

This subroutine has the interface for calling the function *lmder* from MINPACK. *lmder* is a modified levenberg-marquardt algorithm with analytically calculated jacobian.

[called by: [solvers](#).]

[calls: [packdof](#).]

General

Levenberg-Marquardt algorithm is one of the most famous minimization algorithms. There is a brief introduction on Wikipedia. In FOCUS, we use the subroutine *lmder* from MINPACK.

Documentation

The cost functions (targets) are stored in **LM_fvec(1:LM_mfvec)**, and the jacobian is stored in **LM_fjac(1:LM_mfvec, 1:Ndof)**. The number of targets (**LM_mfvec**) must be not be smaller than the number of parameters (**Ndof**).

The targets are consistant of different terms. The following table lists the details. Here are the comments from *lmder*. The four

Table 1: **LM_fvec** components

cost functions	physiccal meaning	switch	length
bnormal	$\mathbf{B} \cdot \mathbf{n}$ on each surface element	weight_bnorm > 0	Nteta*Nzeta
bmnharm	$wBmn_i(Bmn_i - Bmn_i^o)$ for each reasonant harmonics	weight_bharm > 0	2*NBmn in <i>target.harmonics</i>
torflux	$\Psi_i - \Psi_o$ at each toroidal cross-sections	weight_tflux > 0	Nzeta
length	length penalty of each coil, $L_i - L_o$ or $\exp(L_i)/\exp L_o$	weight_ttlen > 0	Ncoils - Nfixgeo
surfsep	potential energy between each coil and a control surface	weight_cssep > 0	Ncoils - Nfixgeo

input parameters for L-M optimizer are **LM_maxiter**, **LM_xtol**, **LM_ftol** and **LM_factor**. Please look at [initial](#) for more details.

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c      the subroutine statement is
c
c      subroutine lmder (fcn , m , n , x , fvec , fjac , ldfjac , ftol , xtol , gtol ,
c                      maxfev , diag , mode , factor , nprint , info , nfev ,
c                      njev , ipvt , qtf , wa1 , wa2 , wa3 , wa4 )
c
c      where
c
c      fcn is the name of the user supplied subroutine which
c      calculates the functions and the jacobian. fcn must
c      be declared in an external statement in the user
c      calling program, and should be written as follows.
c
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      if iflag = 1 calculate the functions at x and
c      return this vector in fvec. do not alter fjac.
c      if iflag = 2 calculate the jacobian at x and
c      return this matrix in fjac. do not alter fvec.
c
c      return
c      end
c
c      the value of iflag should not be changed by fcn unless
c      the user wants to terminate execution of lmder.
c      in this case set iflag to a negative integer.
c
c      m is a positive integer input variable set to the number
c      of functions.
c
c      n is a positive integer input variable set to the number
c      of variables. n must not exceed m.
c
c      x is an array of length n. on input x must contain
c      an initial estimate of the solution vector. on output x
c      contains the final estimate of the solution vector.
c

```

c fvec is an output array of length m which **contains**
 c the functions evaluated at the output x.
 c

c fjac is an output m by n array. the upper n by n submatrix
 c of fjac **contains** an upper triangular matrix r with
 c diagonal elements of nonincreasing magnitude such that
 c

$$c \quad \quad \quad \begin{matrix} t & & t & & t \\ p & *(jac & *jac)*p = r & *r, \end{matrix}$$

c **where** p is a permutation matrix and jac is the final
 c calculated jacobian. column j of p is column ipvt(j)
 c (see below) of the identity matrix. the lower trapezoidal
 c part of fjac **contains** information generated during
 c the computation of r.
 c

c ldjfjac is a positive **integer** input variable not less than m
 c which specifies the leading **dimension** of the array fjac.
 c

c ftol is a nonnegative input variable. termination
 c occurs when both the actual and predicted relative
 c reductions **in** the sum of squares are at most ftol.
 c therefore, ftol measures the relative error desired
 c **in** the sum of squares.
 c

c xtol is a nonnegative input variable. termination
 c occurs when the relative error between two consecutive
 c iterates is at most xtol. therefore, xtol measures the
 c relative error desired **in** the approximate solution.
 c

c gtol is a nonnegative input variable. termination
 c occurs when the cosine of the angle between fvec and
 c any column of the jacobian is at most gtol **in** absolute
 c value. therefore, gtol measures the orthogonality
 c desired between the **function** vector and the columns
 c of the jacobian.
 c

c maxfev is a positive **integer** input variable. termination
 c occurs when the **number** of calls to fcn with iflag = 1
 c has reached maxfev.
 c

c diag is an array of length n. **if** mode = 1 (see
 c below), diag is internally set. **if** mode = 2, diag
 c must contain positive entries that serve as
 c multiplicative scale factors for the variables.
 c

c mode is an **integer** input variable. **if** mode = 1, the
 c variables will be scaled internally. **if** mode = 2,
 c the scaling is specified by the input diag. other
 c values of mode are equivalent to mode = 1.
 c

c factor is a positive input variable used **in** determining the
 c initial step bound. this bound is set to the product of
 c factor and the euclidean norm of diag*x **if** nonzero, or **else**
 c to factor itself. **in** most cases factor should lie **in** the
 c interval (.1,100.).100. is a generally recommended value.
 c

c nprint is an **integer** input variable that enables controlled
 c printing of iterates **if** it is positive. **in** this **case**,
 c fcn is called with iflag = 0 at the beginning of the first
 c iteration and every nprint iterations thereafter and
 c immediately prior to **return**, with x, fvec, and fjac
 c available for printing. fvec and fjac should not be
 c altered. **if** nprint is not positive, no special calls
 c of fcn with iflag = 0 are made.
 c

c info is an **integer** output variable. **if** the user has
 c terminated execution, info is set to the (negative)
 c value of iflag. see description of fcn. otherwise,
 c info is set as follows.
 c

```

c      info = 0  improper input parameters.
c
c      info = 1  both actual and predicted relative reductions
c                in the sum of squares are at most ftol.
c
c      info = 2  relative error between two consecutive iterates
c                is at most xtol.
c
c      info = 3  conditions for info = 1 and info = 2 both hold.
c
c      info = 4  the cosine of the angle between fvec and any
c                column of the jacobian is at most gtol in
c                absolute value.
c
c      info = 5  number of calls to fcn with iflag = 1 has
c                reached maxfev.
c
c      info = 6  ftol is too small. no further reduction in
c                the sum of squares is possible.
c
c      info = 7  xtol is too small. no further improvement in
c                the approximate solution x is possible.
c
c      info = 8  gtol is too small. fvec is orthogonal to the
c                columns of the jacobian to machine precision.
c
c      nfev is an integer output variable set to the number of
c                calls to fcn with iflag = 1.
c
c      njev is an integer output variable set to the number of
c                calls to fcn with iflag = 2.
c
c      ipvt is an integer output array of length n. ipvt
c                defines a permutation matrix p such that jac*p = q*r,
c                where jac is the final calculated jacobian, q is
c                orthogonal (not stored), and r is upper triangular
c                with diagonal elements of nonincreasing magnitude.
c                column j of p is column ipvt(j) of the identity matrix.
c
c      qtf is an output array of length n which contains
c                the first n elements of the vector (q transpose)*fvec.
c
c      wa1, wa2, and wa3 are work arrays of length n.
c
c      wa4 is a work array of length m.
c
c      subprograms called
c
c      user supplied ..... fcn
c
c      minpack supplied ... dpmpar,enorm,lmpar,qrfac
c
c      fortran supplied ... dabs,dmax1,dmin1,dsqrt,mod
c
c      argonne national laboratory. minpack project. march 1980.
c      burton s. garbow, kenneth e. hillstom, jorge j. more

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