUPDT(N,FJAC,LDFJAC,WA3,QTF,TEMP,WA1,WA2)	LMSR2560
	IFLAG = IFLAG + 1	LMSR2570
70	CONTINUE	LMSR2580
	NJEV = NJEV + 1	LMSR2590
C		LMSR2600
C	IF THE JACOBIAN IS RANK DEFICIENT, CALL QRFAC TO	LMSR2610
C	REORDER ITS COLUMNS AND UPDATE THE COMPONENTS OF QTF.	LMSR2620
C		LMSR2630
	SING = .FALSE.	LMSR2640
	DO 80 J = 1, N	LMSR2650
	IF (FJAC(J,J) .EQ. ZERO) SING = .TRUE.	LMSR2660
	IPVT(J) = J	LMSR2670
	WA2(J) = ENORM(J,FJAC(1,J))	LMSR2680
80	CONTINUE	LMSR2690
	IF (.NOT.SING) GO TO 130	LMSR2700

CALL QRFAC(N,N,FJAC,LDFJAC,.TRUE.,IPVT,N,WA1,WA2,WA3)	LMSR2710
DO 120 J = 1, N	LMSR2720
IF (FJAC(J,J) .EQ. ZERO) GO TO 110	LMSR2730
SUM = ZERO	LMSR2740
DO 90 I = J, N	LMSR2750
SUM = SUM + FJAC(I,J)*QTF(I)	LMSR2760
90 CONTINUE	LMSR2770
TEMP = -SUM/FJAC(J,J)	LMSR2780
DO 100 I = J, N	LMSR2790
QTF(I) = QTF(I) + FJAC(I,J)*TEMP	LMSR2800
100 CONTINUE	LMSR2810
110 CONTINUE	LMSR2820
FJAC(J,J) = WA1(J)	LMSR2830
120 CONTINUE	LMSR2840
130 CONTINUE	LMSR2850
C	LMSR2860
C ON THE FIRST ITERATION AND IF MODE IS 1, SCALE ACCORDING	LMSR2870
C TO THE NORMS OF THE COLUMNS OF THE INITIAL JACOBIAN.	LMSR2880
C	LMSR2890
IF (ITER .NE. 1) GO TO 170	LMSR2900
IF (MODE .EQ. 2) GO TO 150	LMSR2910
DO 140 J = 1, N	LMSR2920
DIAG(J) = WA2(J)	LMSR2930
IF (WA2(J) .EQ. ZERO) DIAG(J) = ONE	LMSR2940
140 CONTINUE	LMSR2950
150 CONTINUE	LMSR2960
C	LMSR2970
C ON THE FIRST ITERATION, CALCULATE THE NORM OF THE SCALED X	LMSR2980
C AND INITIALIZE THE STEP BOUND DELTA.	LMSR2990
C	LMSR3000
DO 160 J = 1, N	LMSR3010
WA3(J) = DIAG(J)*X(J)	LMSR3020
160 CONTINUE	LMSR3030
XNORM = ENORM(N,WA3)	LMSR3040
DELTA = FACTOR*XNORM	LMSR3050
IF (DELTA .EQ. ZERO) DELTA = FACTOR	LMSR3060
170 CONTINUE	LMSR3070
C	LMSR3080
C COMPUTE THE NORM OF THE SCALED GRADIENT.	LMSR3090
C	LMSR3100
GNORM = ZERO	LMSR3110
IF (FNORM .EQ. ZERO) GO TO 210	LMSR3120
DO 200 J = 1, N	LMSR3130
L = IPVT(J)	LMSR3140
IF (WA2(L) .EQ. ZERO) GO TO 190	LMSR3150
SUM = ZERO	LMSR3160
DO 180 I = 1, J	LMSR3170
SUM = SUM + FJAC(I,J)*(QTF(I)/FNORM)	LMSR3180
180 CONTINUE	LMSR3190
GNORM = DMAX1(GNORM,DABS(SUM/WA2(L)))	LMSR3200
190 CONTINUE	LMSR3210
200 CONTINUE	LMSR3220
210 CONTINUE	LMSR3230
C	LMSR3240

C	TEST FOR CONVERGENCE OF THE GRADIENT NORM.	LMSR3250
C		LMSR3260
	IF (GNORM .LE. GTOL) INFO = 4	LMSR3270
	IF (INFO .NE. 0) GO TO 340	LMSR3280
C		LMSR3290
C	RESCALE IF NECESSARY.	LMSR3300
C		LMSR3310
	IF (MODE .EQ. 2) GO TO 230	LMSR3320
	DO 220 J = 1, N	LMSR3330
	DIAG(J) = DMAX1(DIAG(J),WA2(J))	LMSR3340
220	CONTINUE	LMSR3350
230	CONTINUE	LMSR3360
C		LMSR3370
C	BEGINNING OF THE INNER LOOP.	LMSR3380
C		LMSR3390
240	CONTINUE	LMSR3400
C		LMSR3410
C	DETERMINE THE LEVENBERG-MARQUARDT PARAMETER.	LMSR3420
C		LMSR3430
	CALL LMPAR(N,FJAC,LDFJAC,IPVT,DIAG,QTF,DELTA,PAR,WA1,WA2,	LMSR3440
	* WA3,WA4)	LMSR3450
C		LMSR3460
C	STORE THE DIRECTION P AND X + P. CALCULATE THE NORM OF P.	LMSR3470
C		LMSR3480
	DO 250 J = 1, N	LMSR3490
	WA1(J) = -WA1(J)	LMSR3500
	WA2(J) = X(J) + WA1(J)	LMSR3510
	WA3(J) = DIAG(J)*WA1(J)	LMSR3520
250	CONTINUE	LMSR3530
	PNORM = ENORM(N,WA3)	LMSR3540
C		LMSR3550
C	ON THE FIRST ITERATION, ADJUST THE INITIAL STEP BOUND.	LMSR3560
C		LMSR3570
	IF (ITER .EQ. 1) DELTA = DMIN1(DELTA,PNORM)	LMSR3580
C		LMSR3590
C	EVALUATE THE FUNCTION AT X + P AND CALCULATE ITS NORM.	LMSR3600
C		LMSR3610
	IFLAG = 1	LMSR3620
	CALL FCN(M,N,WA2,WA4,WA3,IFLAG)	LMSR3630
	NFEV = NFEV + 1	LMSR3640
	IF (IFLAG .LT. 0) GO TO 340	LMSR3650
	FNORM1 = ENORM(M,WA4)	LMSR3660
C		LMSR3670
C	COMPUTE THE SCALED ACTUAL REDUCTION.	LMSR3680
C		LMSR3690
	ACTRED = -ONE	LMSR3700
	IF (P1*FNORM1 .LT. FNORM) ACTRED = ONE - (FNORM1/FNORM)**2	LMSR3710
C		LMSR3720
C	COMPUTE THE SCALED PREDICTED REDUCTION AND	LMSR3730
C	THE SCALED DIRECTIONAL DERIVATIVE.	LMSR3740
C		LMSR3750
	DO 270 J = 1, N	LMSR3760
	WA3(J) = ZERO	LMSR3770
	L = IPVT(J)	LMSR3780

	TEMP = WA1(L)	LMSR3790
	DO 260 I = 1, J	LMSR3800
	WA3(I) = WA3(I) + FJAC(I,J)*TEMP	LMSR3810
260	CONTINUE	LMSR3820
270	CONTINUE	LMSR3830
	TEMP1 = ENORM(N,WA3)/FNORM	LMSR3840
	TEMP2 = (DSQRT(PAR)*PNORM)/FNORM	LMSR3850
	PRERED = TEMP1**2 + TEMP2**2/P5	LMSR3860
	DIRDER = -(TEMP1**2 + TEMP2**2)	LMSR3870
C		LMSR3880
C	COMPUTE THE RATIO OF THE ACTUAL TO THE PREDICTED	LMSR3890
C	REDUCTION.	LMSR3900
C		LMSR3910
	RATIO = ZERO	LMSR3920
	IF (PRERED .NE. ZERO) RATIO = ACTRED/PRERED	LMSR3930
C		LMSR3940
C	UPDATE THE STEP BOUND.	LMSR3950
C		LMSR3960
	IF (RATIO .GT. P25) GO TO 280	LMSR3970
	IF (ACTRED .GE. ZERO) TEMP = P5	LMSR3980
	IF (ACTRED .LT. ZERO)	LMSR3990
*	TEMP = P5*DIRDER/(DIRDER + P5*ACTRED)	LMSR4000
	IF (P1*FNORM1 .GE. FNORM .OR. TEMP .LT. P1) TEMP = P1	LMSR4010
	DELTA = TEMP*DMIN1(DELTA,PNORM/P1)	LMSR4020
	PAR = PAR/TEMP	LMSR4030
	GO TO 300	LMSR4040
280	CONTINUE	LMSR4050
	IF (PAR .NE. ZERO .AND. RATIO .LT. P75) GO TO 290	LMSR4060
	DELTA = PNORM/P5	LMSR4070
	PAR = P5*PAR	LMSR4080
290	CONTINUE	LMSR4090
300	CONTINUE	LMSR4100
C		LMSR4110
C	TEST FOR SUCCESSFUL ITERATION.	LMSR4120
C		LMSR4130
	IF (RATIO .LT. P0001) GO TO 330	LMSR4140
C		LMSR4150
C	SUCCESSFUL ITERATION. UPDATE X, FVEC, AND THEIR NORMS.	LMSR4160
C		LMSR4170
	DO 310 J = 1, N	LMSR4180
	X(J) = WA2(J)	LMSR4190
	WA2(J) = DIAG(J)*X(J)	LMSR4200
310	CONTINUE	LMSR4210
	DO 320 I = 1, M	LMSR4220
	FVEC(I) = WA4(I)	LMSR4230
320	CONTINUE	LMSR4240
	XNORM = ENORM(N,WA2)	LMSR4250
	FNORM = FNORM1	LMSR4260
	ITER = ITER + 1	LMSR4270
330	CONTINUE	LMSR4280
C		LMSR4290
C	TESTS FOR CONVERGENCE.	LMSR4300
C		LMSR4310
	IF (DABS(ACTRED) .LE. FTOL .AND. PRERED .LE. FTOL	LMSR4320

*	.AND. P5*RATIO .LE. ONE) INFO = 1	LMSR4330
	IF (DELTA .LE. XTOL*XNORM) INFO = 2	LMSR4340
	IF (DABS(ACTRED) .LE. FTOL .AND. PRERED .LE. FTOL	LMSR4350
*	.AND. P5*RATIO .LE. ONE .AND. INFO .EQ. 2) INFO = 3	LMSR4360
	IF (INFO .NE. 0) GO TO 340	LMSR4370
C		LMSR4380
C	TESTS FOR TERMINATION AND STRINGENT TOLERANCES.	LMSR4390
C		LMSR4400
	IF (NFEV .GE. MAXFEV) INFO = 5	LMSR4410
	IF (DABS(ACTRED) .LE. EPSMCH .AND. PRERED .LE. EPSMCH	LMSR4420
*	.AND. P5*RATIO .LE. ONE) INFO = 6	LMSR4430
	IF (DELTA .LE. EPSMCH*XNORM) INFO = 7	LMSR4440
	IF (GNORM .LE. EPSMCH) INFO = 8	LMSR4450
	IF (INFO .NE. 0) GO TO 340	LMSR4460
C		LMSR4470
C	END OF THE INNER LOOP. REPEAT IF ITERATION UNSUCCESSFUL.	LMSR4480
C		LMSR4490
	IF (RATIO .LT. P0001) GO TO 240	LMSR4500
C		LMSR4510
C	END OF THE OUTER LOOP.	LMSR4520
C		LMSR4530
	GO TO 30	LMSR4540
	340 CONTINUE	LMSR4550
C		LMSR4560
C	TERMINATION, EITHER NORMAL OR USER IMPOSED.	LMSR4570
C		LMSR4580
	IF (IFLAG .LT. 0) INFO = IFLAG	LMSR4590
	IFLAG = 0	LMSR4600
	IF (NPRINT .GT. 0) CALL FCN(M,N,X,FVEC,WA3,IFLAG)	LMSR4610
	RETURN	LMSR4620
C		LMSR4630
C	LAST CARD OF SUBROUTINE LMSTR.	LMSR4640
C		LMSR4650
	END	LMSR4660

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SUBROUTINE LMSTR1(FCN,M,N,X,FVEC,FJAC,LDFJAC,TOL,INFO,IPVT,WA,
*                LWA)
INTEGER M,N,LDFJAC,INFO,LWA
INTEGER IPVT(N)
DOUBLE PRECISION TOL
DOUBLE PRECISION X(N),FVEC(M),FJAC(LDFJAC,N),WA(LWA)
EXTERNAL FCN
*****

```

SUBROUTINE LMSTR1

THE PURPOSE OF LMSTR1 IS TO MINIMIZE THE SUM OF THE SQUARES OF M NONLINEAR FUNCTIONS IN N VARIABLES BY A MODIFICATION OF THE LEVENBERG-MARQUARDT ALGORITHM WHICH USES MINIMAL STORAGE. THIS IS DONE BY USING THE MORE GENERAL LEAST-SQUARES SOLVER LMSTR. THE USER MUST PROVIDE A SUBROUTINE WHICH CALCULATES THE FUNCTIONS AND THE ROWS OF THE JACOBIAN.

THE SUBROUTINE STATEMENT IS

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SUBROUTINE LMSTR1(FCN,M,N,X,FVEC,FJAC,LDFJAC,TOL,INFO,
                  IPVT,WA,LWA)

```

WHERE

FCN IS THE NAME OF THE USER-SUPPLIED SUBROUTINE WHICH CALCULATES THE FUNCTIONS AND THE ROWS OF THE JACOBIAN. FCN MUST BE DECLARED IN AN EXTERNAL STATEMENT IN THE USER CALLING PROGRAM, AND SHOULD BE WRITTEN AS FOLLOWS.

```

SUBROUTINE FCN(M,N,X,FVEC,FJROW,IFLAG)
INTEGER M,N,IFLAG
DOUBLE PRECISION X(N),FVEC(M),FJROW(N)

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IF IFLAG = 1 CALCULATE THE FUNCTIONS AT X AND
RETURN THIS VECTOR IN FVEC.
IF IFLAG = I CALCULATE THE (I-1)-ST ROW OF THE
JACOBIAN AT X AND RETURN THIS VECTOR IN FJROW.

```

RETURN
END

THE VALUE OF IFLAG SHOULD NOT BE CHANGED BY FCN UNLESS
THE USER WANTS TO TERMINATE EXECUTION OF LMSTR1.
IN THIS CASE SET IFLAG TO A NEGATIVE INTEGER.

M IS A POSITIVE INTEGER INPUT VARIABLE SET TO THE NUMBER
OF FUNCTIONS.

N IS A POSITIVE INTEGER INPUT VARIABLE SET TO THE NUMBER
OF VARIABLES. N MUST NOT EXCEED M.

X IS AN ARRAY OF LENGTH N. ON INPUT X MUST CONTAIN
AN INITIAL ESTIMATE OF THE SOLUTION VECTOR. ON OUTPUT X

LMS10010
LMS10020
LMS10030
LMS10040
LMS10050
LMS10060
LMS10070
LMS10080
LMS10090
LMS10100
LMS10110
LMS10120
LMS10130
LMS10140
LMS10150
LMS10160
LMS10170
LMS10180
LMS10190
LMS10200
LMS10210
LMS10220
LMS10230
LMS10240
LMS10250
LMS10260
LMS10270
LMS10280
LMS10290
LMS10300
LMS10310
LMS10320
LMS10330
LMS10340
LMS10350
LMS10360
LMS10370
LMS10380
LMS10390
LMS10400
LMS10410
LMS10420
LMS10430
LMS10440
LMS10450
LMS10460
LMS10470
LMS10480
LMS10490
LMS10500
LMS10510
LMS10520
LMS10530
LMS10540

C	CONTAINS THE FINAL ESTIMATE OF THE SOLUTION VECTOR.	LMS10550
C		LMS10560
C	FVEC IS AN OUTPUT ARRAY OF LENGTH M WHICH CONTAINS	LMS10570
C	THE FUNCTIONS EVALUATED AT THE OUTPUT X.	LMS10580
C		LMS10590
C	FJAC IS AN OUTPUT N BY N ARRAY. THE UPPER TRIANGLE OF FJAC	LMS10600
C	CONTAINS AN UPPER TRIANGULAR MATRIX R SUCH THAT	LMS10610
C		LMS10620
C	$P^T (JAC^T * JAC) * P = R^T * R,$	LMS10630
C		LMS10640
C		LMS10650
C	WHERE P IS A PERMUTATION MATRIX AND JAC IS THE FINAL	LMS10660
C	CALCULATED JACOBIAN. COLUMN J OF P IS COLUMN IPV T(J)	LMS10670
C	(SEE BELOW) OF THE IDENTITY MATRIX. THE LOWER TRIANGULAR	LMS10680
C	PART OF FJAC CONTAINS INFORMATION GENERATED DURING	LMS10690
C	THE COMPUTATION OF R.	LMS10700
C		LMS10710
C	LDFJAC IS A POSITIVE INTEGER INPUT VARIABLE NOT LESS THAN N	LMS10720
C	WHICH SPECIFIES THE LEADING DIMENSION OF THE ARRAY FJAC.	LMS10730
C		LMS10740
C	TOL IS A NONNEGATIVE INPUT VARIABLE. TERMINATION OCCURS	LMS10750
C	WHEN THE ALGORITHM ESTIMATES EITHER THAT THE RELATIVE	LMS10760
C	ERROR IN THE SUM OF SQUARES IS AT MOST TOL OR THAT	LMS10770
C	THE RELATIVE ERROR BETWEEN X AND THE SOLUTION IS AT	LMS10780
C	MOST TOL.	LMS10790
C		LMS10800
C	INFO IS AN INTEGER OUTPUT VARIABLE. IF THE USER HAS	LMS10810
C	TERMINATED EXECUTION, INFO IS SET TO THE (NEGATIVE)	LMS10820
C	VALUE OF IFLAG. SEE DESCRIPTION OF FCN. OTHERWISE,	LMS10830
C	INFO IS SET AS FOLLOWS.	LMS10840
C		LMS10850
C	INFO = 0 IMPROPER INPUT PARAMETERS.	LMS10860
C		LMS10870
C	INFO = 1 ALGORITHM ESTIMATES THAT THE RELATIVE ERROR	LMS10880
C	IN THE SUM OF SQUARES IS AT MOST TOL.	LMS10890
C		LMS10900
C	INFO = 2 ALGORITHM ESTIMATES THAT THE RELATIVE ERROR	LMS10910
C	BETWEEN X AND THE SOLUTION IS AT MOST TOL.	LMS10920
C		LMS10930
C	INFO = 3 CONDITIONS FOR INFO = 1 AND INFO = 2 BOTH HOLD.	LMS10940
C		LMS10950
C	INFO = 4 FVEC IS ORTHOGONAL TO THE COLUMNS OF THE	LMS10960
C	JACOBIAN TO MACHINE PRECISION.	LMS10970
C		LMS10980
C	INFO = 5 NUMBER OF CALLS TO FCN WITH IFLAG = 1 HAS	LMS10990
C	REACHED 100*(N+1).	LMS11000
C		LMS11010
C	INFO = 6 TOL IS TOO SMALL. NO FURTHER REDUCTION IN	LMS11020
C	THE SUM OF SQUARES IS POSSIBLE.	LMS11030
C		LMS11040
C	INFO = 7 TOL IS TOO SMALL. NO FURTHER IMPROVEMENT IN	LMS11050
C	THE APPROXIMATE SOLUTION X IS POSSIBLE.	LMS11060
C		LMS11070
C	IPVT IS AN INTEGER OUTPUT ARRAY OF LENGTH N. IPV T	LMS11080

```

C      DEFINES A PERMUTATION MATRIX P SUCH THAT JAC*P = Q*R, LMS11090
C      WHERE JAC IS THE FINAL CALCULATED JACOBIAN, Q IS LMS11100
C      ORTHOGONAL (NOT STORED), AND R IS UPPER TRIANGULAR. LMS11110
C      COLUMN J OF P IS COLUMN IPVT(J) OF THE IDENTITY MATRIX. LMS11120
C LMS11130
C      WA IS A WORK ARRAY OF LENGTH LWA. LMS11140
C LMS11150
C      LWA IS A POSITIVE INTEGER INPUT VARIABLE NOT LESS THAN 5*N+M. LMS11160
C LMS11170
C SUBPROGRAMS CALLED LMS11180
C LMS11190
C      USER-SUPPLIED ..... FCN LMS11200
C LMS11210
C      MINPACK-SUPPLIED ... LMSTR LMS11220
C LMS11230
C ARGONNE NATIONAL LABORATORY. MINPACK PROJECT. MARCH 1980. LMS11240
C BURTON S. GARBOW, DUDLEY V. GOETSCHER, KENNETH E. HILLSTROM, LMS11250
C JORGE J. MORE LMS11260
C LMS11270
C ***** LMS11280
C INTEGER MAXFEV,MODE,NFEV,NJEV,NPRINT LMS11290
C DOUBLE PRECISION FACTOR,FTOL,GTOL,XTOL,ZERO LMS11300
C DATA FACTOR,ZERO /1.0D2,0.0D0/ LMS11310
C INFO = 0 LMS11320
C LMS11330
C CHECK THE INPUT PARAMETERS FOR ERRORS. LMS11340
C LMS11350
C IF (N .LE. 0 .OR. M .LT. N .OR. LDFJAC .LT. N .OR. TOL .LT. ZERO LMS11360
C * .OR. LWA .LT. 5*N + M) GO TO 10 LMS11370
C LMS11380
C CALL LMSTR. LMS11390
C LMS11400
C MAXFEV = 100*(N + 1) LMS11410
C FTOL = TOL LMS11420
C XTOL = TOL LMS11430
C GTOL = ZERO LMS11440
C MODE = 1 LMS11450
C NPRINT = 0 LMS11460
C CALL LMSTR(FCN,M,N,X,FVEC,FJAC,LDFJAC,FTOL,XTOL,GTOL,MAXFEV, LMS11470
C * WA(1),MODE,FACTOR,NPRINT,INFO,NFEV,NJEV,IPVT,WA(N+1), LMS11480
C * WA(2*N+1),WA(3*N+1),WA(4*N+1),WA(5*N+1)) LMS11490
C IF (INFO .EQ. 8) INFO = 4 LMS11500
C 10 CONTINUE LMS11510
C RETURN LMS11520
C LMS11530
C LAST CARD OF SUBROUTINE LMSTR1. LMS11540
C LMS11550
C END LMS11560

```

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```

SUBROUTINE QFORM(M,N,Q,LDQ,WA)
INTEGER M,N,LDQ
DOUBLE PRECISION Q(LDQ,M),WA(M)
*****

```

```

SUBROUTINE QFORM

```

```

THIS SUBROUTINE PROCEEDS FROM THE COMPUTED QR FACTORIZATION OF
AN M BY N MATRIX A TO ACCUMULATE THE M BY M ORTHOGONAL MATRIX
Q FROM ITS FACTORED FORM.

```

```

THE SUBROUTINE STATEMENT IS

```

```

SUBROUTINE QFORM(M,N,Q,LDQ,WA)

```

```

WHERE

```

```

M IS A POSITIVE INTEGER INPUT VARIABLE SET TO THE NUMBER
OF ROWS OF A AND THE ORDER OF Q.

```

```

N IS A POSITIVE INTEGER INPUT VARIABLE SET TO THE NUMBER
OF COLUMNS OF A.

```

```

Q IS AN M BY M ARRAY. ON INPUT THE FULL LOWER TRAPEZOID IN
THE FIRST MIN(M,N) COLUMNS OF Q CONTAINS THE FACTORED FORM.
ON OUTPUT Q HAS BEEN ACCUMULATED INTO A SQUARE MATRIX.

```

```

LDQ IS A POSITIVE INTEGER INPUT VARIABLE NOT LESS THAN M
WHICH SPECIFIES THE LEADING DIMENSION OF THE ARRAY Q.

```

```

WA IS A WORK ARRAY OF LENGTH M.

```

```

SUBPROGRAMS CALLED

```

```

FORTRAN-SUPPLIED ... MINO

```

```

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```

```

*****

```

```

INTEGER I,J,JM1,K,L,MINMN,NP1
DOUBLE PRECISION ONE,SUM,TEMP,ZERO
DATA ONE,ZERO /1.0D0,0.0D0/

```

```

ZERO OUT UPPER TRIANGLE OF Q IN THE FIRST MIN(M,N) COLUMNS.

```

```

MINMN = MINO(M,N)

```

```

IF (MINMN .LT. 2) GO TO 30

```

```

DO 20 J = 2, MINMN

```

```

JM1 = J - 1

```

```

DO 10 I = 1, JM1

```

```

Q(I,J) = ZERO

```

```

10 CONTINUE

```

```

20 CONTINUE

```

```

QFRM0010
QFRM0020
QFRM0030
QFRM0040
QFRM0050
QFRM0060
QFRM0070
QFRM0080
QFRM0090
QFRM0100
QFRM0110
QFRM0120
QFRM0130
QFRM0140
QFRM0150
QFRM0160
QFRM0170
QFRM0180
QFRM0190
QFRM0200
QFRM0210
QFRM0220
QFRM0230
QFRM0240
QFRM0250
QFRM0260
QFRM0270
QFRM0280
QFRM0290
QFRM0300
QFRM0310
QFRM0320
QFRM0330
QFRM0340
QFRM0350
QFRM0360
QFRM0370
QFRM0380
QFRM0390
QFRM0400
QFRM0410
QFRM0420
QFRM0430
QFRM0440
QFRM0450
QFRM0460
QFRM0470
QFRM0480
QFRM0490
QFRM0500
QFRM0510
QFRM0520
QFRM0530
QFRM0540

```

30	CONTINUE	QFRM0550
C		QFRM0560
C	INITIALIZE REMAINING COLUMNS TO THOSE OF THE IDENTITY MATRIX.	QFRM0570
C		QFRM0580
	NP1 = N + 1	QFRM0590
	IF (M .LT. NP1) GO TO 60	QFRM0600
	DO 50 J = NP1, M	QFRM0610
	DO 40 I = 1, M	QFRM0620
	Q(I,J) = ZERO	QFRM0630
40	CONTINUE	QFRM0640
	Q(J,J) = ONE	QFRM0650
50	CONTINUE	QFRM0660
60	CONTINUE	QFRM0670
C		QFRM0680
C	ACCUMULATE Q FROM ITS FACTORED FORM.	QFRM0690
C		QFRM0700
	DO 120 L = 1, MINMN	QFRM0710
	K = MINMN - L + 1	QFRM0720
	DO 70 I = K, M	QFRM0730
	WA(I) = Q(I,K)	QFRM0740
	Q(I,K) = ZERO	QFRM0750
70	CONTINUE	QFRM0760
	Q(K,K) = ONE	QFRM0770
	IF (WA(K) .EQ. ZERO) GO TO 110	QFRM0780
	DO 100 J = K, M	QFRM0790
	SUM = ZERO	QFRM0800
	DO 80 I = K, M	QFRM0810
	SUM = SUM + Q(I,J)*WA(I)	QFRM0820
80	CONTINUE	QFRM0830
	TEMP = SUM/WA(K)	QFRM0840
	DO 90 I = K, M	QFRM0850
	Q(I,J) = Q(I,J) - TEMP*WA(I)	QFRM0860
90	CONTINUE	QFRM0870
100	CONTINUE	QFRM0880
110	CONTINUE	QFRM0890
120	CONTINUE	QFRM0900
	RETURN	QFRM0910
C		QFRM0920
C	LAST CARD OF SUBROUTINE QFORM.	QFRM0930
C		QFRM0940
	END	QFRM0950

```

SUBROUTINE QRFAC(M,N,A,LDA,PIVOT,IPVT,LIPVT,RDIAG,ACNORM,WA)
INTEGER M,N,LDA,LIPVT
INTEGER IPVT(LIPVT)
LOGICAL PIVOT
DOUBLE PRECISION A(LDA,N),RDIAG(N),ACNORM(N),WA(N)
*****

```

```

SUBROUTINE QRFAC

```

```

THIS SUBROUTINE USES HOUSEHOLDER TRANSFORMATIONS WITH COLUMN
PIVOTING (OPTIONAL) TO COMPUTE A QR FACTORIZATION OF THE
M BY N MATRIX A. THAT IS, QRFAC DETERMINES AN ORTHOGONAL
MATRIX Q, A PERMUTATION MATRIX P, AND AN UPPER TRAPEZOIDAL
MATRIX R WITH DIAGONAL ELEMENTS OF NONINCREASING MAGNITUDE,
SUCH THAT  $A^*P = Q^*R$ . THE HOUSEHOLDER TRANSFORMATION FOR
COLUMN K,  $K = 1, 2, \dots, \min(M, N)$ , IS OF THE FORM

```

$$I - \frac{1}{U(K)} U^T U$$

```

WHERE U HAS ZEROS IN THE FIRST K-1 POSITIONS. THE FORM OF
THIS TRANSFORMATION AND THE METHOD OF PIVOTING FIRST
APPEARED IN THE CORRESPONDING LINPACK SUBROUTINE.

```

```

THE SUBROUTINE STATEMENT IS

```

```

SUBROUTINE QRFAC(M,N,A,LDA,PIVOT,IPVT,LIPVT,RDIAG,ACNORM,WA)

```

```

WHERE

```

```

M IS A POSITIVE INTEGER INPUT VARIABLE SET TO THE NUMBER
OF ROWS OF A.

```

```

N IS A POSITIVE INTEGER INPUT VARIABLE SET TO THE NUMBER
OF COLUMNS OF A.

```

```

A IS AN M BY N ARRAY. ON INPUT A CONTAINS THE MATRIX FOR
WHICH THE QR FACTORIZATION IS TO BE COMPUTED. ON OUTPUT
THE STRICT UPPER TRAPEZOIDAL PART OF A CONTAINS THE STRICT
UPPER TRAPEZOIDAL PART OF R, AND THE LOWER TRAPEZOIDAL
PART OF A CONTAINS A FACTORED FORM OF Q (THE NON-TRIVIAL
ELEMENTS OF THE U VECTORS DESCRIBED ABOVE).

```

```

LDA IS A POSITIVE INTEGER INPUT VARIABLE NOT LESS THAN M
WHICH SPECIFIES THE LEADING DIMENSION OF THE ARRAY A.

```

```

PIVOT IS A LOGICAL INPUT VARIABLE. IF PIVOT IS SET TRUE,
THEN COLUMN PIVOTING IS ENFORCED. IF PIVOT IS SET FALSE,
THEN NO COLUMN PIVOTING IS DONE.

```

```

IPVT IS AN INTEGER OUTPUT ARRAY OF LENGTH LIPVT. IPVT
DEFINES THE PERMUTATION MATRIX P SUCH THAT  $A^*P = Q^*R$ .
COLUMN J OF P IS COLUMN IPVT(J) OF THE IDENTITY MATRIX.
IF PIVOT IS FALSE, IPVT IS NOT REFERENCED.

```

```

QRFA0010
QRFA0020
QRFA0030
QRFA0040
QRFA0050
QRFA0060
QRFA0070
QRFA0080
QRFA0090
QRFA0100
QRFA0110
QRFA0120
QRFA0130
QRFA0140
QRFA0150
QRFA0160
QRFA0170
QRFA0180
QRFA0190
QRFA0200
QRFA0210
QRFA0220
QRFA0230
QRFA0240
QRFA0250
QRFA0260
QRFA0270
QRFA0280
QRFA0290
QRFA0300
QRFA0310
QRFA0320
QRFA0330
QRFA0340
QRFA0350
QRFA0360
QRFA0370
QRFA0380
QRFA0390
QRFA0400
QRFA0410
QRFA0420
QRFA0430
QRFA0440
QRFA0450
QRFA0460
QRFA0470
QRFA0480
QRFA0490
QRFA0500
QRFA0510
QRFA0520
QRFA0530
QRFA0540

```


C		QRFA0550
C	LIPVT IS A POSITIVE INTEGER INPUT VARIABLE. IF PIVOT IS FALSE,	QRFA0560
C	THEN LIPVT MAY BE AS SMALL AS 1. IF PIVOT IS TRUE, THEN	QRFA0570
C	LIPVT MUST BE AT LEAST N.	QRFA0580
C		QRFA0590
C	RDIAG IS AN OUTPUT ARRAY OF LENGTH N WHICH CONTAINS THE	QRFA0600
C	DIAGONAL ELEMENTS OF R.	QRFA0610
C		QRFA0620
C	ACNORM IS AN OUTPUT ARRAY OF LENGTH N WHICH CONTAINS THE	QRFA0630
C	NORMS OF THE CORRESPONDING COLUMNS OF THE INPUT MATRIX A.	QRFA0640
C	IF THIS INFORMATION IS NOT NEEDED, THEN ACNORM CAN COINCIDE	QRFA0650
C	WITH RDIAG.	QRFA0660
C		QRFA0670
C	WA IS A WORK ARRAY OF LENGTH N. IF PIVOT IS FALSE, THEN WA	QRFA0680
C	CAN COINCIDE WITH RDIAG.	QRFA0690
C		QRFA0700
C	SUBPROGRAMS CALLED	QRFA0710
C		QRFA0720
C	MINPACK-SUPPLIED ... DPMPAR,ENORM	QRFA0730
C		QRFA0740
C	FORTTRAN-SUPPLIED ... DMAX1,DSQRT,MINO	QRFA0750
C		QRFA0760
C	ARGONNE NATIONAL LABORATORY. MINPACK PROJECT. MARCH 1980.	QRFA0770
C	BURTON S. GARBOW, KENNETH E. HILLSTROM, JORGE J. MORE	QRFA0780
C		QRFA0790
C	*****	QRFA0800
C	INTEGER I,J,JP1,K,KMAX,MINMN	QRFA0810
C	DOUBLE PRECISION AJNORM,EPSMCH,ONE,P05,SUM,TEMP,ZERO	QRFA0820
C	DOUBLE PRECISION DPMPAR,ENORM	QRFA0830
C	DATA ONE,P05,ZERO /1.0D0,5.0D-2,0.0D0/	QRFA0840
C		QRFA0850
C	EPSMCH IS THE MACHINE PRECISION.	QRFA0860
C		QRFA0870
C	EPSMCH = DPMPAR(1)	QRFA0880
C		QRFA0890
C	COMPUTE THE INITIAL COLUMN NORMS AND INITIALIZE SEVERAL ARRAYS.	QRFA0900
C		QRFA0910
C	DO 10 J = 1, N	QRFA0920
C	ACNORM(J) = ENORM(M,A(1,J))	QRFA0930
C	RDIAG(J) = ACNORM(J)	QRFA0940
C	WA(J) = RDIAG(J)	QRFA0950
C	IF (PIVOT) IPVT(J) = J	QRFA0960
C	10 CONTINUE	QRFA0970
C		QRFA0980
C	REDUCE A TO R WITH HOUSEHOLDER TRANSFORMATIONS.	QRFA0990
C		QRFA1000
C	MINMN = MINO(M,N)	QRFA1010
C	DO 110 J = 1, MINMN	QRFA1020
C	IF (.NOT.PIVOT) GO TO 40	QRFA1030
C		QRFA1040
C	BRING THE COLUMN OF LARGEST NORM INTO THE PIVOT POSITION.	QRFA1050
C		QRFA1060
C	KMAX = J	QRFA1070
C	DO 20 K = J, N	QRFA1080

	IF (RDIAG(K) .GT. RDIAG(KMAX)) KMAX = K	QRFA1090
20	CONTINUE	QRFA1100
	IF (KMAX .EQ. J) GO TO 40	QRFA1110
	DO 30 I = 1, M	QRFA1120
	TEMP = A(I,J)	QRFA1130
	A(I,J) = A(I,KMAX)	QRFA1140
	A(I,KMAX) = TEMP	QRFA1150
30	CONTINUE	QRFA1160
	RDIAG(KMAX) = RDIAG(J)	QRFA1170
	WA(KMAX) = WA(J)	QRFA1180
	K = IPVT(J)	QRFA1190
	IPVT(J) = IPVT(KMAX)	QRFA1200
	IPVT(KMAX) = K	QRFA1210
40	CONTINUE	QRFA1220
C		QRFA1230
C	COMPUTE THE HOUSEHOLDER TRANSFORMATION TO REDUCE THE	QRFA1240
C	J-TH COLUMN OF A TO A MULTIPLE OF THE J-TH UNIT VECTOR.	QRFA1250
C		QRFA1260
	AJNORM = ENORM(M-J+1,A(J,J))	QRFA1270
	IF (AJNORM .EQ. ZERO) GO TO 100	QRFA1280
	IF (A(J,J) .LT. ZERO) AJNORM = -AJNORM	QRFA1290
	DO 50 I = J, M	QRFA1300
	A(I,J) = A(I,J)/AJNORM	QRFA1310
50	CONTINUE	QRFA1320
	A(J,J) = A(J,J) + ONE	QRFA1330
C		QRFA1340
C	APPLY THE TRANSFORMATION TO THE REMAINING COLUMNS	QRFA1350
C	AND UPDATE THE NORMS.	QRFA1360
C		QRFA1370
	JP1 = J + 1	QRFA1380
	IF (N .LT. JP1) GO TO 100	QRFA1390
	DO 90 K = JP1, N	QRFA1400
	SUM = ZERO	QRFA1410
	DO 60 I = J, M	QRFA1420
	SUM = SUM + A(I,J)*A(I,K)	QRFA1430
60	CONTINUE	QRFA1440
	TEMP = SUM/A(J,J)	QRFA1450
	DO 70 I = J, M	QRFA1460
	A(I,K) = A(I,K) - TEMP*A(I,J)	QRFA1470
70	CONTINUE	QRFA1480
	IF (.NOT.PIVOT .OR. RDIAG(K) .EQ. ZERO) GO TO 80	QRFA1490
	TEMP = A(J,K)/RDIAG(K)	QRFA1500
	RDIAG(K) = RDIAG(K)*DSQRT(DMAX1(ZERO,ONE-TEMP**2))	QRFA1510
	IF (PO5*(RDIAG(K)/WA(K))**2 .GT. EPSMCH) GO TO 80	QRFA1520
	RDIAG(K) = ENORM(M-J,A(JP1,K))	QRFA1530
	WA(K) = RDIAG(K)	QRFA1540
80	CONTINUE	QRFA1550
90	CONTINUE	QRFA1560
100	CONTINUE	QRFA1570
	RDIAG(J) = -AJNORM	QRFA1580
110	CONTINUE	QRFA1590
	RETURN	QRFA1600
C		QRFA1610
C	LAST CARD OF SUBROUTINE QRFAC.	QRFA1620

```

SUBROUTINE QRSOLV(N,R,LDR,IPVT,DIAG,QT,B,X,SDIAG,WA)
INTEGER N,LDR
INTEGER IPVT(N)
DOUBLE PRECISION R(LDR,N),DIAG(N),QT(B(N),X(N),SDIAG(N),WA(N)
*****

```

```

SUBROUTINE QRSOLV

```

```

GIVEN AN M BY N MATRIX A, AN N BY N DIAGONAL MATRIX D,
AND AN M-VECTOR B, THE PROBLEM IS TO DETERMINE AN X WHICH
SOLVES THE SYSTEM

```

$$A * X = B, \quad D * X = 0,$$

```

IN THE LEAST SQUARES SENSE.

```

```

THIS SUBROUTINE COMPLETES THE SOLUTION OF THE PROBLEM
IF IT IS PROVIDED WITH THE NECESSARY INFORMATION FROM THE
QR FACTORIZATION, WITH COLUMN PIVOTING, OF A. THAT IS, IF
 $A * P = Q * R$ , WHERE P IS A PERMUTATION MATRIX, Q HAS ORTHOGONAL
COLUMNS, AND R IS AN UPPER TRIANGULAR MATRIX WITH DIAGONAL
ELEMENTS OF NONINCREASING MAGNITUDE, THEN QRSOLV EXPECTS
THE FULL UPPER TRIANGLE OF R, THE PERMUTATION MATRIX P,
AND THE FIRST N COMPONENTS OF  $(Q \text{ TRANSPOSE}) * B$ . THE SYSTEM
 $A * X = B, D * X = 0$ , IS THEN EQUIVALENT TO

```

$$R^T * Z = Q^T * B, \quad P^T * D * P * Z = 0,$$

```

WHERE  $X = P * Z$ . IF THIS SYSTEM DOES NOT HAVE FULL RANK,
THEN A LEAST SQUARES SOLUTION IS OBTAINED. ON OUTPUT QRSOLV
ALSO PROVIDES AN UPPER TRIANGULAR MATRIX S SUCH THAT

```

$$P^T * (A^T * A + D^T * D) * P = S^T * S.$$

```

S IS COMPUTED WITHIN QRSOLV AND MAY BE OF SEPARATE INTEREST.

```

```

THE SUBROUTINE STATEMENT IS

```

```

SUBROUTINE QRSOLV(N,R,LDR,IPVT,DIAG,QT,B,X,SDIAG,WA)

```

```

WHERE

```

```

N IS A POSITIVE INTEGER INPUT VARIABLE SET TO THE ORDER OF R.

```

```

R IS AN N BY N ARRAY. ON INPUT THE FULL UPPER TRIANGLE
MUST CONTAIN THE FULL UPPER TRIANGLE OF THE MATRIX R.
ON OUTPUT THE FULL UPPER TRIANGLE IS UNALTERED, AND THE
STRICT LOWER TRIANGLE CONTAINS THE STRICT UPPER TRIANGLE
(TRANPOSED) OF THE UPPER TRIANGULAR MATRIX S.

```

```

LDR IS A POSITIVE INTEGER INPUT VARIABLE NOT LESS THAN N
WHICH SPECIFIES THE LEADING DIMENSION OF THE ARRAY R.

```

```

QRSL0010
QRSL0020
QRSL0030
QRSL0040
QRSL0050
QRSL0060
QRSL0070
QRSL0080
QRSL0090
QRSL0100
QRSL0110
QRSL0120
QRSL0130
QRSL0140
QRSL0150
QRSL0160
QRSL0170
QRSL0180
QRSL0190
QRSL0200
QRSL0210
QRSL0220
QRSL0230
QRSL0240
QRSL0250
QRSL0260
QRSL0270
QRSL0280
QRSL0290
QRSL0300
QRSL0310
QRSL0320
QRSL0330
QRSL0340
QRSL0350
QRSL0360
QRSL0370
QRSL0380
QRSL0390
QRSL0400
QRSL0410
QRSL0420
QRSL0430
QRSL0440
QRSL0450
QRSL0460
QRSL0470
QRSL0480
QRSL0490
QRSL0500
QRSL0510
QRSL0520
QRSL0530
QRSL0540

```

C		QRSL0550
C	IPVT IS AN INTEGER INPUT ARRAY OF LENGTH N WHICH DEFINES THE	QRSL0560
C	PERMUTATION MATRIX P SUCH THAT $A \cdot P = Q \cdot R$. COLUMN J OF P	QRSL0570
C	IS COLUMN IPVT(J) OF THE IDENTITY MATRIX.	QRSL0580
C		QRSL0590
C	DIAG IS AN INPUT ARRAY OF LENGTH N WHICH MUST CONTAIN THE	QRSL0600
C	DIAGONAL ELEMENTS OF THE MATRIX D.	QRSL0610
C		QRSL0620
C	QTB IS AN INPUT ARRAY OF LENGTH N WHICH MUST CONTAIN THE FIRST	QRSL0630
C	N ELEMENTS OF THE VECTOR $(Q \text{ TRANSPOSE}) \cdot B$.	QRSL0640
C		QRSL0650
C	X IS AN OUTPUT ARRAY OF LENGTH N WHICH CONTAINS THE LEAST	QRSL0660
C	SQUARES SOLUTION OF THE SYSTEM $A \cdot X = B$, $D \cdot X = 0$.	QRSL0670
C		QRSL0680
C	SDIAG IS AN OUTPUT ARRAY OF LENGTH N WHICH CONTAINS THE	QRSL0690
C	DIAGONAL ELEMENTS OF THE UPPER TRIANGULAR MATRIX S.	QRSL0700
C		QRSL0710
C	WA IS A WORK ARRAY OF LENGTH N.	QRSL0720
C		QRSL0730
C	SUBPROGRAMS CALLED	QRSL0740
C		QRSL0750
C	FORTTRAN-SUPPLIED ... DABS,DSQRT	QRSL0760
C		QRSL0770
C	ARGONNE NATIONAL LABORATORY. MINPACK PROJECT. MARCH 1980.	QRSL0780
C	BURTON S. GARBOW, KENNETH E. HILLSTROM, JORGE J. MORE	QRSL0790
C		QRSL0800
C	*****	QRSL0810
C	INTEGER I,J,JP1,K,KP1,L,NSING	QRSL0820
C	DOUBLE PRECISION COS,COTAN,P5,P25,QTBPJ,SIN,SUM,TAN,TEMP,ZERO	QRSL0830
C	DATA P5,P25,ZERO /5.0D-1,2.5D-1,0.0D0/	QRSL0840
C		QRSL0850
C	COPY R AND $(Q \text{ TRANSPOSE}) \cdot B$ TO PRESERVE INPUT AND INITIALIZE S.	QRSL0860
C	IN PARTICULAR, SAVE THE DIAGONAL ELEMENTS OF R IN X.	QRSL0870
C		QRSL0880
	DO 20 J = 1, N	QRSL0890
	DO 10 I = J, N	QRSL0900
	R(I,J) = R(J,I)	QRSL0910
10	CONTINUE	QRSL0920
	X(J) = R(J,J)	QRSL0930
	WA(J) = QTB(J)	QRSL0940
20	CONTINUE	QRSL0950
C		QRSL0960
C	ELIMINATE THE DIAGONAL MATRIX D USING A GIVENS ROTATION.	QRSL0970
C		QRSL0980
	DO 100 J = 1, N	QRSL0990
C		QFSL1000
C	PREPARE THE ROW OF D TO BE ELIMINATED, LOCATING THE	QRSL1010
C	DIAGONAL ELEMENT USING P FROM THE QR FACTORIZATION.	QRSL1020
C		QRSL1030
	L = IPVT(J)	QRSL1040
	IF (DIAG(L) .EQ. ZERO) GO TO 90	QRSL1050
	DO 30 K = J, N	QRSL1060
	SDIAG(K) = ZERO	QRSL1070
30	CONTINUE	QRSL1080

	SDIAG(J) = DIAG(L)	QRSL1090
C		QRSL1100
C	THE TRANSFORMATIONS TO ELIMINATE THE ROW OF D	QRSL1110
C	MODIFY ONLY A SINGLE ELEMENT OF (Q TRANSPOSE)*B	QRSL1120
C	BEYOND THE FIRST N, WHICH IS INITIALLY ZERO.	QRSL1130
C		QRSL1140
	QTBPJ = ZERO	QRSL1150
	DO 80 K = J, N	QRSL1160
C		QRSL1170
C	DETERMINE A GIVENS ROTATION WHICH ELIMINATES THE	QRSL1180
C	APPROPRIATE ELEMENT IN THE CURRENT ROW OF D.	QRSL1190
C		QRSL1200
	IF (SDIAG(K) .EQ. ZERO) GO TO 70	QRSL1210
	IF (DABS(R(K,K)) .GE. DABS(SDIAG(K))) GO TO 40	QRSL1220
	COTAN = R(K,K)/SDIAG(K)	QRSL1230
	SIN = P5/DSQRT(P25+P25*COTAN**2)	QRSL1240
	COS = SIN*COTAN	QRSL1250
	GO TO 50	QRSL1260
40	CONTINUE	QRSL1270
	TAN = SDIAG(K)/R(K,K)	QRSL1280
	COS = P5/DSQRT(P25+P25*TAN**2)	QRSL1290
	SIN = COS*TAN	QRSL1300
50	CONTINUE	QRSL1310
C		QRSL1320
C	COMPUTE THE MODIFIED DIAGONAL ELEMENT OF R AND	QRSL1330
C	THE MODIFIED ELEMENT OF ((Q TRANSPOSE)*B,0).	QRSL1340
C		QRSL1350
	R(K,K) = COS*R(K,K) + SIN*SDIAG(K)	QRSL1360
	TEMP = COS*WA(K) + SIN*QTBPJ	QRSL1370
	QTBPJ = -SIN*WA(K) + COS*QTBPJ	QRSL1380
	WA(K) = TEMP	QRSL1390
C		QRSL1400
C	ACCUMULATE THE TRANSFORMATION IN THE ROW OF S.	QRSL1410
C		QRSL1420
	KP1 = K + 1	QRSL1430
	IF (N .LT. KP1) GO TO 70	QRSL1440
	DO 60 I = KP1, N	QRSL1450
	TEMP = COS*R(I,K) + SIN*SDIAG(I)	QRSL1460
	SDIAG(I) = -SIN*R(I,K) + COS*SDIAG(I)	QRSL1470
	R(I,K) = TEMP	QRSL1480
60	CONTINUE	QRSL1490
70	CONTINUE	QRSL1500
80	CONTINUE	QRSL1510
90	CONTINUE	QRSL1520
C		QRSL1530
C	STORE THE DIAGONAL ELEMENT OF S AND RESTORE	QRSL1540
C	THE CORRESPONDING DIAGONAL ELEMENT OF R.	QRSL1550
C		QRSL1560
	SDIAG(J) = R(J,J)	QRSL1570
	R(J,J) = X(J)	QRSL1580
100	CONTINUE	QRSL1590
C		QRSL1600
C	SOLVE THE TRIANGULAR SYSTEM FOR Z. IF THE SYSTEM IS	QRSL1610
C	SINGULAR, THEN OBTAIN A LEAST SQUARES SOLUTION.	QRSL1620

C	NSING = N	QRSL1630
	DO 110 J = 1, N	QRSL1640
	IF (SDIAG(J) .EQ. ZERO .AND. NSING .EQ. N) NSING = J - 1	QRSL1650
	IF (NSING .LT. N) WA(J) = ZERO	QRSL1660
110	CONTINUE	QRSL1670
	IF (NSING .LT. 1) GO TO 150	QRSL1680
	DO 140 K = 1, NSING	QRSL1690
	J = NSING - K + 1	QRSL1700
	SUM = ZERO	QRSL1710
	JP1 = J + 1	QRSL1720
	IF (NSING .LT. JP1) GO TO 130	QRSL1730
	DO 120 I = JP1, NSING	QRSL1740
	SUM = SUM + R(I,J)*WA(I)	QRSL1750
120	CONTINUE	QRSL1760
130	CONTINUE	QRSL1770
	WA(J) = (WA(J) - SUM)/SDIAG(J)	QRSL1780
140	CONTINUE	QRSL1790
150	CONTINUE	QRSL1800
C		QRSL1810
C	PERMUTE THE COMPONENTS OF Z BACK TO COMPONENTS OF X.	QRSL1820
C		QRSL1830
	DO 160 J = 1, N	QRSL1840
	L = IPVT(J)	QRSL1850
	X(L) = WA(J)	QRSL1860
160	CONTINUE	QRSL1870
	RETURN	QRSL1880
C		QRSL1890
C	LAST CARD OF SUBROUTINE QRSOLV.	QRSL1900
C		QRSL1910
	END	QRSL1920
		QRSL1930

```

SUBROUTINE RWUPDT(N,R,LDR,W,B,ALPHA,COS,SIN)
INTEGER N,LDR
DOUBLE PRECISION ALPHA
DOUBLE PRECISION R(LDR,N),W(N),B(N),COS(N),SIN(N)
*****

```

```

SUBROUTINE RWUPDT

```

```

GIVEN AN N BY N UPPER TRIANGULAR MATRIX R, THIS SUBROUTINE
COMPUTES THE QR DECOMPOSITION OF THE MATRIX FORMED WHEN A ROW
IS ADDED TO R. IF THE ROW IS SPECIFIED BY THE VECTOR W, THEN
RWUPDT DETERMINES AN ORTHOGONAL MATRIX Q SUCH THAT WHEN THE
N+1 BY N MATRIX COMPOSED OF R AUGMENTED BY W IS PREMULIPLIED
BY (Q TRANSPOSE), THE RESULTING MATRIX IS UPPER TRAPEZOIDAL.
THE MATRIX (Q TRANSPOSE) IS THE PRODUCT OF N TRANSFORMATIONS

```

```

      G(N)*G(N-1)* ... *G(1)

```

```

WHERE G(I) IS A GIVENS ROTATION IN THE (I,N+1) PLANE WHICH
ELIMINATES ELEMENTS IN THE (N+1)-ST PLANE. RWUPDT ALSO
COMPUTES THE PRODUCT (Q TRANSPOSE)*C WHERE C IS THE
(N+1)-VECTOR (B,ALPHA). Q ITSELF IS NOT ACCUMULATED, RATHER
THE INFORMATION TO RECOVER THE G ROTATIONS IS SUPPLIED.

```

```

THE SUBROUTINE STATEMENT IS

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```

      SUBROUTINE RWUPDT(N,R,LDR,W,B,ALPHA,COS,SIN)

```

```

WHERE

```

```

      N IS A POSITIVE INTEGER INPUT VARIABLE SET TO THE ORDER OF R.

```

```

      R IS AN N BY N ARRAY. ON INPUT THE UPPER TRIANGULAR PART OF
      R MUST CONTAIN THE MATRIX TO BE UPDATED. ON OUTPUT R
      CONTAINS THE UPDATED TRIANGULAR MATRIX.

```

```

      LDR IS A POSITIVE INTEGER INPUT VARIABLE NOT LESS THAN N
      WHICH SPECIFIES THE LEADING DIMENSION OF THE ARRAY R.

```

```

      W IS AN INPUT ARRAY OF LENGTH N WHICH MUST CONTAIN THE ROW
      VECTOR TO BE ADDED TO R.

```

```

      B IS AN ARRAY OF LENGTH N. ON INPUT B MUST CONTAIN THE
      FIRST N ELEMENTS OF THE VECTOR C. ON OUTPUT B CONTAINS
      THE FIRST N ELEMENTS OF THE VECTOR (Q TRANSPOSE)*C.

```

```

      ALPHA IS A VARIABLE. ON INPUT ALPHA MUST CONTAIN THE
      (N+1)-ST ELEMENT OF THE VECTOR C. ON OUTPUT ALPHA CONTAINS
      THE (N+1)-ST ELEMENT OF THE VECTOR (Q TRANSPOSE)*C.

```

```

      COS IS AN OUTPUT ARRAY OF LENGTH N WHICH CONTAINS THE
      COSINES OF THE TRANSFORMING GIVENS ROTATIONS.

```

```

      SIN IS AN OUTPUT ARRAY OF LENGTH N WHICH CONTAINS THE

```

```

RWUP0010
RWUP0020
RWUP0030
RWUP0040
RWUP0050
RWUP0060
RWUP0070
RWUP0080
RWUP0090
RWUP0100
RWUP0110
RWUP0120
RWUP0130
RWUP0140
RWUP0150
RWUP0160
RWUP0170
RWUP0180
RWUP0190
RWUP0200
RWUP0210
RWUP0220
RWUP0230
RWUP0240
RWUP0250
RWUP0260
RWUP0270
RWUP0280
RWUP0290
RWUP0300
RWUP0310
RWUP0320
RWUP0330
RWUP0340
RWUP0350
RWUP0360
RWUP0370
RWUP0380
RWUP0390
RWUP0400
RWUP0410
RWUP0420
RWUP0430
RWUP0440
RWUP0450
RWUP0460
RWUP0470
RWUP0480
RWUP0490
RWUP0500
RWUP0510
RWUP0520
RWUP0530
RWUP0540

```

C	SINES OF THE TRANSFORMING GIVENS ROTATIONS.	RWUP0550
C		RWUP0560
C	SUBPROGRAMS CALLED	RWUP0570
C		RWUP0580
C	FORTTRAN-SUPPLIED ... DABS,DSQRT	RWUP0590
C		RWUP0600
C	ARGONNE NATIONAL LABORATORY. MINPACK PROJECT. MARCH 1980.	RWUP0610
C	BURTON S. GARBOW, DUDLEY V. GOETSCHEL, KENNETH E. HILLSTROM,	RWUP0620
C	JORGE J. MORE	RWUP0630
C		RWUP0640
C	*****	RWUP0650
	INTEGER I,J,JM1	RWUP0660
	DOUBLE PRECISION COTAN,ONE,P5,P25,ROWJ,TAN,TEMP,ZERO	RWUP0670
	DATA ONE,P5,P25,ZERO /1.0D0,5.0D-1,2.5D-1,0.0D0/	RWUP0680
C		RWUP0690
	DO 60 J = 1, N	RWUP0700
	ROWJ = W(J)	RWUP0710
	JM1 = J - 1	RWUP0720
C		RWUP0730
C	APPLY THE PREVIOUS TRANSFORMATIONS TO	RWUP0740
C	R(I,J), I=1,2,...,J-1, AND TO W(J).	RWUP0750
C		RWUP0760
	IF (JM1 .LT. 1) GO TO 20	RWUP0770
	DO 10 I = 1, JM1	RWUP0780
	TEMP = COS(I)*R(I,J) + SIN(I)*ROWJ	RWUP0790
	ROWJ = -SIN(I)*R(I,J) + COS(I)*ROWJ	RWUP0800
	R(I,J) = TEMP	RWUP0810
10	CONTINUE	RWUP0820
20	CONTINUE	RWUP0830
C		RWUP0840
C	DETERMINE A GIVENS ROTATION WHICH ELIMINATES W(J).	RWUP0850
C		RWUP0860
	COS(J) = ONE	RWUP0870
	SIN(J) = ZERO	RWUP0880
	IF (ROWJ .EQ. ZERO) GO TO 50	RWUP0890
	IF (DABS(R(J,J)) .GE. DABS(ROWJ)) GO TO 30	RWUP0900
	COTAN = R(J,J)/ROWJ	RWUP0910
	SIN(J) = P5/DSQRT(P25+P25*COTAN**2)	RWUP0920
	COS(J) = SIN(J)*COTAN	RWUP0930
	GO TO 40	RWUP0940
30	CONTINUE	RWUP0950
	TAN = ROWJ/R(J,J)	RWUP0960
	COS(J) = P5/DSQRT(P25+P25*TAN**2)	RWUP0970
	SIN(J) = COS(J)*TAN	RWUP0980
40	CONTINUE	RWUP0990
C		RWUP1000
C	APPLY THE CURRENT TRANSFORMATION TO R(J,J), B(J), AND ALPHA.	RWUP1010
C		RWUP1020
	R(J,J) = COS(J)*R(J,J) + SIN(J)*ROWJ	RWUP1030
	TEMP = COS(J)*B(J) + SIN(J)*ALPHA	RWUP1040
	ALPHA = -SIN(J)*B(J) + COS(J)*ALPHA	RWUP1050
	B(J) = TEMP	RWUP1060
50	CONTINUE	RWUP1070
60	CONTINUE	RWUP1080

C
C
C
RETURN
LAST CARD OF SUBROUTINE RWUPDT.
END

RWUP1090
RWUP1100
RWUP1110
RWUP1120
RWUP1130

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SUBROUTINE R1MPYQ(M,N,A,LDA,V,W)
 INTEGER M,N,LDA
 DOUBLE PRECISION A(LDA,N),V(N),W(N)

SUBROUTINE R1MPYQ

GIVEN AN M BY N MATRIX A, THIS SUBROUTINE COMPUTES $A*Q$ WHERE
 Q IS THE PRODUCT OF $2*(N - 1)$ TRANSFORMATIONS

$GV(N-1)*...*GV(1)*GW(1)*...*GW(N-1)$

AND $GV(I)$, $GW(I)$ ARE GIVENS ROTATIONS IN THE (I,N) PLANE WHICH
 ELIMINATE ELEMENTS IN THE I-TH AND N-TH PLANES, RESPECTIVELY.
 Q ITSELF IS NOT GIVEN, RATHER THE INFORMATION TO RECOVER THE
 GV, GW ROTATIONS IS SUPPLIED.

THE SUBROUTINE STATEMENT IS

SUBROUTINE R1MPYQ(M,N,A,LDA,V,W)

WHERE

M IS A POSITIVE INTEGER INPUT VARIABLE SET TO THE NUMBER
 OF ROWS OF A.

N IS A POSITIVE INTEGER INPUT VARIABLE SET TO THE NUMBER
 OF COLUMNS OF A.

A IS AN M BY N ARRAY. ON INPUT A MUST CONTAIN THE MATRIX
 TO BE POSTMULTIPLIED BY THE ORTHOGONAL MATRIX Q
 DESCRIBED ABOVE. ON OUTPUT $A*Q$ HAS REPLACED A.

LDA IS A POSITIVE INTEGER INPUT VARIABLE NOT LESS THAN M
 WHICH SPECIFIES THE LEADING DIMENSION OF THE ARRAY A.

V IS AN INPUT ARRAY OF LENGTH N. $V(I)$ MUST CONTAIN THE
 INFORMATION NECESSARY TO RECOVER THE GIVENS ROTATION $GV(I)$
 DESCRIBED ABOVE.

W IS AN INPUT ARRAY OF LENGTH N: $W(I)$ MUST CONTAIN THE
 INFORMATION NECESSARY TO RECOVER THE GIVENS ROTATION $GW(I)$
 DESCRIBED ABOVE.

SUBROUTINES CALLED

FORTRAN-SUPPLIED ... DABS,DSQRT

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 BURTON S. GARBOW, KENNETH E. HILLSTROM, JORGE J. MORE

INTEGER I,J,NMJ,NM1
 DOUBLE PRECISION COS,ONE,SIN,TEMP

R1MQ0010
 R1MQ0020
 R1MQ0030
 R1MQ0040
 R1MQ0050
 R1MQ0060
 R1MQ0070
 R1MQ0080
 R1MQ0090
 R1MQ0100
 R1MQ0110
 R1MQ0120
 R1MQ0130
 R1MQ0140
 R1MQ0150
 R1MQ0160
 R1MQ0170
 R1MQ0180
 R1MQ0190
 R1MQ0200
 R1MQ0210
 R1MQ0220
 R1MQ0230
 R1MQ0240
 R1MQ0250
 R1MQ0260
 R1MQ0270
 R1MQ0280
 R1MQ0290
 R1MQ0300
 R1MQ0310
 R1MQ0320
 R1MQ0330
 R1MQ0340
 R1MQ0350
 R1MQ0360
 R1MQ0370
 R1MQ0380
 R1MQ0390
 R1MQ0400
 R1MQ0410
 R1MQ0420
 R1MQ0430
 R1MQ0440
 R1MQ0450
 R1MQ0460
 R1MQ0470
 R1MQ0480
 R1MQ0490
 R1MQ0500
 R1MQ0510
 R1MQ0520
 R1MQ0530
 R1MQ0540

C	DATA ONE /1.0D0/	R1MQ0550
C	APPLY THE FIRST SET OF GIVENS ROTATIONS TO A.	R1MQ0560
C		R1MQ0570
	NM1 = N - 1	R1MQ0580
	IF (NM1 .LT. 1) GO TO 50	R1MQ0590
	DO 20 NMJ = 1, NM1	R1MQ0600
	J = N - NMJ	R1MQ0610
	IF (DABS(V(J)) .GT. ONE) COS = ONE/V(J)	R1MQ0620
	IF (DABS(V(J)) .GT. ONE) SIN = DSQRT(ONE-COS**2)	R1MQ0630
	IF (DABS(V(J)) .LE. ONE) SIN = V(J)	R1MQ0640
	IF (DABS(V(J)) .LE. ONE) COS = DSQRT(ONE-SIN**2)	R1MQ0650
	DO 10 I = 1, M	R1MQ0660
	TEMP = COS*A(I,J) - SIN*A(I,N)	R1MQ0670
	A(I,N) = SIN*A(I,J) + COS*A(I,N)	R1MQ0680
	A(I,J) = TEMP	R1MQ0690
10	CONTINUE	R1MQ0700
20	CONTINUE	R1MQ0710
C		R1MQ0720
C	APPLY THE SECOND SET OF GIVENS ROTATIONS TO A.	R1MQ0730
C		R1MQ0740
	DO 40 J = 1, NM1	R1MQ0750
	IF (DABS(W(J)) .GT. ONE) COS = ONE/W(J)	R1MQ0760
	IF (DABS(W(J)) .GT. ONE) SIN = DSQRT(ONE-COS**2)	R1MQ0770
	IF (DABS(W(J)) .LE. ONE) SIN = W(J)	R1MQ0780
	IF (DABS(W(J)) .LE. ONE) COS = DSQRT(ONE-SIN**2)	R1MQ0790
	DO 30 I = 1, M	R1MQ0800
	TEMP = COS*A(I,J) + SIN*A(I,N)	R1MQ0810
	A(I,N) = -SIN*A(I,J) + COS*A(I,N)	R1MQ0820
	A(I,J) = TEMP	R1MQ0830
30	CONTINUE	R1MQ0840
40	CONTINUE	R1MQ0850
50	CONTINUE	R1MQ0860
	RETURN	R1MQ0870
C		R1MQ0880
C	LAST CARD OF SUBROUTINE R1MPYQ.	R1MQ0890
C		R1MQ0900
	END	R1MQ0910
		R1MQ0920

SUBROUTINE R1UPDT(M,N,S,LS,U,V,W,SING)
 INTEGER M,N,LS
 LOGICAL SING
 DOUBLE PRECISION S(LS),U(M),V(N),W(M)

SUBROUTINE R1UPDT

GIVEN AN M BY N LOWER TRAPEZOIDAL MATRIX S, AN M-VECTOR U,
 AND AN N-VECTOR V, THE PROBLEM IS TO DETERMINE AN
 ORTHOGONAL MATRIX Q SUCH THAT

$$(S + U^T V)^T Q$$

IS AGAIN LOWER TRAPEZOIDAL.

THIS SUBROUTINE DETERMINES Q AS THE PRODUCT OF $2*(N - 1)$
 TRANSFORMATIONS

$$GV(N-1)*...*GV(1)*GW(1)*...*GW(N-1)$$

WHERE GV(I), GW(I) ARE GIVENS ROTATIONS IN THE (I,N) PLANE
 WHICH ELIMINATE ELEMENTS IN THE I-TH AND N-TH PLANES,
 RESPECTIVELY. Q ITSELF IS NOT ACCUMULATED, RATHER THE
 INFORMATION TO RECOVER THE GV, GW ROTATIONS IS RETURNED.

THE SUBROUTINE STATEMENT IS

SUBROUTINE R1UPDT(M,N,S,LS,U,V,W,SING)

WHERE

M IS A POSITIVE INTEGER INPUT VARIABLE SET TO THE NUMBER
 OF ROWS OF S.

N IS A POSITIVE INTEGER INPUT VARIABLE SET TO THE NUMBER
 OF COLUMNS OF S. N MUST NOT EXCEED M.

S IS AN ARRAY OF LENGTH LS. ON INPUT S MUST CONTAIN THE LOWER
 TRAPEZOIDAL MATRIX S STORED BY COLUMNS. ON OUTPUT S CONTAINS
 THE LOWER TRAPEZOIDAL MATRIX PRODUCED AS DESCRIBED ABOVE.

LS IS A POSITIVE INTEGER INPUT VARIABLE NOT LESS THAN
 $(N*(2*M-N+1))/2$.

U IS AN INPUT ARRAY OF LENGTH M WHICH MUST CONTAIN THE
 VECTOR U.

V IS AN ARRAY OF LENGTH N. ON INPUT V MUST CONTAIN THE VECTOR
 V. ON OUTPUT V(I) CONTAINS THE INFORMATION NECESSARY TO
 RECOVER THE GIVENS ROTATION GV(I) DESCRIBED ABOVE.

W IS AN OUTPUT ARRAY OF LENGTH M. W(I) CONTAINS INFORMATION

R1UP0010
 R1UP0020
 R1UP0030
 R1UP0040
 R1UP0050
 R1UP0060
 R1UP0070
 R1UP0080
 R1UP0090
 R1UP0100
 R1UP0110
 R1UP0120
 R1UP0130
 R1UP0140
 R1UP0150
 R1UP0160
 R1UP0170
 R1UP0180
 R1UP0190
 R1UP0200
 R1UP0210
 R1UP0220
 R1UP0230
 R1UP0240
 R1UP0250
 R1UP0260
 R1UP0270
 R1UP0280
 R1UP0290
 R1UP0300
 R1UP0310
 R1UP0320
 R1UP0330
 R1UP0340
 R1UP0350
 R1UP0360
 R1UP0370
 R1UP0380
 R1UP0390
 R1UP0400
 R1UP0410
 R1UP0420
 R1UP0430
 R1UP0440
 R1UP0450
 R1UP0460
 R1UP0470
 R1UP0480
 R1UP0490
 R1UP0500
 R1UP0510
 R1UP0520
 R1UP0530
 R1UP0540

C	NECESSARY TO RECOVER THE GIVENS ROTATION GW(I) DESCRIBED	R1UP0550
C	ABOVE.	R1UP0560
C		R1UP0570
C	SING IS A LOGICAL OUTPUT VARIABLE. SING IS SET TRUE IF ANY	R1UP0580
C	OF THE DIAGONAL ELEMENTS OF THE OUTPUT S ARE ZERO. OTHERWISE	R1UP0590
C	SING IS SET FALSE.	R1UP0600
C		R1UP0610
C	SUBPROGRAMS CALLED	R1UP0620
C		R1UP0630
C	MINPACK-SUPPLIED ... DPMPAR	R1UP0640
C		R1UP0650
C	FORTTRAN-SUPPLIED ... DABS,DSQRT	R1UP0660
C		R1UP0670
C	ARGONNE NATIONAL LABORATORY. MINPACK PROJECT. MARCH 1980.	R1UP0680
C	BURTON S. GARBOW, KENNETH E. HILLSTROM, JORGE J. MORE,	R1UP0690
C	JOHN L. NAZARETH	R1UP0700
C		R1UP0710
C	*****	R1UP0720
	INTEGER I,J,JJ,L,NMJ,NM1	R1UP0730
	DOUBLE PRECISION COS,COTAN,GIANT,ONE,P5,P25,SIN,TAN,TAU,TEMP,	R1UP0740
	* ZERO	R1UP0750
	DOUBLE PRECISION DPMPAR	R1UP0760
	DATA ONE,P5,P25,ZERO /1.0D0,5.0D-1,2.5D-1,0.0D0/	R1UP0770
C		R1UP0780
C	GIANT IS THE LARGEST MAGNITUDE.	R1UP0790
C		R1UP0800
	GIANT = DPMPAR(3)	R1UP0810
C		R1UP0820
C	INITIALIZE THE DIAGONAL ELEMENT POINTER.	R1UP0830
C		R1UP0840
	JJ = (N*(2*M - N + 1))/2 - (M - N)	R1UP0850
C		R1UP0860
C	MOVE THE NONTRIVIAL PART OF THE LAST COLUMN OF S INTO W.	R1UP0870
C		R1UP0880
	L = JJ	R1UP0890
	DO 10 I = N, M	R1UP0900
	W(I) = S(L)	R1UP0910
	L = L + 1	R1UP0920
10	CONTINUE	R1UP0930
C		R1UP0940
C	ROTATE THE VECTOR V INTO A MULTIPLE OF THE N-TH UNIT VECTOR	R1UP0950
C	IN SUCH A WAY THAT A SPIKE IS INTRODUCED INTO W.	R1UP0960
C		R1UP0970
	NM1 = N - 1	R1UP0980
	IF (NM1 .LT. 1) GO TO 70	R1UP0990
	DO 60 NMJ = 1, NM1	R1UP1000
	J = N - NMJ	R1UP1010
	JJ = JJ - (M - J + 1)	R1UP1020
	W(J) = ZERO	R1UP1030
	IF (V(J) .EQ. ZERO) GO TO 50	R1UP1040
C		R1UP1050
C	DETERMINE A GIVENS ROTATION WHICH ELIMINATES THE	R1UP1060
C	J-TH ELEMENT OF V.	R1UP1070
C		R1UP1080

	IF (DABS(V(N)) .GE. DABS(V(J))) GO TO 20	R1UP1090
	COTAN = V(N)/V(J)	R1UP1100
	SIN = P5/DSQRT(P25+P25*COTAN**2)	R1UP1110
	COS = SIN*COTAN	R1UP1120
	TAU = ONE	R1UP1130
	IF (DABS(COS)*GIANT .GT. ONE) TAU = ONE/COS	R1UP1140
	GO TO 30	R1UP1150
20	CONTINUE	R1UP1160
	TAN = V(J)/V(N)	R1UP1170
	COS = P5/DSQRT(P25+P25*TAN**2)	R1UP1180
	SIN = COS*TAN	R1UP1190
	TAU = SIN	R1UP1200
30	CONTINUE	R1UP1210
C		R1UP1220
C	APPLY THE TRANSFORMATION TO V AND STORE THE INFORMATION	R1UP1230
C	NECESSARY TO RECOVER THE GIVENS ROTATION.	R1UP1240
C		R1UP1250
	V(N) = SIN*V(J) + COS*V(N)	R1UP1260
	V(J) = TAU	R1UP1270
C		R1UP1280
C	APPLY THE TRANSFORMATION TO S AND EXTEND THE SPIKE IN W.	R1UP1290
C		R1UP1300
	L = JJ	R1UP1310
	DO 40 I = J, M	R1UP1320
	TEMP = COS*S(L) - SIN*W(I)	R1UP1330
	W(I) = SIN*S(L) + COS*W(I)	R1UP1340
	S(L) = TEMP	R1UP1350
	L = L + 1	R1UP1360
40	CONTINUE	R1UP1370
50	CONTINUE	R1UP1380
60	CONTINUE	R1UP1390
70	CONTINUE	R1UP1400
C		R1UP1410
C	ADD THE SPIKE FROM THE RANK 1 UPDATE TO W.	R1UP1420
C		R1UP1430
	DO 80 I = 1, M	R1UP1440
	W(I) = W(I) + V(N)*U(I)	R1UP1450
80	CONTINUE	R1UP1460
C		R1UP1470
C	ELIMINATE THE SPIKE.	R1UP1480
C		R1UP1490
	SING = .FALSE.	R1UP1500
	IF (NM1 .LT. 1) GO TO 140	R1UP1510
	DO 130 J = 1, NM1	R1UP1520
	IF (W(J) .EQ. ZERO) GO TO 120	R1UP1530
C		R1UP1540
C	DETERMINE A GIVENS ROTATION WHICH ELIMINATES THE	R1UP1550
C	J-TH ELEMENT OF THE SPIKE.	R1UP1560
C		R1UP1570
	IF (DABS(S(JJ)) .GE. DABS(W(J))) GO TO 90	R1UP1580
	COTAN = S(JJ)/W(J)	R1UP1590
	SIN = P5/DSQRT(P25+P25*COTAN**2)	R1UP1600
	COS = SIN*COTAN	R1UP1610
	TAU = ONE	R1UP1620

	IF (DABS(COS)*GIANT .GT. ONE) TAU = ONE/COS	R1UP1630
	GO TO 100	R1UP1640
90	CONTINUE	R1UP1650
	TAN = W(J)/S(JJ)	R1UP1660
	COS = P5/DSQRT(P25+P25*TAN**2)	R1UP1670
	SIN = COS*TAN	R1UP1680
	TAU = SIN	R1UP1690
100	CONTINUE	R1UP1700
C		R1UP1710
C	APPLY THE TRANSFORMATION TO S AND REDUCE THE SPIKE IN W.	R1UP1720
C		R1UP1730
	L = JJ	R1UP1740
	DO 110 I = J, M	R1UP1750
	TEMP = COS*S(L) + SIN*W(I)	R1UP1760
	W(I) = -SIN*S(L) + COS*W(I)	R1UP1770
	S(L) = TEMP	R1UP1780
	L = L + 1	R1UP1790
110	CONTINUE	R1UP1800
C		R1UP1810
C	STORE THE INFORMATION NECESSARY TO RECOVER THE	R1UP1820
C	GIVENS ROTATION.	R1UP1830
C		R1UP1840
	W(J) = TAU	R1UP1850
120	CONTINUE	R1UP1860
C		R1UP1870
C	TEST FOR ZERO DIAGONAL ELEMENTS IN THE OUTPUT S.	R1UP1880
C		R1UP1890
	IF (S(JJ) .EQ. ZERO) SING = .TRUE.	R1UP1900
	JJ = JJ + (M - J + 1)	R1UP1910
130	CONTINUE	R1UP1920
140	CONTINUE	R1UP1930
C		R1UP1940
C	MOVE W BACK INTO THE LAST COLUMN OF THE OUTPUT S.	R1UP1950
C		R1UP1960
	L = JJ	R1UP1970
	DO 150 I = N, M	R1UP1980
	S(L) = W(I)	R1UP1990
	L = L + 1	R1UP2000
150	CONTINUE	R1UP2010
	IF (S(JJ) .EQ. ZERO) SING = .TRUE.	R1UP2020
	RETURN	R1UP2030
C		R1UP2040
C	LAST CARD OF SUBROUTINE R1UPDT.	R1UP2050
C		R1UP2060
	END	R1UP2070

REAL FUNCTION SPMPAR(I)

INTEGER I

FUNCTION SPMPAR

THIS FUNCTION PROVIDES SINGLE PRECISION MACHINE PARAMETERS WHEN THE APPROPRIATE SET OF DATA STATEMENTS IS ACTIVATED (BY REMOVING THE C FROM COLUMN 1) AND ALL OTHER DATA STATEMENTS ARE RENDERED INACTIVE. MOST OF THE PARAMETER VALUES WERE OBTAINED FROM THE CORRESPONDING BELL LABORATORIES PORT LIBRARY FUNCTION.

THE FUNCTION STATEMENT IS

REAL FUNCTION SPMPAR(I)

WHERE

I IS AN INTEGER INPUT VARIABLE SET TO 1, 2, OR 3 WHICH SELECTS THE DESIRED MACHINE PARAMETER. IF THE MACHINE HAS T BASE B DIGITS AND ITS SMALLEST AND LARGEST EXPONENTS ARE EMIN AND EMAX, RESPECTIVELY, THEN THESE PARAMETERS ARE

SPMPAR(1) = B**(1 - T), THE MACHINE PRECISION,

SPMPAR(2) = B**(EMIN - 1), THE SMALLEST MAGNITUDE,

SPMPAR(3) = B**EMAX*(1 - B**(-T)), THE LARGEST MAGNITUDE.

ARGONNE NATIONAL LABORATORY. MINPACK PROJECT. MARCH 1980.
BURTON S. GARBOW, KENNETH E. HILLSTROM, JORGE J. MORE

INTEGER MCHEPS(2)

INTEGER MINMAG(2)

INTEGER MAXMAG(2)

REAL RMACH(3)

EQUIVALENCE (RMACH(1),MCHEPS(1))

EQUIVALENCE (RMACH(2),MINMAG(1))

EQUIVALENCE (RMACH(3),MAXMAG(1))

MACHINE CONSTANTS FOR THE IBM 360/370 SERIES,
THE AMDAHL 470/V6, THE ICL 2900, THE ITTEL AS/6,
THE XEROX SIGMA 5/7/9 AND THE SEL SYSTEMS 85/86.

DATA RMACH(1) / Z3C100000 /

DATA RMACH(2) / Z00100000 /

DATA RMACH(3) / Z7FFFFFFF /

MACHINE CONSTANTS FOR THE HONEYWELL 600/6000 SERIES.

DATA RMACH(1) / 0716400000000 /

DATA RMACH(2) / 0402400000000 /

DATA RMACH(3) / 037677777777 /

SPPR0010
SPPR0020
SPPR0030
SPPR0040
SPPR0050
SPPR0060
SPPR0070
SPPR0080
SPPR0090
SPPR0100
SPPR0110
SPPR0120
SPPR0130
SPPR0140
SPPR0150
SPPR0160
SPPR0170
SPPR0180
SPPR0190
SPPR0200
SPPR0210
SPPR0220
SPPR0230
SPPR0240
SPPR0250
SPPR0260
SPPR0270
SPPR0280
SPPR0290
SPPR0300
SPPR0310
SPPR0320
SPPR0330
SPPR0340
SPPR0350
SPPR0360
SPPR0370
SPPR0380
SPPR0390
SPPR0400
SPPR0410
SPPR0420
SPPR0430
SPPR0440
SPPR0450
SPPR0460
SPPR0470
SPPR0480
SPPR0490
SPPR0500
SPPR0510
SPPR0520
SPPR0530
SPPR0540

C		SPPR0550
C	MACHINE CONSTANTS FOR THE CDC 6000/7000 SERIES.	SPPR0560
C		SPPR0570
C	DATA RMACH(1) / 1641400000000000000B /	SPPR0580
C	DATA RMACH(2) / 0001400000000000000B /	SPPR0590
C	DATA RMACH(3) / 3776777777777777777B /	SPPR0600
C		SPPR0610
C	MACHINE CONSTANTS FOR THE PDP-10 (KA OR KI PROCESSOR).	SPPR0620
C		SPPR0630
C	DATA RMACH(1) / "147400000000 /	SPPR0640
C	DATA RMACH(2) / "000400000000 /	SPPR0650
C	DATA RMACH(3) / "377777777777 /	SPPR0660
C		SPPR0670
C	MACHINE CONSTANTS FOR THE PDP-11 FORTRAN SUPPORTING	SPPR0680
C	32-BIT INTEGERS (EXPRESSED IN INTEGER AND OCTAL).	SPPR0690
C		SPPR0700
C	DATA MCHEPS(1) / 889192448 /	SPPR0710
C	DATA MINMAG(1) / 8388608 /	SPPR0720
C	DATA MAXMAG(1) / 2147483647 /	SPPR0730
C		SPPR0740
C	DATA RMACH(1) / 006500000000 /	SPPR0750
C	DATA RMACH(2) / 000040000000 /	SPPR0760
C	DATA RMACH(3) / 017777777777 /	SPPR0770
C		SPPR0780
C	MACHINE CONSTANTS FOR THE PDP-11 FORTRAN SUPPORTING	SPPR0790
C	16-BIT INTEGERS (EXPRESSED IN INTEGER AND OCTAL).	SPPR0800
C		SPPR0810
C	DATA MCHEPS(1),MCHEPS(2) / 13568, 0 /	SPPR0820
C	DATA MINMAG(1),MINMAG(2) / 128, 0 /	SPPR0830
C	DATA MAXMAG(1),MAXMAG(2) / 32767, -1 /	SPPR0840
C		SPPR0850
C	DATA MCHEPS(1),MCHEPS(2) / 0032400, 0000000 /	SPPR0860
C	DATA MINMAG(1),MINMAG(2) / 0000200, 0000000 /	SPPR0870
C	DATA MAXMAG(1),MAXMAG(2) / 0077777, 0177777 /	SPPR0880
C		SPPR0890
C	MACHINE CONSTANTS FOR THE BURROUGHS 5700/6700/7700 SYSTEMS.	SPPR0900
C		SPPR0910
C	DATA RMACH(1) / 013010000000000000 /	SPPR0920
C	DATA RMACH(2) / 017710000000000000 /	SPPR0930
C	DATA RMACH(3) / 007777777777777777 /	SPPR0940
C		SPPR0950
C	MACHINE CONSTANTS FOR THE BURROUGHS 1700 SYSTEM.	SPPR0960
C		SPPR0970
C	DATA RMACH(1) / Z4EA800000 /	SPPR0980
C	DATA RMACH(2) / Z400800000 /	SPPR0990
C	DATA RMACH(3) / Z5FFFFFFFF /	SPPR1000
C		SPPR1010
C	MACHINE CONSTANTS FOR THE UNIVAC 1100 SERIES.	SPPR1020
C		SPPR1030
C	DATA RMACH(1) / 01474000000000 /	SPPR1040
C	DATA RMACH(2) / 00004000000000 /	SPPR1050
C	DATA RMACH(3) / 03777777777777 /	SPPR1060
C		SPPR1070
C	MACHINE CONSTANTS FOR THE DATA GENERAL ECLIPSE S/200.	SPPR1080

C		SPPR1090
C	NOTE - IT MAY BE APPROPRIATE TO INCLUDE THE FOLLOWING CARD -	SPPR1100
C	STATIC RMACH(3)	SPPR1110
C		SPPR1120
C	DATA MINMAG/20K,0/,MAXMAG/77777K,177777K/	SPPR1130
C	DATA MCHEPS/36020K,0/	SPPR1140
C		SPPR1150
C	MACHINE CONSTANTS FOR THE HARRIS 220.	SPPR1160
C		SPPR1170
C	DATA MCHEPS(1),MCHEPS(2) / '20000000, '00000353 /	SPPR1180
C	DATA MINMAG(1),MINMAG(2) / '20000000, '00000201 /	SPPR1190
C	DATA MAXMAG(1),MAXMAG(2) / '37777777, '00000177 /	SPPR1200
C		SPPR1210
C	MACHINE CONSTANTS FOR THE CRAY-1.	SPPR1220
C		SPPR1230
C	DATA RMACH(1) / 037722400000000000000000B /	SPPR1240
C	DATA RMACH(2) / 020003400000000000000000B /	SPPR1250
C	DATA RMACH(3) / 05777777777777777777776B /	SPPR1260
C		SPPR1270
C	MACHINE CONSTANTS FOR THE PRIME 400.	SPPR1280
C		SPPR1290
C	DATA MCHEPS(1) / :10000000153 /	SPPR1300
C	DATA MINMAG(1) / :10000000000 /	SPPR1310
C	DATA MAXMAG(1) / :1777777777 /	SPPR1320
C		SPPR1330
	SPMPAR = RMACH(I)	SPPR1340
	RETURN	SPPR1350
C		SPPR1360
C	LAST CARD OF FUNCTION SPMPAR.	SPPR1370
C		SPPR1380
	END	SPPR1390

DOUBLE PRECISION FUNCTION DPMPAR(I)
INTEGER I

FUNCTION DPMPAR

THIS FUNCTION PROVIDES DOUBLE PRECISION MACHINE PARAMETERS
WHEN THE APPROPRIATE SET OF DATA STATEMENTS IS ACTIVATED (BY
REMOVING THE C FROM COLUMN 1) AND ALL OTHER DATA STATEMENTS ARE
RENDERED INACTIVE. MOST OF THE PARAMETER VALUES WERE OBTAINED
FROM THE CORRESPONDING BELL LABORATORIES PORT LIBRARY FUNCTION.

THE FUNCTION STATEMENT IS

DOUBLE PRECISION FUNCTION DPMPAR(I)

WHERE

I IS AN INTEGER INPUT VARIABLE SET TO 1, 2, OR 3 WHICH
SELECTS THE DESIRED MACHINE PARAMETER. IF THE MACHINE HAS
T BASE B DIGITS AND ITS SMALLEST AND LARGEST EXPONENTS ARE
EMIN AND EMAX, RESPECTIVELY, THEN THESE PARAMETERS ARE

$DPMPAR(1) = B^{*(1 - T)}$, THE MACHINE PRECISION,

$DPMPAR(2) = B^{*(EMIN - 1)}$, THE SMALLEST MAGNITUDE,

$DPMPAR(3) = B^{*EMAX*(1 - B^{*(-T)})}$, THE LARGEST MAGNITUDE.

ARGONNE NATIONAL LABORATORY. MINPACK PROJECT. MARCH 1980.
BURTON S. GARBOW, KENNETH E. HILLSTROM, JORGE J. MORE

INTEGER MCHEPS(4)

INTEGER MINMAG(4)

INTEGER MAXMAG(4)

DOUBLE PRECISION DMACH(3)

EQUIVALENCE (DMACH(1),MCHEPS(1))

EQUIVALENCE (DMACH(2),MINMAG(1))

EQUIVALENCE (DMACH(3),MAXMAG(1))

MACHINE CONSTANTS FOR THE /IBM 360/370 SERIES,
THE AMDAHL 470/V6, THE ICL 2900, THE ITCL AS/6,
THE XEROX SIGMA 5/7/9 AND THE SEL SYSTEMS 85/86.

DATA MCHEPS(1),MCHEPS(2) / Z34100000, Z00000000 /
DATA MINMAG(1),MINMAG(2) / Z00100000, Z00000000 /
DATA MAXMAG(1),MAXMAG(2) / Z7FFFFFFF, ZFFFFFFF /

MACHINE CONSTANTS FOR THE HONEYWELL 600/6000 SERIES.

DATA MCHEPS(1),MCHEPS(2) / 0606400000000, 0000000000000 /
DATA MINMAG(1),MINMAG(2) / 0402400000000, 0000000000000 /
DATA MAXMAG(1),MAXMAG(2) / 0376777777777, 0777777777777 /

DPPR0010
DPPR0020
DPPR0030
DPPR0040
DPPR0050
DPPR0060
DPPR0070
DPPR0080
DPPR0090
DPPR0100
DPPR0110
DPPR0120
DPPR0130
DPPR0140
DPPR0150
DPPR0160
DPPR0170
DPPR0180
DPPR0190
DPPR0200
DPPR0210
DPPR0220
DPPR0230
DPPR0240
DPPR0250
DPPR0260
DPPR0270
DPPR0280
DPPR0290
DPPR0300
DPPR0310
DPPR0320
DPPR0330
DPPR0340
DPPR0350
DPPR0360
DPPR0370
DPPR0380
DPPR0390
DPPR0400
DPPR0410
DPPR0420
DPPR0430
DPPR0440
DPPR0450
DPPR0460
DPPR0470
DPPR0480
DPPR0490
DPPR0500
DPPR0510
DPPR0520
DPPR0530
DPPR0540

C		DPPR0550
C	MACHINE CONSTANTS FOR THE CDC 6000/7000 SERIES.	DPPR0560
C		DPPR0570
C	DATA MCHEPS(1) / 15614000000000000000B /	DPPR0580
C	DATA MCHEPS(2) / 15010000000000000000B /	DPPR0590
C		DPPR0600
C	DATA MINMAG(1) / 00604000000000000000B /	DPPR0610
C	DATA MINMAG(2) / 00000000000000000000B /	DPPR0620
C		DPPR0630
C	DATA MAXMAG(1) / 3776777777777777777B /	DPPR0640
C	DATA MAXMAG(2) / 3716777777777777777B /	DPPR0650
C		DPPR0660
C	MACHINE CONSTANTS FOR THE PDP-10 (KA PROCESSOR).	DPPR0670
C		DPPR0680
C	DATA MCHEPS(1),MCHEPS(2) / "114400000000, "000000000000 /	DPPR0690
C	DATA MINMAG(1),MINMAG(2) / "033400000000, "000000000000 /	DPPR0700
C	DATA MAXMAG(1),MAXMAG(2) / "377777777777, "344777777777 /	DPPR0710
C		DPPR0720
C	MACHINE CONSTANTS FOR THE PDP-10 (KI PROCESSOR).	DPPR0730
C		DPPR0740
C	DATA MCHEPS(1),MCHEPS(2) / "104400000000, "000000000000 /	DPPR0750
C	DATA MINMAG(1),MINMAG(2) / "000400000000, "000000000000 /	DPPR0760
C	DATA MAXMAG(1),MAXMAG(2) / "377777777777, "377777777777 /	DPPR0770
C		DPPR0780
C	MACHINE CONSTANTS FOR THE PDP-11 FORTRAN SUPPORTING	DPPR0790
C	32-BIT INTEGERS (EXPRESSED IN INTEGER AND OCTAL).	DPPR0800
C		DPPR0810
C	DATA MCHEPS(1),MCHEPS(2) / 620756992, 0 /	DPPR0820
C	DATA MINMAG(1),MINMAG(2) / 8388608, 0 /	DPPR0830
C	DATA MAXMAG(1),MAXMAG(2) / 2147483647, -1 /	DPPR0840
C		DPPR0850
C	DATA MCHEPS(1),MCHEPS(2) / 004500000000, 000000000000 /	DPPR0860
C	DATA MINMAG(1),MINMAG(2) / 000040000000, 000000000000 /	DPPR0870
C	DATA MAXMAG(1),MAXMAG(2) / 017777777777, 037777777777 /	DPPR0880
C		DPPR0890
C	MACHINE CONSTANTS FOR THE PDP-11 FORTRAN SUPPORTING	DPPR0900
C	16-BIT INTEGERS (EXPRESSED IN INTEGER AND OCTAL).	DPPR0910
C		DPPR0920
C	DATA MCHEPS(1),MCHEPS(2) / 9472, 0 /	DPPR0930
C	DATA MCHEPS(3),MCHEPS(4) / 0, 0 /	DPPR0940
C		DPPR0950
C	DATA MINMAG(1),MINMAG(2) / 128, 0 /	DPPR0960
C	DATA MINMAG(3),MINMAG(4) / 0, 0 /	DPPR0970
C		DPPR0980
C	DATA MAXMAG(1),MAXMAG(2) / 32767, -1 /	DPPR0990
C	DATA MAXMAG(3),MAXMAG(4) / -1, -1 /	DPPR1000
C		DPPR1010
C	DATA MCHEPS(1),MCHEPS(2) / 0022400, 0000000 /	DPPR1020
C	DATA MCHEPS(3),MCHEPS(4) / 0000000, 0000000 /	DPPR1030
C		DPPR1040
C	DATA MINMAG(1),MINMAG(2) / 0000200, 0000000 /	DPPR1050
C	DATA MINMAG(3),MINMAG(4) / 0000000, 0000000 /	DPPR1060
C		DPPR1070
C	DATA MAXMAG(1),MAXMAG(2) / 0077777, 0177777 /	DPPR1080

C	DATA MAXMAG(3),MAXMAG(4) / 0177777, 0177777 /	DPPR1090
C		DPPR1100
C	MACHINE CONSTANTS FOR THE BURROUGHS 6700/7700 SYSTEMS.	DPPR1110
C		DPPR1120
C	DATA MCHEPS(1) / 014510000000000000 /	DPPR1130
C	DATA MCHEPS(2) / 000000000000000000 /	DPPR1140
C		DPPR1150
C	DATA MINMAG(1) / 017710000000000000 /	DPPR1160
C	DATA MINMAG(2) / 077700000000000000 /	DPPR1170
C		DPPR1180
C	DATA MAXMAG(1) / 007777777777777777 /	DPPR1190
C	DATA MAXMAG(2) / 077777777777777777 /	DPPR1200
C		DPPR1210
C	MACHINE CONSTANTS FOR THE BURROUGHS 5700 SYSTEM.	DPPR1220
C		DPPR1230
C	DATA MCHEPS(1) / 014510000000000000 /	DPPR1240
C	DATA MCHEPS(2) / 000000000000000000 /	DPPR1250
C		DPPR1260
C	DATA MINMAG(1) / 017710000000000000 /	DPPR1270
C	DATA MINMAG(2) / 000000000000000000 /	DPPR1280
C		DPPR1290
C	DATA MAXMAG(1) / 007777777777777777 /	DPPR1300
C	DATA MAXMAG(2) / 000077777777777777 /	DPPR1310
C		DPPR1320
C	MACHINE CONSTANTS FOR THE BURROUGHS 1700 SYSTEM.	DPPR1330
C		DPPR1340
C	DATA MCHEPS(1) / ZCC6800000 /	DPPR1350
C	DATA MCHEPS(2) / Z000000000 /	DPPR1360
C		DPPR1370
C	DATA MINMAG(1) / ZC00800000 /	DPPR1380
C	DATA MINMAG(2) / Z000000000 /	DPPR1390
C		DPPR1400
C	DATA MAXMAG(1) / ZDFFFFFFF /	DPPR1410
C	DATA MAXMAG(2) / ZFFFFFFF /	DPPR1420
C		DPPR1430
C	MACHINE CONSTANTS FOR THE UNIVAC 1100 SERIES.	DPPR1440
C		DPPR1450
C	DATA MCHEPS(1),MCHEPS(2) / 0170640000000, 0000000000000 /	DPPR1460
C	DATA MINMAG(1),MINMAG(2) / 0000040000000, 0000000000000 /	DPPR1470
C	DATA MAXMAG(1),MAXMAG(2) / 0377777777777, 0777777777777 /	DPPR1480
C		DPPR1490
C	MACHINE CONSTANTS FOR THE DATA GENERAL ECLIPSE S/200.	DPPR1500
C		DPPR1510
C	NOTE - IT MAY BE APPROPRIATE TO INCLUDE THE FOLLOWING CARD -	DPPR1520
C	STATIC DMACH(3)	DPPR1530
C		DPPR1540
C	DATA MINMAG/20K,3*0/,MAXMAG/77777K,3*177777K/	DPPR1550
C	DATA MCHEPS/32020K,3*0/	DPPR1560
C		DPPR1570
C	MACHINE CONSTANTS FOR THE HARRIS 220.	DPPR1580
C		DPPR1590
C	DATA MCHEPS(1),MCHEPS(2) / '20000000, '00000334 /	DPPR1600
C	DATA MINMAG(1),MINMAG(2) / '20000000, '00000201 /	DPPR1610
C	DATA MAXMAG(1),MAXMAG(2) / '37777777, '37777577 /	DPPR1620

C		DPPR1630
C	MACHINE CONSTANTS FOR THE CRAY-1.	DPPR1640
C		DPPR1650
C	DATA MCHEPS(1) / 037642400000000000000000B /	DPPR1660
C	DATA MCHEPS(2) / 000000000000000000000000B /	DPPR1670
C		DPPR1680
C	DATA MINMAG(1) / 020003400000000000000000B /	DPPR1690
C	DATA MINMAG(2) / 000000000000000000000000B /	DPPR1700
C		DPPR1710
C	DATA MAXMAG(1) / 057777777777777777777777B /	DPPR1720
C	DATA MAXMAG(2) / 0000007777777777777777776B /	DPPR1730
C		DPPR1740
C	MACHINE CONSTANTS FOR THE PRIME 400.	DPPR1750
C		DPPR1760
C	DATA MCHEPS(1),MCHEPS(2) / :10000000000, :00000000123 /	DPPR1770
C	DATA MINMAG(1),MINMAG(2) / :10000000000, :00000100000 /	DPPR1780
C	DATA MAXMAG(1),MAXMAG(2) / :17777777777, :37777677776 /	DPPR1790
C		DPPR1800
	DPMPAR = DMACH(I)	DPPR1810
	RETURN	DPPR1820
C		DPPR1830
C	LAST CARD OF FUNCTION DPMPAR.	DPPR1840
C		DPPR1850
	END	DPPR1860

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