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USER GUIDE FOR MINPACK-1

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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 Hillstrom [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, Iltel AS/6, and ICL 2980. At Argonne, software performance has been further measured with the help of WATFIV and BRANGL (Fosdick [1974]). WATFIV detects run-time errors such as undefined variables and out-of-range subscripts, while BRANGL 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 FORTRAN 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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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 Belaire Blvd.
Houston, TX 77036
Phone: (713) 777-1977

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

\[
f_i(x_1, x_2, \ldots, x_n) = 0, \quad 1 \leq i \leq n.
\]

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

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

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 MNPACK-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

\[
f_i(x_1, x_2, \ldots, x_n) = 0, \quad 1 \leq i \leq n
\]
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
$f_1, f_2, \ldots, f_n$. 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
$f_1, f_2, \ldots, f_n$ 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

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

by a modification of the Levenberg-Marquardt algorithm. The principal requirements of the subroutines are as follows (see also Figure 7).

**LMDIF1, LMDIF**

The user must provide a subroutine to calculate the functions $f_1, f_2, \ldots, f_m$. 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 $f_1, f_2, \ldots, f_m$ 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 $f_1, f_2, \ldots, f_m$ 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.
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:

\[ \beta^{1-z} \], the machine precision,
\[ \beta^{e_{\text{min}} - 1} \], the smallest magnitude,
\[ (1 - \beta^{-z}) \beta^{e_{\text{max}}} \], the largest magnitude,

where \( z \) is the number of base \( \beta \) digits on the machine, \( e_{\text{min}} \) is the smallest machine exponent, and \( e_{\text{max}} \) is the largest machine exponent.

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

\[ |b-a| \leq c_m |a| , \]
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.

DOLEG
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.
LMFAR
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 \( \Delta \), 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 \( A \).

R1MPYQ
This subroutine multiplies a matrix by an orthogonal matrix given as a product of Givens rotations.

RIJUPDT
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 \( A \).
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 \( \mathbb{R}^n \) 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 \( \mathbb{R}^n \) and range in \( \mathbb{R}^m \) is denoted by \( F: \mathbb{R}^n \rightarrow \mathbb{R}^m \). 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 \( f_i: \mathbb{R}^n \rightarrow \mathbb{R} \) 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 \( F: \mathbb{R}^n \rightarrow \mathbb{R}^n \), and a solution vector \( x^* \) in \( \mathbb{R}^n \) is such that

\[ F(x^*) = 0. \]

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

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

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 \( F: \mathbb{R}^n \rightarrow \mathbb{R}^m \); that is, the \( m \times n \) 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 \( f: \mathbb{R}^n \rightarrow \mathbb{R} \), which is the mapping \( \nabla f: \mathbb{R}^n \rightarrow \mathbb{R}^n \) defined by

\[ \nabla f(x) = \begin{bmatrix} \frac{\partial f(x)}{\partial x_1} \\ \frac{\partial f(x)}{\partial x_2} \\ \vdots \\ \frac{\partial f(x)}{\partial x_n} \end{bmatrix}. \]

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 $F: \mathbb{R}^n \times \mathbb{R}^m$, 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

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

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 \( \Delta \), and an approximation \( J \) to the Jacobian matrix of \( F \) at \( x \). Users of the core subroutines can specify initial values \( D_0 \) and \( \Delta_0 \); in the easy-to-use drivers \( D_0 \) and \( \Delta_0 \) 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

\[ \min \{ \|f + Jp\| : \|Dp\| \leq \Delta \} \tag{2} \]

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 \( \Delta \) 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, \( D \), \( \Delta \), and \( J \) are also replaced.

The motivation for using (2) to obtain the correction \( p \) is that for appropriate choices of \( J \) and \( \Delta \), 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

\[ \|D(x-x^*)\| \leq \Delta \tag{3} \]

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 \( p \) that minimizes \( \| x^* p \| \) in a two-dimensional subspace of the ellipsoid \( \{ p : \| D p \| \leq \Lambda \} \). The nonlinear least squares algorithm obtains a \( p \) that is the exact solution of (2) with a small (10%) perturbation of \( \Delta \). 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

\[
\| D(x-x^*) \| \leq \text{XTOL} \cdot \| D x^* \|,
\]

where \( \text{XTOL} \) 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) \[ \| F(x) \| \leq (1 + FTOL) \cdot \| F(x^*) \| , \]

where $FTOL$ is a second user-supplied tolerance.

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

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

where $a_1, a_2, \ldots, a_n$ 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 = 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 $\Delta$. That is, the actual convergence test is

$$\Delta \leq \text{XTOL} \cdot \|Dx\|.$$  

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 $\text{FTOL} = 10^{-k}$, then $\|F(x)\|$ has $k$ significant digits, but $x$ may not be as accurate. For example, if $\text{FTOL} = 10^{-6}$ 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 $\text{FTOL} = 10^{-6}$, but (1) is only satisfied with $\text{XTOL} = 10^{-3}$.

In many least squares problems, if $\text{FTOL} = (\text{XTOL})^2$ 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 $\text{XTOL} = 10^{-3}$ 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

\[
\text{ACTRED} = \left( \| \mathbf{f} \| - \| \mathbf{f}_+ \| / \| \mathbf{f} \| ,
\]

while the (relative) predicted reduction is

\[
\text{PRERED} = \left( \| \mathbf{f} \| - \| \mathbf{f}_+ J \mathbf{p} \| / \| \mathbf{f} \| .
\]

The \( F \)-convergence test then requires that

\[
\text{PRERED} \leq \text{FTOL}
\]

\[
|\text{ACTRED}| \leq \text{FTOL}
\]

\[
\text{ACTRED} \leq 2 \cdot \text{PRERED}
\]

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

\[
(4) \quad ||r|| \leq AFTOL,
\]

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

$$f(x + h e_j) - f(x)$$

\[ h_j \]

(1)

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,

\[ h_j = (EPSFCN)^{1/2} |x_j| \]

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 \( a_1, a_2, \ldots, a_n \) are the columns of \( A \). It is now easy to verify that the solution of the problem
\[ \min \{ \| J - J \|_D : \tilde{J}p = F(x^p) - F(x) \} , \]

is given by
\[ J_+ = J + \left( \frac{F(x^p) - F(x) - Jp}{\| Dp \|^2} \right) (D^T Dp)^T . \]

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
\[ \tilde{F}(x) = \alpha F(D_V x) \]
\[ \tilde{x}_o = D_V^{-1} x_o , \]

where \( \alpha \) is a positive scalar and \( D_V \) is a diagonal matrix with positive entries, the approximations \( \tilde{x} \) and \( \tilde{x}_o \) 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
\[ (1) \quad \tilde{D}_o = \alpha D_V D_o , \]

where \( D_o \) and \( \tilde{D}_o \) are the initial scaling matrices of the respective problems defined by \( F \) and \( x_o \) and by \( \tilde{F} \) and \( \tilde{x}_o \). If the user of the core subroutines has
requested internal scaling (MODE = 1), then the internal scaling matrix is set to

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

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

$$\tilde{F}(x) = D_0 F(x),$$

$$\tilde{x}_0 = x_0,$$
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

$$\|F(x_*)\| > \|F(x)\|.$$

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 MTNPACK-1 algorithms require that the user provide a subroutine with name of his choosing, say FCN, to calculate the residuals of the function $F: \mathbb{R}^m \to \mathbb{R}^m$, where $m = n$ for systems of nonlinear equations and $m > n$ 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.

$$\tau = g(x)$$

For $i = 1, 2, \ldots, m$

$$f_i(x) = \tau + h_i(x).$$

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 \( \alpha_{ij} \) and \( \beta_{ij} \) are given constants. The following program segment evaluates the \( f_i \) efficiently.

For \( i = 1, 2, \ldots, m \)
\[
f_i(x) = 0
\]
For \( j = 1, 2, \ldots, n \)
\[
    \gamma = \cos(x_j) \\
    \omega = \sin(x_j)
\]
For \( i = 1, 2, \ldots, m \)
\[
f_i(x) = f_i(x) + \gamma \alpha_{ij} + \omega \beta_{ij} .
\]

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 \( \alpha_{ij} \) and \( \beta_{ij} \) 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 \( j = 1, 2, \ldots, n \)
\[
\gamma = \cos(x_j) \\
\nu = \sin(x_j)
\]
For \( i = 1, 2, \ldots, m \)
\[
\frac{\partial f_i(x)}{\partial x_j} = -\alpha_{ij} + \beta_{ij}.
\]

The previous example illustrates further the possibility of common subexpressions 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
\[
\tau = g(x)
\]
Save \( \tau \) in COMMON
For \( i = 1, 2, \ldots, m \)
\[
f_i(x) = \tau^2 + h_i(x)
\]
If JACOBIAN EVALUATION then
\[
v = \nabla g(x)
\]
For \( i = 1, 2, \ldots, m \)
\[
\nabla f_i(x) = 2\tau v + \nabla h_i(x).
\]
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 $\mathbb{R}^n$.

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 $\mu$ 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
\[ \|D_0 p_0\| \leq \Delta_0 , \]

where \( D_0 \) is a diagonal scaling matrix and \( \Delta_0 \) is a step bound. The contents of \( D_0 \) are governed by the parameter MODE. If \( \text{MODE} = 1 \) then \( D_0 \) is internally set, while if \( \text{MODE} = 2 \) then \( D_0 \) is specified by the user through the array DIAG. The step bound \( \Delta_0 \) is determined from the parameter FACTOR. By definition

\[ \Delta_0 = \text{FACTOR} \cdot \|D_0 x_0\| , \]

unless \( x_0 \) is the zero vector, in which case

\[ \Delta_0 = \text{FACTOR} . \]

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 \( x_0 + p_0 \) will be found that belongs to \( D \).

Be aware that the step restriction is on \( D_0 p_0 \) and not on \( p_0 \) directly. A small element of \( D_0 \), which can be set by internal scaling when \( \text{MODE} = 1 \), may lead to a large component in the correction \( p_0 \). In many cases it is not necessary to control \( p_0 \) directly, but if this is desired then \( \text{MODE} = 2 \) must be used.

When \( \text{MODE} = 2 \), the contents of \( D_0 \) are specified by the user, and this allows direct control of \( p_0 \). If, for example, it is desired to restrict the components of \( p_0 \) to small relative corrections of the corresponding components of \( x_0 \) (assumed nonzero), then this can be done by setting

\[ D_0 = \text{diag} \left( \frac{1}{|z_1|}, \frac{1}{|z_2|}, \ldots, \frac{1}{|z_n|} \right) , \]

where \( z_i \) is the \( i \)-th component of \( x_0 \), and by choosing FACTOR appropriately. To justify this choice, note that \( p_0 \) satisfies

\[ \|D_0 p_0\| \leq \Delta_0 = \text{FACTOR} \cdot \|D_0 x_0\| , \]

and that the choice of \( D_0 \) guarantees that...
\[ \|D_0 x_0\| = n^{\frac{1}{2}}. \]

Thus, if \( \rho_i \) is the \( i \)-th component of \( p_0 \), then
\[ |\rho_i| \leq n^{\frac{1}{2}} \text{FACTOR} \cdot |\xi_i|, \]

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 \( F: \mathbb{R}^n \rightarrow \mathbb{R}^m \) define a nonlinear least squares problem \((m \geq n)\), and let \( x^* \) be a solution. Given \( \epsilon > 0 \), the problem is to determine sensitivity (upper) bounds \( \sigma_1, \sigma_2, \ldots, \sigma_n \) 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
\[ \|F(x)\| \leq (1 + \epsilon)F(x^*)\|. \]

Of particular interest are values of \( \sigma_i \) 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 \( \sigma_i \) shows that
\[
(1) \quad \sigma_i = c^{\frac{1}{2}} \left( \frac{\|F(x^*)\|}{\|F'(x^*)e_i\|} \right),
\]

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 \( \|F'(x^*)e_i\| \) 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

$$
\sigma_i \approx \varepsilon \frac{\|F(x)\|}{\|J_{i*}\|}
$$

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

$$
JP = QR
$$

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

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

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

$$
J_{e_p(j)} = QR e_j,
$$

and hence,

$$
\|J_{e_p(j)}\| = \|Re_j\|.
$$

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

```plaintext
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 $\varepsilon > 0$ and a vector $v$ with $\|v\| = 1$, the problem is to determine a bound $\sigma$ such that

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

A first order estimate of $\sigma$ is now

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

if $\|F'(x^*)\cdot v\|$ is small relative to $\|F(x^*)\|$, then $\sigma$ 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

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

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

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

is used for this purpose.
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

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

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 $R$

$$ |r_{kk}| > |r_{ij}|, \quad k \leq i \leq j, \quad (5) $$
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,LDJAC,.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,LDK,IPVT,TOL,WA)
INTEGER N,LDK
INTEGER IPVT(N)
DOUBLE PRECISION TOL
DOUBLE PRECISION R(LDR,N),WA(N)

**************

SUBROUTINE COVAR
GIVEN AN M BY N MATRIX A, THE PROBLEM IS TO DETERMINE
THE COVARIANCE MATRIX CORRESPONDING TO A, DEFINED AS

T
INVERSE(A *A) .

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*A = 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 COVAR EXPECTS
THE FULL UPPER TRIANGLE OF R AND THE PERMUTATION MATRIX P.
THE COVARIANCE MATRIX IS THEN COMPUTED AS

T
P*INVERSE(R *R)*P
.

IF A IS NEARLY RANK DEFICIENT, IT MAY BE DESIRABLE TO COMPUTE
THE COVARIANCE MATRIX CORRESPONDING TO THE LINEARLY INDEPENDENT
COLUMNS OF A. TO DEFINE THE NUMERICAL RANK OF A, COVAR USES
THE TOLERANCE TOL. IF L IS THE LARGEST INTEGER SUCH THAT

ABS(R(L,L)) .GT. TOL*ABS(R(1,1)) ,

THEN COVAR COMPUTES THE COVARIANCE MATRIX CORRESPONDING TO
THE FIRST L COLUMNS OF R. FOR K GREATER THAN L, COLUMN
AND ROW IPVT(K) OF THE COVARIANCE MATRIX ARE SET TO ZERO.

THE SUBROUTINE STATEMENT IS

SUBROUTINE COVAR(N,R,LDK,IPVT,TOL,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
R CONTAINS THE SQUARE SYMMETRIC COVARIANCE MATRIX.

LDK IS A POSITIVE INTEGER INPUT VARIABLE NOT LESS THAN N
WHICH SPECIFIES THE LEADING DIMENSION OF THE ARRAY R.

IPVT IS AN INTEGER INPUT ARRAY OF LENGTH N WHICH DEFINES THE
PERMUTATION MATRIX P SUCH THAT A*P = Q*R. COLUMN J OF P
IS COLUMN IPVT(J) OF THE IDENTITY MATRIX.

TOL IS A NONNEGATIVE INPUT VARIABLE, USED TO DEFINE THE
NUMERICAL RANK OF A IN THE MANNER DESCRIBED ABOVE.

WA IS A WORK ARRAY OF LENGTH N.

SUBPROGRAMS CALLED

FORTRAN-SUPPLIED ... DABS

ARGONNE NATIONAL LABORATORY. MINPACK PROJECT. AUGUST 1980.
BURTON S. GARROW, KENNETH E. HILLSTROM, JORGE J. MORE

************
INTEGER I,II,J,JJ,K,KM1,L
LOGICAL SING
DOUBLE PRECISION ONE,TEMP,TOLR,ZERO
DATA ONE,ZERO /1.0D0,0.0D0/

FORM THE INVERSE OF R IN THE FULL UPPER TRIANGLE OF R.

TOLR = TOL*DABS(R(1,1))
L = 0
DO 40 K = 1, N
   IF (DABS(R(K,K)) .LE. TOLR) GO TO 50
   R(K,K) = ONE/R(K,K)
   KM1 = K - 1
   IF (KM1 .LT. 1) GO TO 30
   DO 20 J = 1, KM1
      TEMP = R(K,K)*R(J,K)
      R(J,K) = ZERO
      DO 10 I = 1, J
         R(I,K) = R(I,K) - TEMP*R(I,J)
          10 CONTINUE
    20 CONTINUE
30 CONTINUE
L = K
40 CONTINUE
50 CONTINUE

FORM THE FULL UPPER TRIANGLE OF THE INVERSE OF (R TRANSPOSE)*R
IN THE FULL UPPER TRIANGLE OF R.

IF (L .LT. 1) GO TO 110
DO 100 K = 1, L
   KM1 = K - 1
   IF (KM1 .LT. 1) GO TO 80
   DO 70 J = 1, KM1
      TEMP = R(J,K)
      DO 60 I = 1, J
         R(I,J) = R(I,J) + TEMP*R(I,K)
            60 CONTINUE
   70 CONTINUE
100 CONTINUE
110 CONTINUE
70     CONTINUE
80     CONTINUE
      TEMP = R(K,K)
   DO 90 I = 1, K
      R(I,K) = TEMP*R(I,K)
   90     CONTINUE
100    CONTINUE
110    CONTINUE

C FORM THE FULL LOWER TRIANGLE OF THE COVARIANCE MATRIX
C IN THE STRICT LOWER TRIANGLE OF R AND IN WA.
C
DO 130 J = 1, N
   JJ = IPVT(J)
   SING = J .GT. L
   DO 120 I = 1, J
      IF (SING) R(I,J) = ZERO
      II = IPVT(I)
      IF (II .GT. JJ) R(II,JJ) = R(I,J)
      IF (II .LT. JJ) R(JJ,II) = R(I,J)
   120    CONTINUE
   WA(JJ) = R(J,J)
130    CONTINUE

C SYMMETRIZE THE COVARIANCE MATRIX IN R.
C
DO 150 J = 1, N
   DO 140 I = 1, J
      R(I,J) = R(J,I)
   140    CONTINUE
   R(J,J) = WA(J)
150    CONTINUE
RETURN

C LAST CARD OF SUBROUTINE COVAR.
C
END
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 Bluee'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 RWUPDT is based on the work of Gill, Golub, Murray, and Saunders [1974].

References


