

Package ‘nleqslv’

August 10, 2014

Type Package

Title Solve systems of non linear equations

Version 2.4

Date 2014-08-10

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Description Solve a system of non linear equations using a Broyden or a Newton method with a choice of global strategies such as line search and trust region. There are options for using a numerical or user supplied Jacobian and for specifying that a numerical Jacobian is banded.

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NeedsCompilation yes

Repository CRAN

Date/Publication 2014-08-10 00:24:19

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Description

The **nleqslv** package provides two algorithms for solving (dense) non linear systems of equations. The methods provided are

- a Broyden Secant method where the matrix of derivatives is updated after each major iteration using the Broyden rank 1 update.
- a full Newton method where the Jacobian matrix of derivatives is recalculated at each iteration

Both methods utilise global strategies such as line search or trust region methods whenever the standard Newton/Broyden step does not lead to a point closer to a root of the equation system. Line search may be either quadratic or geometric. The trust region methods are either the double dogleg, the Powell single dogleg method or a Levenberg-Marquardt type method.

There is a facility for specifying that the jacobian is banded; this can significantly speedup the calculation of a numerical Jacobian when the number of sub- and super diagonals is small compared to the size of the system of equations. For example the Jacobian of a tridiagonal system can be calculated with only three evaluations of the function.

The algorithms provided in this package are derived from Dennis and Schnabel (1996). The code is written in Fortran 77 and Fortran 95 and uses Lapack and BLAS routines as provided by the R system.

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References

Dennis, J.E. Jr and Schnabel, R.B. (1996), *Numerical Methods for Unconstrained Optimization and Nonlinear Equations*, Siam.

Description

The function solves a system of non linear equations with either a Broyden or a full Newton method. It provides line search and trust region global strategies for difficult systems.

Usage

```
nleqslv(x, fn, jac=NULL,...,
        method = c("Broyden", "Newton"),
        global = c("dbldog", "pwldog", "cline", "qline", "gline", "hook", "none"),
        xscalm = c("fixed", "auto"),
        jacobian=FALSE,
        control = list()
)
```

Arguments

x	A list or numeric vector of starting estimates.
fn	A function of x returning the function values.
jac	A function to return the Jacobian for the fn function. If not supplied numerical derivatives will be used.
...	Further arguments to be passed to fn and jac.
method	The method used for finding a solution. See ‘Details’.
global	The global strategy to apply. See ‘Details’.
xscalm	The type of x scaling to use. See ‘Details’.
jacobian	A logical indicating if the estimated (approximate) jacobian in the solution should be returned. See ‘Details’.
control	A list of control parameters. See ‘Details’.

Details

The algorithms implemented in `nleqslv` are based on Dennis and Schnabel (1996).

Method Broyden starts with a computed Jacobian of the function and then updates this Jacobian after each successful iteration using the so-called Broyden update. This method often shows super linear convergence towards a solution. When `nleqslv` determines that it cannot continue with the current Broyden matrix it will compute a new Jacobian.

Method Newton calculates a Jacobian of the function `fn` at each iteration. Close to a solution this method will usually show quadratic convergence.

Both methods apply a so-called (backtracking) global strategy to find a better (more acceptable) iterate. The function criterion used by the algorithm is the sum of squares of the function values and “acceptable” means sufficient decrease of the current function criterion value compared to that of the previous iteration. A comprehensive discussion of these issues can be found in Dennis and Schnabel (1996). Both methods apply a QR-decomposition to the Jacobian as implemented in Lapack. The Broyden method applies a rank-1 update to the Jacobian at the end of each iteration and uses a modified version of the algorithm described in Dennis and Schnabel (1996).

The `global` argument indicates which global strategy to use or to use no global strategy

`cline` a cubic line search

`qline` a quadratic line search

`gline` a geometric line search

`dbldog` a trust region method using the double dogleg method as described in Dennis and Schnabel (1996)

`pwldog` a trust region method using the Powell dogleg method as developed by Powell (1970).

`hook` a trust region method described by Dennis and Schnabel (1996) as *The locally constrained optimal ("hook") step*. It is equivalent to a Levenberg-Marquardt algorithm described in Moré (1978) and Nocedal and Wright (2006).

`none` Only a pure local Newton or Broyden iteration is used. The maximum stepsize (see below) is taken into account. The default maximum number of iterations (see below) is set to 20.

The double dogleg method is the default global strategy employed by this package.

Which global strategy to use in a particular situation is a matter of trial and error. When one of the trust region methods fails, one of the line search strategies should be tried. Sometimes a trust region will work and sometimes a line search method; neither has a clear advantage but in many cases the double dogleg method works quite well.

The parameters x may be scaled during the search for a zero of fn . The `xscal` argument provides two possibilities for scaling

`fixed` the scaling factors are set to the values supplied in the `control` argument and remain unchanged during the iterations. The scaling factor of any element of x should be set to the inverse of the typical value of that element of x , ensuring that all elements of x are approximately equal in size.

`auto` the scaling factors are calculated from the euclidean norms of the columns of the Jacobian matrix. When a new Jacobian is computed, the scaling values will be set to the euclidean norm of the corresponding column if that is larger than the current scaling value. Thus the scaling values will not decrease during the iteration. This is the method described in Moré (1978). Usually manual scaling is preferable.

The algorithm cannot cope with a singular or ill-conditioned Jacobian. When a Jacobian becomes singular or very ill-conditioned the algorithm will return an error. A Jacobian is considered to be very ill-conditioned when the estimated inverse condition is less than or equal to a specified tolerance with a default value equal to 10^{-12} .

When the function to be solved returns non-finite function values for a parameter vector x and the algorithm is *not* evaluating a numerical Jacobian, then any non-finite values will be replaced by a large number forcing the algorithm to backtrack, i.e. decrease the line search factor or decrease the trust region radius. When the algorithm is evaluating a numerical Jacobian, it will stop with an error message on detecting non-finite function values. An error message will also be issued when a user supplied jacobian contains non-finite entries.

When the `jacobian` argument is set to `TRUE` the final Jacobian or Broyden matrix will be returned in the return list. The default value is `FALSE`; i.e. to not return the final matrix. There is no guarantee that the final Broyden matrix resembles the actual Jacobian.

The `control` argument is a list that can supply any of the following components:

`xtol` The relative steplength tolerance. When the relative steplength of all scaled x values is smaller than this value convergence is declared. The default value is 10^{-8} .

`ftol` The function value tolerance. Convergence is declared when the largest absolute function value is smaller than `ftol`. The default value is 10^{-8} .

- btol** The backtracking tolerance. When the relative steplength in a backtracking step to find an acceptable point is smaller than the backtracking tolerance, the backtracking is terminated. In the Broyden method a new Jacobian will be calculated if the Jacobian is outdated. The default value is 10^{-3} .
- cndtol** The tolerance of the test for ill conditioning of the Jacobian or Broyden approximation. If less than the machine precision it will be silently set to the machine precision. When the estimated inverse condition of the (approximated) Jacobian matrix is less than or equal to the value of **cndtol** the matrix is deemed to be ill-conditioned. The default value is 10^{-12} .
- sigma** Reduction factor for the geometric line search. The default value is 0.5.
- scalex** a vector of scaling values for the parameters. The inverse of a scale value is an indication of the size of a parameter. The default value is 1.0 for all scale values.
- maxit** The maximum number of major iterations. The default value is 150 if a global strategy has been specified. If no global strategy has been specified the default is 20.
- trace** Non-negative integer. A value of 1 will give a detailed report of the progress of the iteration. For a description see [Iteration report](#).
- chkjac** A logical value indicating whether to check a user supplied Jacobian, if supplied. The default value is FALSE. The first 10 errors are printed. The code for this check is derived from the code in Bouaricha and Schnabel (1997).
- delta** Initial (scaled) trust region radius. A value of -1.0 or "cauchy" is replaced by the length of the Cauchy step in the initial point. A value of -2.0 or "newton" is replaced by the length of the Newton step in the initial point. Any numeric value less than or equal to 0 and not equal to -2.0 , will be replaced by -1.0 ; the algorithm will then start with the length of the Cauchy step in the initial point. If it is numeric and positive it will be set to the smaller of the value supplied or the maximum stepsize. If it is not numeric and not one of the permitted character strings then an error message will be issued. The default is -2.0 .
- stepmax** Maximum scaled stepsize. If this is negative then the maximum stepsize is set to the largest positive representable number. The default is -1.0 , so there is no default maximum stepsize.
- dsub** Number of non zero subdiagonals of a banded Jacobian. The default is to assume that the Jacobian is *not* banded. Must be specified if **dsuper** has been specified and must be larger than zero when **dsuper** is zero.
- dsuper** Number of non zero super diagonals of a banded Jacobian. The default is to assume that the Jacobian is *not* banded. Must be specified if **dsub** has been specified and must be larger than zero when **dsub** is zero.

Value

A list containing components

- | | |
|---------------|--|
| x | final values for x |
| fvec | function values |
| termcd | termination code as integer. The values returned are |
| | 1 Function criterion is near zero. Convergence of function values has been achieved. |

	2 x-values within tolerance. This means that the relative distance between two consecutive x-values is smaller than <code>xtol</code> .
	3 No better point found. This means that the algorithm has stalled and cannot find an acceptable new point. This may or may not indicate acceptably small function values.
	4 Iteration limit <code>maxit</code> exceeded.
	5 Jacobian is too ill-conditioned.
	6 Jacobian is singular.
	-10 User supplied Jacobian is most likely incorrect.
<code>message</code>	a string describing the termination code
<code>scalex</code>	a vector containing the scaling factors, which will be the final values when automatic scaling was selected
<code>njcmt</code>	number of Jacobian evaluations
<code>nfcmt</code>	number of function evaluations, excluding those required for calculating a Jacobian and excluding the initial function evaluation (at iteration 0)
<code>iter</code>	number of outer iterations used by the algorithm. This excludes the initial iteration. The number of backtracks can be calculated as the difference between items <code>nfcmt</code> and <code>iter</code> of the outputlist.
<code>jac</code>	the final Jacobian or the Broyden approximation if <code>jacobian</code> was set to <code>TRUE</code> . If no iterations were executed, as may happen when the initial starting values are sufficiently close the solution, there is no Broyden approximation and the returned matrix will always be the actual Jacobian. If the matrix is singular or too ill-conditioned the returned matrix is of no value.

Warning

You cannot use this function recursively. Thus function `fn` should not in its turn call `nleqslv`.

References

- Bouaricha, A. and Schnabel, R.B. (1997), Algorithm 768: TENSOLVE: A Software Package for Solving Systems of Nonlinear Equations and Nonlinear Least-squares Problems Using Tensor Methods, *Transactions on Mathematical Software*, **23**, 2, pp. 174–195.
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Examples

```
# Dennis Schnabel example 6.5.1 page 149
dslnex <- function(x) {
  y <- numeric(2)
  y[1] <- x[1]^2 + x[2]^2 - 2
  y[2] <- exp(x[1]-1) + x[2]^3 - 2
  y
}

jacdsln <- function(x) {
  n <- length(x)
  Df <- matrix(numeric(n*n),n,n)
  Df[1,1] <- 2*x[1]
  Df[1,2] <- 2*x[2]
  Df[2,1] <- exp(x[1]-1)
  Df[2,2] <- 3*x[2]^2

  Df
}

BADjacdsln <- function(x) {
  n <- length(x)
  Df <- matrix(numeric(n*n),n,n)
  Df[1,1] <- 4*x[1]
  Df[1,2] <- 2*x[2]
  Df[2,1] <- exp(x[1]-1)
  Df[2,2] <- 5*x[2]^2

  Df
}

xstart <- c(2,0.5)
fstart <- dslnex(xstart)
xstart
fstart

# a solution is c(1,1)

nleqslv(xstart, dslnex, control=list(btol=.01))

# Cauchy start
nleqslv(xstart, dslnex, control=list(trace=1,btol=.01,delta=-1.0))

# Newton start
nleqslv(xstart, dslnex, control=list(trace=1,btol=.01,delta=-2.0))

# final Broyden approximation of Jacobian (quite good)
z <- nleqslv(xstart, dslnex, jacobian=TRUE,control=list(btol=.01))
z$x
z$jac
jacdsln(z$x)
```

```

# different initial start; not a very good final approximation
xstart <- c(0.5,2)
z <- nleqslv(xstart, dslnex, jacobian=TRUE,control=list(btol=.01))
z$x
z$jac
jacdsln(z$x)

## Not run:
# no global strategy but limit stepsize
# but look carefully: a different solution is found
nleqslv(xstart, dslnex, method="Newton", global="none", control=list(trace=1,stepmax=5))

# but if the stepsize is limited even more the c(1,1) solution is found
nleqslv(xstart, dslnex, method="Newton", global="none", control=list(trace=1,stepmax=2))

# Broyden also finds the c(1,1) solution when the stepsize is limited
nleqslv(xstart, dslnex, jacdsln, method="Broyden", global="none", control=list(trace=1,stepmax=2))

## End(Not run)

```

nleqslv-iterationreport

Detailed iteration report of nleqslv

Description

The format of the iteration report provided by nleqslv when the trace component of the control argument has been set to 1.

Details

All iteration reports consist of a series of columns with a header summarising the contents. Common column headers are

Iter Iteration counter

Jac Jacobian type. The Jacobian type is indicated by N for a Newton Jacobian or B for a Broyden updated matrix; optionally followed by the letter s indicating a totally singular matrix or the letter i indicating an ill-conditioned matrix. Unless the Jacobian is singular, the Jacobian type is followed by an estimate of the inverse condition number of the Jacobian in parentheses as computed by Lapack. This column will be blank when backtracking is active.

Fnorm square of the euclidean norm of function values / 2

Largest |f| infinity norm of $f(x)$ at the current point

Report for linesearch methods

A sample iteration report for the linesearch global methods (cline, qline and gline) is (some intercolumn space has been removed to make the table fit)

Iter	Jac	Lambda	Ftarg	Fnorm	Largest f
0				2.886812e+00	2.250000e+00
1	N(9.6e-03)	1.0000	2.886235e+00	5.787362e+05	1.070841e+03
1		0.1000	2.886754e+00	9.857947e+00	3.214799e+00
1		0.0100	2.886806e+00	2.866321e+00	2.237878e+00
2	B(2.2e-02)	1.0000	2.865748e+00	4.541965e+03	9.341610e+01

The column headed by Lambda shows the value of the line search parameter. The column headed by Ftarg follows from a sufficient decrease requirement and is the value below which Fnorm must drop if the current step is to be accepted.

Report for the pure method

The iteration report for the global method none is almost the same as the above report, except that the column labelled Ftarg is omitted. The column Lambda gives the ratio of the maximum stepsize and the length of the full Newton step. It is either exactly 1.0, indicating that the Newton step is smaller than the maximum stepsize and therefore used unmodified, or smaller than 1.0, indicating that the Newton step is larger than the maximum stepsize and therefore truncated.

Report for the double dogleg global method

A sample iteration report for the global method dbldog is (some intercolumn space has been removed to make the table fit)

Iter	Jac	Lambda	Eta	Dlt0	Dltn	Fnorm	Largest f
0						2.886812e+00	2.250000e+00
1	N(9.6e-03)	C	0.9544	0.4671	0.9343	1.699715e-01	5.421673e-01
1		W 0.0833	0.9544	0.9343	0.4671	1.699715e-01	5.421673e-01
2	B(1.1e-02)	W 0.1154	0.4851	0.4671	0.4671	1.277667e-01	5.043571e-01
3	B(7.3e-02)	W 0.7879	0.7289	0.4671	0.0759	5.067893e-01	7.973542e-01
3		C	0.7289	0.0759	0.1519	5.440250e-02	2.726084e-01
4	B(8.3e-02)	W 0.5307	0.3271	0.1519	0.3037	3.576547e-02	2.657553e-01
5	B(1.8e-01)	N	0.6674	0.2191	0.4383	6.566182e-03	8.555110e-02
6	B(1.8e-01)	N	0.9801	0.0376	0.0752	4.921645e-04	3.094104e-02
7	B(1.9e-01)	N	0.7981	0.0157	0.0313	4.960629e-06	2.826064e-03
8	B(1.6e-01)	N	0.3942	0.0029	0.0058	1.545503e-08	1.757498e-04
9	B(1.5e-01)	N	0.6536	0.0001	0.0003	2.968676e-11	5.983765e-06
10	B(1.5e-01)	N	0.4730	0.0000	0.0000	4.741792e-14	2.198380e-07
11	B(1.5e-01)	N	0.9787	0.0000	0.0000	6.451792e-19	8.118586e-10

After the column for the Jacobian the letters indicate the following

C a fraction (≤ 1.0) of the Cauchy or steepest descent step is taken where the fraction is the ratio of the trust region radius and the Cauchy steplength.

W a convex combination of the Cauchy and eta*(Newton step) is taken. The number in the column headed by Lambda is the weight of the partial Newton step.

P a fraction (≥ 1.0) of the partial Newton step, equal to eta*(Newton step), is taken where the fraction is the ratio of the trust region radius and the partial Newton steplength.

N a normal full Newton step is taken.

The number in the column headed by Eta is calculated from an upper limit on the ratio of the length of the steepest descent direction and the length of the Newton step. See Dennis and Schnabel (1996) pp.139ff for the details.

The column headed by Dlt0 gives the size of the trust region at the start of the current iteration. The column headed by DltN gives the size of the trust region when the current step has been accepted by the dogleg algorithm. The size of the trust region is decreased when the actual reduction of the function value norm does not agree well with the predicted reduction from the linear approximation of the function. And increased when the actual and predicted reduction are sufficiently close.

Normally the initial trust region radius is the same as the final trust region radius of the previous iteration but the size of the trust region is restricted by the size of the current Newton step. So when full Newton steps are being taken, the trust region radius at the start of an iteration may be less than the final value of the previous iteration.

Report for the single (Powell) dogleg global method

A sample iteration report for the global method pwldog is (some intercolumn space has been removed to make the table fit)

Iter	Jac	Lambda	Dlt0	DltN	Fnorm	Largest	f
0					2.886812e+00	2.250000e+00	
1	N(9.6e-03)	C	0.4671	0.9343	1.699715e-01	5.421673e-01	
1		W 0.0794	0.9343	0.4671	1.699715e-01	5.421673e-01	
2	B(1.1e-02)	W 0.0559	0.4671	0.4671	1.205661e-01	4.890487e-01	
3	B(7.3e-02)	W 0.5662	0.4671	0.0960	4.119560e-01	7.254441e-01	
3		W 0.0237	0.0960	0.1921	4.426507e-02	2.139252e-01	
4	B(8.8e-02)	W 0.2306	0.1921	0.3842	2.303135e-02	2.143943e-01	
4		W 0.4769	0.3842	0.1921	2.303135e-02	2.143943e-01	
5	B(1.9e-01)	N	0.1375	0.2750	8.014508e-04	3.681498e-02	

This is much simpler than the double dogleg report, since the (single) dogleg takes either a steepest descent step, a convex combination of the steepest descent and Newton steps or a full Newton step. The number in the column Lambda is the weight of the Newton step. The single dogleg method is a special case of the double dogleg method with eta equal to 1.

Report for the hook step global method

A sample iteration report for the global method hook is (some intercolumn space has been removed to make the table fit)

Iter	Jac	mu	dnorm	Dlt0	DltN	Fnorm	Largest	f
0						2.886812e+00	2.250000e+00	
1	N(9.6e-03)	H 0.1968	0.4909	0.4671	0.9343	1.806293e-01	5.749418e-01	
1		H 0.0366	0.9381	0.9343	0.4671	1.806293e-01	5.749418e-01	
2	B(2.5e-02)	H 0.1101	0.4745	0.4671	0.2336	1.797759e-01	5.635028e-01	
3	B(1.4e-01)	H 0.0264	0.2341	0.2336	0.4671	3.768809e-02	2.063234e-01	
4	B(1.6e-01)	N	0.0819	0.0819	0.1637	3.002274e-03	7.736213e-02	
5	B(1.8e-01)	N	0.0513	0.0513	0.1025	5.355533e-05	1.018879e-02	
6	B(1.5e-01)	N	0.0090	0.0090	0.0179	1.357039e-06	1.224357e-03	
7	B(1.5e-01)	N	0.0004	0.0004	0.0008	1.846111e-09	6.070166e-05	

```
8 B(1.4e-01) N      0.0000  0.0000  0.0001  3.292896e-12  2.555851e-06
9 B(1.5e-01) N      0.0000  0.0000  0.0000  7.281583e-18  3.800552e-09
```

The column headed by `mu` shows the Levenberg-Marquardt parameter when the Newton step is larger than the trust region radius. The column headed by `dnorm` gives the Euclidean norm of the step (adjustment of the current `x`) taken by the algorithm. The absolute value of the difference with `Dlt0` is less than 0.1 times the trust region radius.

After the column for the Jacobian the letters indicate the following

H a Levenberg-Marquardt restricted step is taken.

N a normal full Newton step is taken.

The meaning of the columns headed by `Dlt0` and `Dltn` is identical to that of the same columns for the double dogleg method.

See Also

[nleqslv](#)

<code>print.test.nleqslv</code>	<i>Printing the result of testnslv</i>
---------------------------------	--

Description

Print method for `test.nleqslv` objects.

Usage

```
## S3 method for class 'test.nleqslv'
print(x, digits=4, ...)
```

Arguments

<code>x</code>	a <code>test.nleqslv</code> object
<code>digits</code>	specifies the minimum number of significant digits to be printed in values.
<code>...</code>	additional arguments to <code>print</code> .

Details

This is the `print` method for objects inheriting from class `test.nleqslv`. It prints the call to `testnslv` followed by the description of the experiment (if the `title` argument was specified in the call to `testnslv`) and the dataframe containing the results of `testnslv`.

Value

It returns the object `x` invisibly.

Examples

```

dslnex <- function(x) {
  y <- numeric(2)
  y[1] <- x[1]^2 + x[2]^2 - 2
  y[2] <- exp(x[1]-1) + x[2]^3 - 2
  y
}
xstart <- c(1.5,0.5)
fstart <- dslnex(xstart)
z <- testnslv(xstart,dslnex)
print(z)

```

testnslv

Test different methods for solving with nleqslv

Description

The function tests different methods and global strategies for solving a system of non linear equations with `nleqslv`

Usage

```

testnslv(x, fn, jac=NULL,...,
         method = c("Newton", "Broyden"),
         global = c("cline", "qline", "gline", "pwlldog", "dblldog", "hook", "none"),
         Nrep=0L, title=NULL
)

```

Arguments

<code>x</code>	A list or numeric vector of starting estimates.
<code>fn</code>	A function of <code>x</code> returning the function values.
<code>jac</code>	A function to return the Jacobian for the <code>fn</code> function. If not supplied numerical derivatives will be used.
<code>...</code>	Further arguments to be passed to <code>fn</code> and <code>jac</code> and nleqslv .
<code>method</code>	The methods to use for finding a solution.
<code>global</code>	The global strategies to test. The argument may consist of several possibly abbreviated items.
<code>Nrep</code>	Number of repetitions to apply. Default is no repetitions.
<code>title</code>	a description of this experiment.

Details

The function solves the function `fn` with `nleqslv` for the specified methods and global strategies. When argument `Nrep` has been set to a number greater than or equal to 1, repetitions of the solving process are performed and the used CPU time in seconds is recorded.

If checking a user supplied jacobian is enabled, then `testnslv` will stop immediately when a possibly incorrect jacobian is detected.

Value

`testnslv` returns an object of class `"test.nleqslv"` which is a list containing the following elements

`call` the matched call

`out` a dataframe containing the results with the following columns

`method` method used.

`global` global strategy used.

`termcd` termination code of `nleqslv`.

`fctcall` number of function evaluations used by the method and global strategy.

`jaccall` number of Jacobian evaluations.

`itercnt` number of outer iterations used by the algorithm.

`message` a string describing the termination code in an abbreviated form.

`fnorm` square of the euclidean norm of the vector of function results divided by 2.

`cpusecs` CPU seconds used by the requested number of repetitions (only present when argument `Nrep` is not 0).

`title` the description if specified

The abbreviated strings are

`Fcrit` Convergence of function values has been achieved.

`Xcrit` This means that the relative distance between two consecutive x-values is smaller than `xtol`.

`Stalled` The algorithm cannot find an acceptable new point.

`Maxiter` Iteration limit `maxit` exceeded.

`Illcond` Jacobian is too ill-conditioned.

`Singular` Jacobian is singular.

Warning

Any `nleqslv` error message will be shown immediately and an error for the particular combination of method and global strategy will be recorded in the final dataframe.

Examples

```
dslnex <- function(x) {  
  y <- numeric(2)  
  y[1] <- x[1]^2 + x[2]^2 - 2  
  y[2] <- exp(x[1]-1) + x[2]^3 - 2  
  y  
}  
xstart <- c(0.5,0.5)  
fstart <- dslnex(xstart)  
testnslv(xstart,dslnex)  
# this will encounter an error  
xstart <- c(2.0,0.5)  
fstart <- dslnex(xstart)  
testnslv(xstart,dslnex)
```

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