The neldermead Package - version 1.0-11

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neldermead is a R port of a module originally developed for Scilab version 5.2.1 by Michael Baudin (INRIA - DIGITEO). Information about this software can be found at www.scilab.org. The following documentation as well as the content of the functions .Rd files are adaptations of the documentation provided with the original Scilab neldermead module.

neldermead currently does not include any adaptation of the Scilab ‘nmplot’ function series that is available in the original neldermead module.

1 Overview

1.1 Description

The goal of this toolbox is to provide several direct search optimization algorithms based on the simplex method. The optimization problem to solve is the minimization of a cost function, with bounds and nonlinear constraints.

\[ \min f(x) \]

\[ l_i \leq x_i \leq h_i, \quad i = 1, n \]

\[ g_j(x) \geq 0, \quad j = 0, nbineq \]

where \( f \) is the cost function, \( x \) is the vector of parameter estimates, \( l \) and \( h \) are vectors of lower and upper bounds for the parameter estimates, \( n \) is the number of parameters and \( nbineq \) the number of inequality constraints \( g(x) \).

The provided algorithms are direct search algorithms, i.e. algorithms which do not use the derivative of the cost function. They are based on the update of a simplex, which is a set of \( k \geq n + 1 \) vertices, where each vertex is associated with one point and one function value.

The following algorithms are available:

- The fixed shape simplex method of Spendley, Hext and Himsworth: this algorithm solves an unconstrained optimization problem with a fixed shape simplex made of \( k = n + 1 \) vertices.

- The variable shape simplex method of Nelder and Mead: this algorithm solves an unconstrained optimization problem with a variable shape simplex made of \( k = n + 1 \) vertices [3].

- Box’s complex method: this algorithm solves an constrained optimization problem with a variable shape simplex made of an arbitrary \( k \) number of vertices (\( k = 2n \) is recommended by Box).
1.2 Basic object

The basic object used by the neldermead package to store the configuration settings and the history of an optimization is a 'neldermead' object, i.e. a list typically created by neldermead and having a strictly defined structure (see ?neldermead for more details).

1.3 The cost function

The function element of the neldermead object allows to configure the cost function. The cost function is used to compute the objective function value \( f \). If the \texttt{nbineqconst} element of the neldermead object is configured to a non-zero value, the cost function must also compute the value of the nonlinear, positive, inequality constraints \( c \). The cost function can also take as input/output an additional argument, if the \texttt{costfargument} element is configured. The function should be defined as described in vignette('optimbase',package='optimbase'):

```r
costf <- function(x, index, fmsfundata){
  # Define f and c here #
  return(list(f, g=NULL, c, gc=NULL, index=index, this=list(costfargument = fmsfundata)))
}
```

where

- \( x \): is the current point, as a column vector,
- \texttt{index}: (optional), an integer representing the value to compute, and
- \texttt{fmsfundata}: an user-provided input/output argument.
- \( f \): the value of the objective function (a scalar),
- \( g \): typically the gradient of the objective function in the context of the optimbase functions; must be set to NULL as the Nelder-Mead is not gradient-based,
- \( c \): the vector of values of non-linear, positive, inequality constraints,
- \( gc \): typically the gradient of the constraints in the context of the optimbase functions; must be set to NULL as the Nelder-Mead is not gradient-based,
- \texttt{this}: must be set to \texttt{list(costfargument = fmsfundata)}.

The index input parameter tells the cost function what to return as output arguments (as described in vignette('optimbase',package='optimbase')). It has the following meaning:

- index = 2: compute \( f \),
- index = 5: compute \( c \),
- index = 6: compute \( f \) and \( c \).
The `fmsdata` argument is both input and output. This feature may be used in the situation where the cost function has to update its environment from call to call. Its simplest use is to count the number of calls to the cost function, but this feature is already available directly. Consider the more practical situation where the optimization requires the execution of an underlying Newton method (a chemical solver for example). This Newton method requires an initial guess $x_0$. If the initial guess for this underlying Newton method is kept constant, the Newton method may have problems to converge when the current optimization point get far away from the its initial point. If a `costfargument` element is defined in the neldermead object, it can be passed to the cost function as the `fmsdata` argument. In this case, the initial guess for the Newton method can be updated so that it gets the value of the previous call. This way, the Newton method will have less problems to converge and the cost function evaluation may be faster.

We now present how the feature works. Everytime the cost function is called back, the `costfargument` element is passed to the cost function as an input argument. If the cost function modifies its content in the output argument, the content of the `costfargument` element is updated accordingly. Once the optimization is performed, the user may call the `neldermead.get` function and get back an updated `costfargument` content.

1.4 The output function

The `outputcommand` element of the neldermead object allows to configure a command which is called back at the start of the optimization, at each iteration and at the end of the optimization. The output function must be defined as follows:

```r
outputcmd <- function(state, data, myobj)

where

state: is a string representing the current state of the algorithm. Available values are 'init', 'iter', and 'done',

data: a list containing at least the following entries:

  x: the current optimum,
  fval: the current function value,
  iteration: the current iteration index,
  funccount: the number of function evaluations,
  simplex: the current simplex,
  step: the previous step in the algorithm. The following values are available: 'init', 'done', 'reflection', 'expansion', 'insidecontraction', 'outsidecontraction', 'reflectionnext', and 'shrink',

myobj: a user-defined parameter. This input parameter is defined with the `outputcommandarg` element of the neldermead object.

The output function may be used when debugging the specialized optimization algorithm, so that a verbose logging is produced. It may also be used to write one or several report files in a specialized format (ASCII, LATEX, Excel, etc...). The user-defined parameter may be used in that case to store file names or logging options.

The `data` list argument may contain more fields than the current presented ones. These additional fields may contain values which are specific to the specialized algorithm, such as the simplex in a Nelder-Mead method, the gradient of the cost function in a BFGS method, etc...
1.5 Termination

The current package takes into account several generic termination criteria. The following termination criteria are enabled by default:

- `maxiter`,
- `maxfunevals`,
- `tolxmethod`,
- `tolsimplexizemethod`.

The `neldermead.termination` function uses a set of rules to compute if the termination occurs and sets optimization status to one of the following: 'continue', 'maxiter', 'maxfunevals', 'tolf', 'tolx', 'tolsize', 'tolsizedeltafv', 'kelleystagnation', 'tolboxf' or 'tolvariance'. The value of the status may also be a user-defined string, in the case where a user-defined termination function has been set.

The following set of rules is examined in this order:

- By default, the status is 'continue' and the terminate flag is FALSE.

- The number of iterations is examined and compared to the `maxiter` element of the neldermead object: if `iterations ≥ maxiter`, then the status is set to 'maxiter' and terminate is set to TRUE.

- The number of function evaluations is examined and compared to the `maxfunevals` elements: if `funevals ≥ maxfunevals`, then the status is set to 'maxfuneval' and terminate is set to TRUE.

- The tolerance on function value is examined depending on the value of the `tolfunmethod`.
  - FALSE: then the criteria is just ignored,
  - TRUE: if `|currentfopt| < tolfunrelative · |previousfopt| + tolfunabsolute`, then the status is set to 'tolf' and terminate is set to TRUE.

  The relative termination criteria on the function value works well if the function value at optimum is near zero. In that case, the function value at initial guess `fx0` may be used as `previousfopt`. This criteria is sensitive to the `tolfunrelative` and `tolfunabsolute` elements.

  The absolute termination criteria on the function value works if the user has an accurate idea of the optimum function value.

- The tolerance on x is examined depending on the value of the `tolxmethod` element.
  - FALSE: then the criteria is just ignored,
  - TRUE: if `norm(currentxopt - previousxopt) < tolxrelative · norm(currentxopt) + tolxabsolute`, then the status is set to 'tolx' and terminate is set to TRUE.

  This criteria is sensitive to the `tolxrelative` and `tolxabsolute` elements. The relative termination criteria on x works well if x at optimum is different from zero. In that case, the condition measures the distance between two iterates. The absolute termination criteria on x works if the user has an accurate idea of the scale of the optimum x. If the optimum x is near 0, the relative tolerance will not work and the absolute tolerance is more appropriate.
• The tolerance on simplex size is examined depending on the value of the tolsimplexizemethod element.

FALSE: then the criteria is just ignored,
TRUE: if \( \text{ssize} < \text{tolsimplexizerelative} \cdot \text{simplexsize0} + \text{tolsimplexizeabsolute} \),
where \( \text{simplexsize0} \) is the size of the simplex at iteration 0, then the status is set to 'tolsize' and terminate is set to TRUE.

The size of the simplex is computed from the 'sigmaplus' method of the optimsimplex package.
This criteria is sensitive to the tolsimplexizeabsolute and the tolsimplexizerelative elements.

• The absolute tolerance on simplex size and absolute difference of function value is examined depending on the value of the tolssizedeltafvmethod element.

FALSE: then the criteria is just ignored,
TRUE: if both the following conditions \( \text{ssize} < \text{tolsimplexizeabsolute} \) and \( \text{shiftfv} < \text{toldeltafv} \) are true where \( \text{ssize} \) is the current simplex size and \( \text{shiftfv} \) is the absolute value of the difference of function value between the highest and lowest vertices, then the status is set to 'tolsizedeltafv' and terminate is set to TRUE.

• The stagnation condition based on Kelley sufficient decrease condition is examined depending on the value of the kelleystagnationflag element.

FALSE: then the criteria is just ignored,
TRUE: if \( \text{newfvmean} \leq \text{oldfvmean} - \alpha \cdot \text{t(sg)} \cdot \text{sg} \) where \( \text{newfvmean} \) (resp. \( \text{oldfvmean} \)) is the function value average in the current iteration (resp. in the previous iteration), then the status is set to 'kelleystagnation' and terminate is set to TRUE. Here, \( \alpha \) is a non-dimensional coefficient and \( \text{sg} \) is the simplex gradient.

• The termination condition suggested by Box is examined depending on the value of the boxtermination element.

FALSE: then the criteria is just ignored,
TRUE: if both the following conditions \( \text{shiftfv} < \text{boxtolf} \) and \( \text{boxkount} == \text{boxnbmatch} \) are true, where \( \text{shiftfv} \) is the difference of function value between the best and worst vertices, and \( \text{boxkount} \) is the number of consecutive iterations where this criteria is met, then the status is set to 'boxtolf' and terminate is set to TRUE. Here, the \( \text{boxtolf} \) parameter is the value associated with the boxtermination element of the neldermead object and is a user-defined absolute tolerance on the function value. The \( \text{boxnbmatch} \) parameter is the value associated with the boxtermination element and is the user-defined number of consecutive match.

• The termination condition based on the variance of the function values in the simplex is examined depending on the value of the tolvarianceflag element.

FALSE: then the criteria is just ignored,
TRUE: if \( \text{var} < \text{tolrelativevariance} \cdot \text{variancesimplex0} + \text{tolabsolutevariance} \), where \( \text{var} \) is the variance of the function values in the simplex, then the status is set to 'tolvariance' and terminate is set to TRUE. Here, the \( \text{tolrelativevariance} \) parameter is the value associated with the tolvarianceflag element of the neldermead
object and is a user-defined relative tolerance on the variance of the function values. The `tolabsolutevariance` parameter is the value associated with the `tolabsolutevariance` element and is the user-defined absolute tolerance of the variance of the function values.

- The user-defined termination condition is examined depending on the value of the `myterminateflag` element.

  FALSE: then the criteria is just ignored,

  TRUE: if the `term` boolean output argument returned by the termination function is TRUE, then the status is set to the user-defined status and terminate is set to TRUE.

### 1.6 Kelley’s stagnation detection

The stagnation detection criteria suggested by Kelley is based on a sufficient decrease condition, which requires a parameter $\alpha > 0$ to be defined [1]. The `kelleynormalizationflag` element of the `neldermead` object allows to configure the method to use to compute this $\alpha$ parameter. Two methods are available, where each method corresponds to a different paper by Kelley:

- **constant:** in ‘Detection and Remediation of Stagnation in the Nelder-Mead Algorithm Using a Sufficient Decrease Condition’, Kelley uses a constant $\alpha$, with the suggested value $1.e-4$, which is the typical choice for line search method.

- **normalized:** in ‘Iterative Methods for Optimization’, Kelley uses a normalized $\alpha$, computed from the following formula: $\alpha = \alpha_0 \cdot \sigma_0 / nsg$, where $\sigma_0$ is the size of the initial simplex and $nsg$ is the norm of the simplex gradient for the initial guess point.

### 1.7 O’Neill’s factorial optimality test

In ‘Algorithm AS47 - Function minimization using a simplex procedure’, O’Neill presents a fortran 77 implementation of the simplex method [5]. A factorial test is used to check if the computed optimum point is a local minimum. If the `restartdetection` element of the `neldermead` object is set to ‘oneill’, that factorial test is used to see if a restart should be performed.

### 1.8 Implementation notes of the method of Spendley et al.

The original paper may be implemented with several variations, which might lead to different results [6]. This section defines what algorithmic choices have been used in the present package.

The paper states the following rules.

- 'Rule 1. Ascertain the lowest reading $y$, of $y_1$ ... $y_{k+1}$ Complete a new simplex $Sp$ by excluding the point $V_p$ corresponding to $y$, and replacing it by $V^*$ defined as above.'

- 'Rule 2. If a result has occurred in $(k + 1)$ successive simplexes, and is not then eliminated by application of Rule 1, do not move in the direction indicated by Rule 1, or at all, but discard the result and replace it by a new observation at the same point.'

- 'Rule 3. If $y$ is the lowest reading in $So$, and if the next observation made, $y^*$, is the lowest reading in the new simplex $S$, do not apply Rule 1 and return to $So$ from $Sp$. Move out of $S$, by rejecting the second lowest reading (which is also the second lowest reading in $So$).'</n

We implement the following 'rules' of the Spendley et al. method:
• Rule 1 is strictly applied, but the reflection is done by reflection of the high point, since we minimize a function instead of maximizing it, like Spendley.

• Rule 2 is NOT implemented, as we expect that the function evaluation is not subject to errors.

• Rule 3 is applied, i.e. reflection with respect to next to the high point. The original paper does not mention any shrink step. When the original algorithm cannot improve the function value with reflection steps, the basic algorithm stops. In order to make the current implementation of practical value, a shrink step is included, with shrinkage factor sigma. This perfectly fits into the spirit of the original paper. Notice that the shrink step makes the rule #3 (reflection with respect to next-to-worst vertex) unnecessary. Indeed, the minimum required steps are the reflection and shrinkage. Nevertheless, the rule #3 has been kept in order to make the algorithm as close as it can be to the original.

1.9 Implementation notes on the method of Nelder and Mead

The purpose of this section is to analyze the current implementation of Nelder-Mead’s algorithm. The algorithm that we use is described in ‘Iterative Methods for Optimization’ by Kelley.

The original paper uses a ‘greedy’ expansion, in which the expansion point is accepted whatever its function value. The current implementation, as most implementations, uses the expansion point only if it improves over the reflection point, that is,

• if \( f_e < f_r \), then the expansion point is accepted,

• if not, the reflection point is accepted.

The termination criteria suggested by Nelder and Mead is based on an absolute tolerance on the standard deviation of the function values in the simplex. We provide this original termination criteria with the \texttt{tolvarianceflag} element of the \texttt{neldermead} object, which is disabled by default.

1.10 Box’s complex algorithm implementation notes

In this section, we analyze the current implementation of Box’s complex method [4]. The initial simplex can be computed as in Box’s paper, but this may not be safe. In his paper, Box suggests that if a vertex of the initial simplex does not satisfy the non linear constraints, then it should be ‘moved halfway toward the centroid of those points already selected’. This behaviour is available when the \texttt{scalingsimplex0} element of the \texttt{neldermead} object is set to 'tocenter'. It may happen, as suggested by Guin [2], that the centroid is not feasible if the constraints are not convex. In this case, the initial simplex cannot be computed. This is why we provide the 'tox0' option, which allows to compute the initial simplex by scaling toward the initial guess, which is always feasible.

In Box’s paper, the scaling into the non linear constraints is performed ‘toward’ the centroid, that is, by using a scaling factor equal to 0.5. This default scaling factor might be sub-optimal in certain situations. This is why we provide the \texttt{boxineqscaling} element, which allows to configure the scaling factor.

In Box’s paper, whether we are concerned with the initial simplex or with the simplex at a given iteration, the scaling for the non linear constraints is performed without end. This is because Box’s hypothesis is that ‘ultimately, a satisfactory point will be found’. As suggested by Guin, if the process fails, the algorithm goes into an infinite loop. In order to avoid this, we perform the scaling until a minimum scaling value is reached, as defined by the \texttt{guinalphamin} element.

We have taken into account the comments by Guin, but it should be emphasized that the current implementation is still as close as possible to Box’s algorithm and is not Guin’s algorithm. More
precisely, during the iterations, the scaling for the non linear constraints is still performed toward the centroid, be it feasible or not.

1.11 User-defined algorithm

The `mymethod` element of the `neldemead` object allows to configure a user-defined simplex-based algorithm. The reason for this option is that many simplex-based variants of Nelder-Mead’s algorithm have been developed over the years, with specific goals. While it is not possible to provide them all, it is very convenient to use the current structure without being forced to make many developments.

The value of the `mymethod` element is expected to be a R function with the following structure:

```r
> myalgorithm <- function( this ){
+   ...
+   return(this)
+ }
```

where `this` is the current `neldermead` object.

In order to use the user-defined algorithm, the `method` element must be set to 'mine'. In this case, the component performs the optimization exactly as if the user-defined algorithm was provided by the component.

The user interested in that feature may use the internal scripts provided in the distribution as templates and tune his own algorithm from that point. There is of course no warranty that the user-defined algorithm improves on the standard algorithm, so that users use this feature at their own risks.

1.12 User-defined termination

Many termination criteria are found in the literature. Users who aim at reproducing the results exhibited in a particular paper may find that that none of the provided termination criteria match the one which is used in the paper. It may also happen that the provided termination criteria are not suitable for the specific test case. In those situation the `myterminate` element of the `neldermead` object allows to configure a user-defined termination function. The value of the `myterminate` element is expected to be a R function with the following structure:

```r
> mystoppingrule <- function( this , simplex ){
+   ...
+   return(list(this=this,terminate=terminate,status=status))
+ }
```

where `this` is the current `neldermead` object and `simplex` is the current simplex. The `terminate` output argument is a logical flag which is FALSE if the algorithm must continue and TRUE if the algorithm must stop. The `status` output argument is a string which is associated with the current termination criteria.

In order to enable the use of the user-defined termination function, the value of the `myterminateflag` element must be set to TRUE in the `neldermead` object. At each iteration, if the `myterminateflag` element has been set to TRUE, the user-defined termination is called. If the terminate output argument is TRUE, then the algorithm is stopped. In that case, the value of the `status` element of the `neldermead.get` function output is the value of the `status` output argument of the user-defined termination function.
2 Specialized functions

2.1 fminsearch

The fminsearch function is based on a specialized use of the more general neldermead function bundle and searches for the unconstrained minimum of a given cost function. This function corresponds to the Matlab (or Scilab) fminsearch function. In the context of fminsearch, the function to be minimized is not a cost function as described in Section 1.3 but an objective function (returning a numeric scalar). Additional information and examples are available in ?fminsearch from a R environment.

2.2 Direct grid search

Direct grid search, performed by fmin.gridsearch, is a functionality added to the original Scilab neldermead module and constitutes another specialized use of the neldermead package. This function allows to explore the search space of an optimization problem around the initial point $x_0$. This optimization problem is defined by an objective function, like for fminsearch, and not a cost function. fmin.gridsearch automatically creates a grid of search points selected around the initial point and evaluates the objective function at each point. The boundaries of the grid are set either by a vector of parameter-specific lower and upper limits, or by a vector of factors $\alpha$ as follows:$[x_0/\alpha, x_0 \times \alpha]$. The number npts of points evaluated for each parameter (or dimension of the optimization problem) can also be defined. The total number of points in the grid is therefore $npts^n$. At the end of the search, fmin.gridsearch returns a table sorted by value of the objective function. The feasibility of the objective function is also determined at each point, as fmin.gridsearch is a wrapper around optimbase.gridsearch which assesses the feasibility of a cost function in addition to calculating its value at each particular search point. Because fmin.gridsearch does not accept constraints, the objective function should always be feasible. Additional information is available in ?fmin.gridsearch from a R environment.

3 Examples

We present in this section basic examples illustrating the use of neldermead functions to optimize unconstrained or constrained systems. More complex examples are described in a Scilab-based document written by Michael Baudin and available at http://forge.scilab.org/index.php/p/docneldermead/. Because the R port of the Scilab neldermead module is almost literal, the user should be able to reproduce the described examples in R with minimal adaptations.

3.1 Example 1: Basic use

In the following example, we solve a simple quadratic test case. We begin by defining the cost function, which takes 3 input arguments and returns the value of the objective function as the f element of a list. The standard starting point [-1.2 1.0] is used. neldermead creates a new neldermead object. Then we use neldermead.set to configure the parameters of the problem. We use all default settings and perform the search for the optimum. neldermead.get is finally used to retrieve the optimum parameters.

```r
> quadratic <- function(x=NULL,index=NULL,fmsfundata=NULL){
+     return(list(f=x[1]^2 + x[2]^2,
+                     g=c(),
+                     },
```

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```r
+x0 <- transpose( c(1.0,1.0) )
> nm <- neldermead()
> nm <- neldermead.set(nm, 'numberofvariables', 2)
> nm <- neldermead.set(nm, 'function', quadratic)
> nm <- neldermead.set(nm, 'x0', x0)
> nm <- neldermead.search(nm)
> summary(nm)

Number of Estimated Variable(s): 2

Estimated Variable(s):
   Initial Final
1 1 -1.010582e-08
2 1 -1.768891e-07

Cost Function:
function(x=NULL,index=NULL,fmsfundata=NULL){
  return(list(f=x[1]^2 + x[2]^2,
              g=c(),
              c=c(),
              gc=c(),
              index=index,
              this=list(costfargument=fmsfundata)))
}
<environment: namespace:tools>

Cost Function Argument(s):

Optimization:
- Status: "maxfuneval"
- Initial Cost Function Value: 2.000000
- Final Cost Function Value: 0.000000
- Number of Iterations (max): 52 (100)
- Number of Function Evaluations (max): 100 (100)

Simplex Information:
- Simplex at Initial Point:
  Dimension: n=2
  Number of vertices: nbve=3
  Vertex #1/3 : fv=2.000000e+00, x=1.000000e+00 1.000000e+00
  Vertex #2/3 : fv=5.000000e+00, x=2.000000e+00 1.000000e+00
  Vertex #3/3 : fv=5.000000e+00, x=1.000000e+00 2.000000e+00
```
Simplex at Optimal Point:
Dimension: n=2
Number of vertices: nbve=3
  Vertex #1/3 : fv=3.139189e-14, x=-1.010582e-08 -1.768891e-07
  Vertex #2/3 : fv=1.290894e-13, x=-3.557479e-07 5.032676e-08
  Vertex #3/3 : fv=1.601186e-13, x=2.637847e-07 3.008924e-07

3.2 Example 2: Customized use
In the following example, we solve the Rosenbrock test case. We begin by defining the Rosenbrock function, which takes 3 input arguments and returns the value of the objective function. The standard starting point [-1.2 1.0] is used. neldermead creates a new neldermead object. Then we use neldermead.set to configure the parameters of the problem. The initial simplex is computed from the axes and the single length 1.0 (this is the default, but is explicitly written here as an example). The variable simplex algorithm by Nelder and Mead is used, which corresponds to the method 'variable' option. neldermead.search performs the search for the minimum. Once the minimum is found, we represent part of the search space using the contour function (this is possible since our problem involves only 2 parameters) and we superimpose the starting point (in red), the optimisation path (in bleu), and the optimum (in green) to the plot. The history of the optimisation can be retrieved (using neldermead.get) because the 'storehistory' option was set to TRUE.

```r
> rosenbrock <- function(x=NULL,index=NULL,fmsfundata=NULL){
+   return(list(f=100*(x[2]-x[1]^2)^2+(1-x[1])^2,
+                 g=c(),
+                 c=c(),
+                 gc=c(),
+                 index=index,
+                 this=list(costfargument=fmsfundata)))
+ }
> x0 <- transpose(c(-1.2,1.0))
> nm <- neldermead()
> nm <- neldermead.set(nm,'numberofvariables',2)
> nm <- neldermead.set(nm,'function',rosenbrock)
> nm <- neldermead.set(nm,'x0',x0)
> nm <- neldermead.set(nm,'maxiter',200)
> nm <- neldermead.set(nm,'maxfunevals',300)
> nm <- neldermead.set(nm,'tolfunrelative',10*.Machine$double.eps)
> nm <- neldermead.set(nm,'tolxrelative',10*.Machine$double.eps)
> nm <- neldermead.set(nm,'simplex0method','axes')
> nm <- neldermead.set(nm,'simplex0length',1.0)
> nm <- neldermead.set(nm,'method','variable')
> nm <- neldermead.set(nm,'verbose',FALSE)
> nm <- neldermead.set(nm,'storehistory',TRUE)
> nm <- neldermead.set(nm,'verbosetermination',FALSE)
> nm <- neldermead.search(nm)
> xmin <- ymin <- -2.0
> xmax <- ymax <- 2.0
> nx <- ny <- 100
```
> stepy <- stepx <- (xmax - xmin)/nx
> ydata <- xdata <- seq(xmin,xmax,stepx)
> zdata <- apply(expand.grid(xdata,ydata),1,
+ function(x) neldermead.function(nm,transpose(x)))
> zdata <- matrix(zdata,ncol=length(ydata))
> optimpath <- matrix(unlist((neldermead.get(nm,
+ historyxopt'))),
+ nrow=2)
> optimpath <- data.frame(x=optimpath[1,],y=optimpath[2,])
> contour(xdata,ydata,zdata,levels=c(1,10,100,500,1000,2000))
> par(new=TRUE,ann=TRUE)
> plot(c(x0[1],optimpath$x[158]), c(x0[2],optimpath$y[158]),
+ col=c('red','green'),pch=16,xlab='x[1]',ylab='x[2]',
+ xlim=c(xmin,xmax),ylim=c(ymin,ymax))
> par(new=TRUE,ann=FALSE)
> plot(optimpath$x,optimpath$y,col='blue',type='l',
+ xlim=c(xmin,xmax),ylim=c(ymin,ymax))

Setting the 'verbose' element of the neldermead object to 1 allows to get detailed information about the current optimization process. The following is a sample output for an optimization based on the Nelder and Mead variable-shape simplex algorithm. Only the output corresponding to the
iteration #156 is displayed. In order to display specific outputs (or to create specific output files and graphics), the 'outputcommand' option should be used.

=================================================================
Iteration \#156 (total = 156)
Function Eval \#298
Xopt: 0.99999999999991 0.999999999999816
Fopt: 8.997809e-27
DeltaFv: 4.492261e-26
Center: 1.00000000000003 1.00000000000007
Size: 4.814034e-13
Vertex \#2/3 : fv=2.649074e-26, x=1.000000e+00 1.000000e+00
Vertex \#3/3 : fv=5.392042e-26, x=1.000000e+00 1.000000e+00
Reflect
xbar=1.00000000000001 1.00000000000003
Function Evaluation \#299 at [0.99999999999996 ]
Function Evaluation \#299 at [0.999999999999907 ]
xr=[0.99999999999996 0.999999999999907], f(xr)=0.000000

> Perform reflection
Sort

3.3 Example 3: Optimization with bound constraints

In the following example, we solve a simple quadratic test case used in Example 1 but in the case where bounds are set for parameter estimates. We begin by defining the cost function, which takes 3 input arguments and returns the value of the objective function as the f element of a list. The starting point [1.2 1.9] is used. neldermead creates a new neldermead object. Then we use neldermead.set to configure the parameters of the problem including the lower -boundsmin and upper -boundsmax bounds. The initial simplex is computed from boxnbpoints random points within the bounds. The variable simplex algorithm by Box is used, which corresponds to the -method 'box' option. neldermead.search finally performs the search for the minimum.

```r
> quadratic <- function(x=NULL,index=NULL,fmsfundata=NULL){
+    return(list(f=x[1]^2 + x[2]^2,
+                 g=c(),
+                 c=c(),
+                 gc=c(),
+                 index=index,
+                 this=list(costfargument=fmsfundata)))
+ }
> set.seed(0)
> x0 <- transpose(c(1.2,1.9))
> nm <- neldermead()
> nm <- neldermead.set(nm,'numberofvariables',2)
> nm <- neldermead.set(nm,'function',quadratic)
> nm <- neldermead.set(nm,'x0',x0)
> nm <- neldermead.set(nm,'verbose',FALSE)
> nm <- neldermead.set(nm,'storehistory',TRUE)
> nm <- neldermead.set(nm,'verbosetermination',FALSE)
```
> nm <- neldermead.set(nm, 'method', 'box')
> nm <- neldermead.set(nm, 'boundsmin', c(1,1))
> nm <- neldermead.set(nm, 'boundsmax', c(2,2))
> nm <- neldermead.search(nm)
> summary(nm)

Number of Estimated Variable(s): 2

Estimated Variable(s):

<table>
<thead>
<tr>
<th></th>
<th>Initial</th>
<th>Final</th>
<th>Lower bound</th>
<th>Upper bound</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.2</td>
<td>1.000001</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>2</td>
<td>1.9</td>
<td>1.000001</td>
<td>1</td>
<td>2</td>
</tr>
</tbody>
</table>

Cost Function:

```r
function(x=NULL, index=NULL, fmsfundata=NULL) {
    return(list(f=x[1]^2 + x[2]^2, 
                 g=c(),
                 c=c(),
                 gc=c(),
                 index=index,
                 this=list(costfargument=fmsfundata)))
}
```

<bytecode: 0x6fb0c78>

Cost Function Argument(s):

| [1] | "" |

Optimization:

- Status: "maxfuneval"
- Initial Cost Function Value: 5.050000
- Final Cost Function Value: 2.000004
- Number of Iterations (max): 90 (100)
- Number of Function Evaluations (max): 100 (100)

Simplex Information:

- Simplex at Initial Point:
  Dimension: n=2
  Number of vertices: nbve=3
  Vertex #1/3 : fv=5.050000e+00, x=1.200000e+00 1.900000e+00
  Vertex #2/3 : fv=7.610000e+00, x=2.000000e+00 1.900000e+00
  Vertex #3/3 : fv=5.440000e+00, x=1.200000e+00 2.000000e+00

- Simplex at Optimal Point:
  Dimension: n=2
  Number of vertices: nbve=3
  Vertex #1/3 : fv=2.000004e+00, x=1.000001e+00 1.000001e+00
  Vertex #2/3 : fv=2.000004e+00, x=1.000001e+00 1.000001e+00
  Vertex #3/3 : fv=2.000004e+00, x=1.000001e+00 1.000001e+00
### 3.4 Example 4: Optimization with nonlinear inequality constraints

In the following example, we solve Michalewicz’s $G_6$ test problem using Box’s methods \[7\]. This problem consists in minimizing: 

$$G_6(x) = (x_1 - 10)^3 + (x_2 - 20)^3,$$

given the nonlinear constraints:

\[c_1: (x_1 - 5)^2 + (x_2 - 5)^2 - 100 \geq 0\]

\[c_2: -(x_1 - 6)^2 - (x_2 - 5)^2 + 82.81 \geq 0\]

and bounds: $13 \leq x_1 \leq 100$, $0 \leq x_2 \leq 100$.

We begin by defining the `michalewicz` function, which takes 3 input arguments and return the value of the objective function and the constraint evaluations as the f and c elements of a list. `neldermead` creates a new `neldermead` object. Then we use `neldermead.set` to configure the parameters of the problem, including the lower `-boundsmin` and upper `-boundsmax` bounds. The initial simplex is computed from `boxnbpoints` random points within the bounds. The variable simplex algorithm by Box is used, which corresponds to the `-method 'box'` option. `neldermead.search` finally performs the search for the minimum. The starting point ([15 4.99]) like all the vertices of the optimization simplex must be feasible, i.e. they must satisfy all constraints and bounds. Constraints are enforced by ensuring that all arguments of c in the cost function output are positive or null. Note that the boundaries were set to stricter ranges to limit the sensitivity of the solution to the initial guesses.

```r
> michalewicz <- function(x=NULL,index=NULL,fmsfundata=NULL){
+ f <- c()
+ c <- c()
+ if (index == 2 | index ==6)
+ f <- (x[1]-10)^3+(x[2]-20)^3
+ + if (index == 5 | index ==6)
+ c <- c((x[1]-5)^2+(x[2]-5)^2 -100,
+ 82.81-((x[1]-6)^2+(x[2]-5)^2))
+ + varargout <- list(f=f,
+ g=c(),
+ c=c,
+ gc=c(),
+ index=index,
+ this=list(costfargument=fmsfundata))
+ return(varargout)
+ }
> set.seed(0)
> x0 <- transpose(c(15,4.99))
> nm <- neldermead()
> nm <- neldermead.set(nm, 'numberofvariables', 2)
> nm <- neldermead.set(nm, 'nbineqconst', 2)
> nm <- neldermead.set(nm, 'function', michalewicz)
> nm <- neldermead.set(nm, 'x0', x0)
> nm <- neldermead.set(nm, 'maxiter', 300)
> nm <- neldermead.set(nm, 'maxfunevals', 1000)
> nm <- neldermead.set(nm, 'simplex0method', 'randbounds')
> nm <- neldermead.set(nm, 'boxnbpoints', 3)
> nm <- neldermead.set(nm, 'storehistory', TRUE)
```

---

1 Example suggested by Pascal Grandeau
```r
> nm <- neldermead.set(nm, 'method', 'box')
> nm <- neldermead.set(nm, 'boundsmin', c(13, 0))
> nm <- neldermead.set(nm, 'boundsmax', c(20, 10))
> nm <- neldermead.search(nm)
> summary(nm)

Number of Estimated Variable(s): 2

Estimated Variable(s):

<table>
<thead>
<tr>
<th>Initial</th>
<th>Final</th>
<th>Lower bound</th>
<th>Upper bound</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 15.00</td>
<td>14.09</td>
<td>13</td>
<td>20</td>
</tr>
<tr>
<td>2 4.99</td>
<td>0.84</td>
<td>0</td>
<td>10</td>
</tr>
</tbody>
</table>

Number of Inequality Contraints: 2

Cost Function:

```r
def function(x=NULL, index=NULL, fmsfundata=NULL){
  f <- c()
  c <- c()
  if (index == 2 | index ==6)
    f <- (x[1]-10)^3+(x[2]-20)^3
  if (index == 5 | index ==6)
    c <- c((x[1]-5)^2+(x[2]-5)^2 -100, 82.81-((x[1]-6)^2+(x[2]-5)^2))
  varargout <- list(f=f,
      g=c(),
      gc=c(),
      index=index,
      this=list(costfargument=fmsfundata))
  return(varargout)
}
```

<bytecode: 0x7135ba0>

Cost Function Argument(s):
[1] ""

Optimization:
- Status: "impossibleimprovement"
- Initial Cost Function Value: -3256.754501
- Final Cost Function Value: -6961.813876
- Number of Iterations (max): 236 (300)
- Number of Function Evaluations (max): 794 (1000)

Simplex Information:
- Simplex at Initial Point:
  Dimension: n=2
```
3.5 Example 5: Passing data to the cost function

In the following example, we use a simple example to illustrate how to pass user-defined arguments to a user-defined cost function. We try to find the mean and standard deviation of some normally distributed data using maximum likelihood (actually a modified negative log-likelihood approach) ².

We begin by defining the negLL function, which takes 3 input arguments and return the value of the objective function. The random dataset is then generated and stored in the list fmsfundata. neldermead creates a new neldermead object. Then we use neldermead.set to configure the parameters of the problem, including costfargument, set to fmsfundata, and the lower -boundsmin and upper -boundsmax bounds (the standard deviations has to be positive). The variable simplex algorithm by Box is used. neldermead.search finally performs the search for the minimum.

```r
> negLL <- function(x=NULL, index=NULL, fmsfundata=NULL)
+ { mn <- x[1]
+ sdv <- x[2]
+ out <- -sum(dnorm(fmsfundata$data, mean=mn, sd=sdv, log=TRUE))
+ return(list(f = out,
+ index = index,
+ this=list(costfargument=fmsfundata)))
+ }
> set.seed(12345)
> fmsfundata <- structure(
+ list(data=rnorm(500,mean=50,sd=2)),
+ class='optimbase.functionargs')
> x0 <- transpose(c(45,3))
> nm <- neldermead()
> nm <- neldermead.set(nm,'numberofvariables',2)
> nm <- neldermead.set(nm,'function',negLL)
> nm <- neldermead.set(nm,'x0',x0)
> nm <- neldermead.set(nm,'costfargument',fmsfundata)
> nm <- neldermead.set(nm,'maxiter',500)
> nm <- neldermead.set(nm,'maxfunevals',1500)
> nm <- neldermead.set(nm,'method','box')
> nm <- neldermead.set(nm,'storehistory',TRUE)
```

²Example suggested by Mark Taper
> nm <- neldermead.set(nm, 'boundsmin', c(-100, 0))
> nm <- neldermead.set(nm, 'boundsmax', c(100, 100))
> nm <- neldermead.search(this=nm)
> summary(nm)

Number of Estimated Variable(s): 2

Estimated Variable(s):

<table>
<thead>
<tr>
<th></th>
<th>Initial</th>
<th>Final</th>
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<td>100</td>
</tr>
<tr>
<td>2</td>
<td>3</td>
<td>1.98</td>
<td>0</td>
<td>100</td>
</tr>
</tbody>
</table>

Cost Function:

```r
function(x=NULL, index=NULL, fmsfundata=NULL) {
  mn <- x[1]
  sdv <- x[2]
  out <- -sum(dnorm(fmsfundata$data, mean=mn, sd=sdv, log=TRUE))
  return(list(f = out,
              index = index,
              this=list(costfargument=fmsfundata))
}
```

Cost Function Argument(s):

```
$\text{data}
[1]  51.17106  51.41893  49.78139  49.09301  51.21177  46.36409  51.26020
[22]  52.91157  48.71134  46.89373  46.80458  53.61020  49.03671  51.24076
[29]  51.22425  49.67538  51.62375  54.39367  54.09838  53.26489  50.50854
[36]  50.98238  49.35183  46.67590  53.53547  50.05160  52.25702  45.23928
[43]  47.87947  51.87428  51.70890  52.92146  47.17380  51.13481  51.16638
[50]  47.38640  48.91923  53.89539  50.10718  50.70333  48.65805  50.55951
[57]  51.38234  51.64759  54.29013  45.30611  50.29918  47.31494  51.10661
[64]  53.17993  48.82624  46.33525  51.77628  53.18698  51.03371  47.40866
[71]  50.10923  48.43070  47.90129  54.66102  52.80541  51.88520  51.65252
[78]  48.37692  50.95250  52.04252  51.29077  52.08629  49.39126  54.95422
[85]  51.94244  53.73420  51.34408  49.38409  51.07305  51.64974  48.07220
[92]  48.28983  53.77389  49.21636  48.03873  51.37466  48.98991  54.31544
[99]  48.80040  48.61091  50.44785  47.68755  50.84484  47.35049  50.28217
[106] 48.92790  49.37679  53.11222  49.10393  50.64225  47.53966  47.35188
[113] 52.52248  52.63846  49.83849  48.98982  49.89569  51.25772  54.36000
[120] 49.86197  53.08973  52.64290  50.64430  50.06191  49.15752  47.68236
[127] 46.30926  52.31465  45.75290  47.60794  53.28438  51.76731  51.04975
[134] 47.63068  55.31158  47.90417  47.97775  51.33784  50.25835  49.15485
[141] 47.71947  47.41257  48.81060  46.99837  50.03171  51.08034  46.90642
[148] 51.69931  51.79203  50.27738  46.76134  50.09680  50.30566  48.38700
[155] 49.78275  49.49811  53.39869  49.31140  50.13554  48.69886  49.02472
```
Optimization:
- Status: "impossibleimprovement"
- Initial Cost Function Value: 1858.501814
- Final Cost Function Value: 1050.592365
- Number of Iterations (max): 137 (500)
- Number of Function Evaluations (max): 268 (1500)

Simplex Information:
- Simplex at Initial Point:
  Dimension: n=2
  Number of vertices: nbve=3
  Vertex #1/3 : fv=1.858502e+03, x=4.500000e+01 3.000000e+00
  Vertex #2/3 : fv=1.599340e+03, x=4.600000e+01 3.000000e+00
  Vertex #3/3 : fv=1.630588e+03, x=4.500000e+01 4.000000e+00

- Simplex at Optimal Point:
  Dimension: n=2
  Number of vertices: nbve=3
  Vertex #1/3 : fv=1.050592e+03, x=5.016492e+01 1.978316e+00
  Vertex #2/3 : fv=1.050592e+03, x=5.016492e+01 1.978316e+00
  Vertex #3/3 : fv=1.050592e+03, x=5.016492e+01 1.978316e+00

3.6 Example 6: Direct grid search

In the following example, we use the Rosenbrock test case introduced as Example 2 to illustrate the
direct grid search capacity of neldermead. We begin by defining the Rosenbrock function, which
takes only one input argument and returns the value of the objective function. We request 6 points
per dimension of the problem and set the range of search around the standard starting point [-1.2
1.0] by providing limits. fmin.gridsearch performs the search and return a table sorted by value
of the cost function.

```r
> rosenbrock <- function(x=NULL){
+   f <- 100*(x[2]-x[1]^2)^2+(1-x[1])^2
+ } 
> x0 <- c(-1.2,1.0)
> npts <- 6
> xmin <- c(-2,-2)
> xmax <- c(2,2)
> grid <- fmin.gridsearch(fun=rosenbrock,x0=x0,xmin=xmin,xmax=xmax,npts=npts,alpha=alpha)
```

The grid contains 30 unique combinations.
  Evaluating combination number: 1/30
  Evaluating combination number: 2/30
| Evaluating combination number: 3/30 |
| Evaluating combination number: 4/30 |
| Evaluating combination number: 5/30 |
| Evaluating combination number: 6/30 |
| Evaluating combination number: 7/30 |
| Evaluating combination number: 8/30 |
| Evaluating combination number: 9/30 |
| Evaluating combination number: 10/30 |
| Evaluating combination number: 11/30 |
| Evaluating combination number: 12/30 |
| Evaluating combination number: 13/30 |
| Evaluating combination number: 14/30 |
| Evaluating combination number: 15/30 |
| Evaluating combination number: 16/30 |
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| Evaluating combination number: 19/30 |
| Evaluating combination number: 20/30 |
| Evaluating combination number: 21/30 |
| Evaluating combination number: 22/30 |
| Evaluating combination number: 23/30 |
| Evaluating combination number: 24/30 |
| Evaluating combination number: 25/30 |
| Evaluating combination number: 26/30 |
| Evaluating combination number: 27/30 |
| Evaluating combination number: 28/30 |
| Evaluating combination number: 29/30 |
| Evaluating combination number: 30/30 |

> grid

<table>
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<th>x1</th>
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<th>feasible</th>
</tr>
</thead>
<tbody>
<tr>
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<td>1.0</td>
<td>0.0</td>
<td>1</td>
</tr>
<tr>
<td>15</td>
<td>0.0</td>
<td>1.0</td>
<td>1</td>
</tr>
<tr>
<td>20</td>
<td>-1.0</td>
<td>4.0</td>
<td>1</td>
</tr>
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<td>1</td>
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<td>-1.2</td>
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</tr>
<tr>
<td>16</td>
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<td>28</td>
<td>1.0</td>
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</table>
4 References


5 Dependencies of fminsearch

We illustrate in the figures below the network of functions of the *neldermead*, *optimbase*, and *optim simplex* packages that are called from the *fminsearch* functions. This large network is broken down in 6 plots, which are shown in the order functions are called. Green boxes represent functions that are not expanded on a given plot but on a previous or later one.
Figure 1: fminsearch function network (1/6)
Figure 2: fminsearch function network (2/6)
Figure 3: fminsearch function network (3/6)
Figure 4: fminsearch function network (4/6)
Figure 5: fminsearch function network (5/6)
Figure 6: fminsearch function network (6/6)
6 Help on neldermead functions

neldermead-package  R port of the Scilab neldermead module

Description

The goal of this package is to provide a Nelder-Mead direct search optimization method. That Nelder-Mead algorithm may be used in the following optimization context:

- there is no need to provide the derivatives of the objective function,
- the number of parameters is small (up to 10-20),
- there are bounds and/or non linear constraints.

Design

This package provides the following components:

- neldermead provides various Nelder-Mead variants and manages for Nelder-Mead specific settings, such as the method to compute the initial simplex, the specific termination criteria,
- fminsearch provides a simplified Nelder-Mead algorithm. Specific termination criteria, initial simplex and auxiliary settings are automatically configured.
- fminbnd provides a simplified Box algorithm, ie the equivalent of fminsearch for unconstrained search.
- optimset, optimget provide commands to emulate their Scilab counterparts.
- optimplotfunccount, optimplotx and optimplotfval provide plotting features for the fminsearch function (Not implemented yet).
- nmplot provides a high-level component which provides directly output pictures for Nelder-Mead algorithm. (Not implemented yet).

The current component is based on the following packages

- optimbase: provides an abstract class for a general optimization component, including the number of variables, the minimum and maximum bounds, the number of non linear inequality constraints, the loggin system, various termination criteria, the cost function, etc...
- optimsimplex: provides a class to manage a simplex made of an arbitrary number of vertices, including the computation of a simplex by various methods (axes, regular, Pfeffer’s, randomized bounds), the computation of the size by various methods (diameter, sigma+, sigma-, etc...),

Features

The following is a list of features the Nelder-Mead prototype algorithm currently provides:

- Provides 3 algorithms, including
  - the fixed shape algorithm of Spendley et al.,
  - the variable shape algorithm of Nelder and Mead,
- Box’s ‘complex’ algorithm managing bounds and nonlinear inequality constraints based on arbitrary number of vertices in the simplex.

- **Manage various simplex initializations:**
  - initial simplex given by user,
  - initial simplex computed with a length and along the coordinate axes,
  - initial regular simplex computed with formula of Spendley et al.,
  - initial simplex computed by a small perturbation around the initial guess point.

- **Manage cost function:**
  - optional additional argument,
  - direct communication of the task to perform: cost function or inequality constraints.

- **Manage various termination criteria, including maximum number of iterations, tolerance on function value (relative or absolute):**
  - tolerance on x (relative or absolute),
  - tolerance on standard deviation of function value (original termination criteria in Box 1965),
  - maximum number of evaluations of cost function,
  - absolute or relative simplex size.

- **Manage the history of the convergence, including:**
  - history of function values,
  - history of optimum point,
  - history of simplices,
  - history of termination criteria.

- **Provide a plot command which allows to graphically see the history of the simplices toward the optimum (Not yet implemented).**

- **Provide query features for the status of the optimization process: number of iterations, number of function evaluations, status of execution, function value at initial point, function value at optimal point, etc...**

- **Kelley restart based on simplex gradient.**

- **O’Neill restart based on factorial search around optimum.**

**Details**

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See `vignette('neldermead', package='neldermead')` for more information.
Author(s)

Author of Scilab neldermead module: Michael Baudin (INRIA - Digiteo)
Author of R adaptation: Sebastien Bihorel (<sb.pmlab@gmail.com>)

References

'Detection and Remediation of Stagnation in the Nelder–Mead Algorithm Using a Sufficient Decrease Condition’, Kelley C. T., SIAM J. on Optimization, 1999

See Also

optimbase optimsimplex

costf.transpose x Cost Function Call

Description

Call the cost function after transposition of the value of the point estimate x, so that the input row vector, given by optimsimplex, is transposed into a column vector as required by the cost function.

Usage

```
costf.transpose(x = NULL, this = NULL)
```

Arguments

x The point estimate provide as a row matrix.
this A neldermead object.
Value

Return the value of the cost function (called by \texttt{neldermead.costf}).

Author(s)

Author of Scilab neldermead module: Michael Baudin (INRIA - Digiteo)
Author of R adaptation: Sebastien Bihorel (<sb.pmlab@gmail.com>)

See Also

\texttt{neldermead.costf}

\begin{verbatim}
\texttt{fmin.gridsearch} \hspace{1cm} \textit{Grid evaluation of an unconstrained cost function}
\end{verbatim}

Description

Evaluate an unconstrained cost function on a grid of points around a given initial point estimate.

Usage

\begin{verbatim}
fmin.gridsearch(fun = NULL, x0 = NULL, xmin = NULL, xmax = NULL, npts = 3, alpha = 10)
\end{verbatim}

Arguments

- \texttt{fun} \hspace{1cm} An unconstrained cost function returning a numeric scalar, similar to those used in the \texttt{fminsearch} function.
- \texttt{x0} \hspace{1cm} The initial point estimate, provided as a numeric vector.
- \texttt{xmin} \hspace{1cm} Optional: a vector of lower bounds.
- \texttt{xmax} \hspace{1cm} Optional: a vector of upper bounds.
- \texttt{npts} \hspace{1cm} An integer scalar greater than 2, indicating the number of evaluation points will be used on each dimension to build the search grid.
- \texttt{alpha} \hspace{1cm} A vector of numbers greater than 1, which give the factor(s) used to calculate the evaluation range of each dimension of the search grid (see Details). If \texttt{alpha} length is lower than that of \texttt{x0}, elements of \texttt{alpha} are recycled. If its length is higher than that of \texttt{x0}, \texttt{alpha} is truncated.

Details

\texttt{fmin.gridsearch} evaluates the cost function at each point of a grid of \texttt{npts} \^{ \texttt{length(x0)}} points. If lower (\texttt{xmin}) and upper (\texttt{ xmax}) bounds are provided, the range of evaluation points is limited by those bounds and \texttt{alpha} is not used. Otherwise, the range of evaluation points is defined as \texttt{[x0/alpha,x0*alpha]}.

The actual evaluation of the cost function is delegated to \texttt{optimbase.gridsearch}. 

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Value

Return a data.frame with the coordinates of the evaluation point, the value of the cost function and its feasibility. Because the cost function is unconstrained, it is always feasible. The data.frame is ordered by feasibility and increasing value of the cost function.

Author(s)

Sebastien Bihorel (<sb.pmlab@gmail.com>)

See Also

fminsearch, optimbase.gridsearch

fminsearch.function fminsearch Cost Function Call

Description

This function calls the cost function and makes it match neldermead requirements. It is used in the fminsearch function as the function element of the neldermead object (see ?neldermead and ?neldermead.set).

Usage

fminsearch.function(x = NULL, index = NULL, fmsfundata = NULL)

Arguments

x A single column vector of parameter estimates.

index An integer variable set to 2, indicating that only the cost function is to be computed by the algorithm.

fmsfundata An object of class 'optimbase.functionargs' and with (at least) a fun element, which contains the user-defined cost function.

Value

Returns a list with the following elements:

f The value of the cost function at the current point estimate.

index The same index variable.

this A list with a single element costargument which contains fmsfundata.

Author(s)

Author of Scilab neldermead module: Michael Baudin (INRIA - Digiteo)

Author of R adaptation: Sebastien Bihorel (<sb.pmlab@gmail.com>)
See Also

fminsearch, neldermead, neldermead.set,

---

fminbnd.outputfun  \textit{fminbnd Output Function Call}

\section*{Description}

This function calls the output function and make it match neldermead requirements. It is used in the \texttt{fminbnd} function as the \texttt{outputcommand} element of the neldermead object (see \texttt{?neldermead} and \texttt{?neldermead.set}).

\section*{Usage}

\begin{verbatim}
fminbnd.outputfun(state = NULL, data = NULL, fmsdata = NULL)
\end{verbatim}

\section*{Arguments}

\begin{itemize}
  \item \texttt{state}  
    The current state of the algorithm either 'init', 'iter' or 'done'.
  \item \texttt{data}  
    The data at the current state. This is an object of class 'neldermead.data', i.e. a list with the following elements:
    \begin{itemize}
    \item \texttt{x}  
      The current parameter estimates.
    \item \texttt{fval}  
      The current value of the cost function.
    \item \texttt{simplex}  
      The current simplex object.
    \item \texttt{iteration}  
      The number of iterations performed.
    \item \texttt{funccount}  
      The number of function evaluations.
    \item \texttt{step}  
      The type of step in the previous iteration.
    \end{itemize}
  \item \texttt{fmsdata}  
    This is an object of class 'optimbase.functionargs' which contains specific data of the \texttt{fminbnd} algorithm:
    \begin{itemize}
    \item \texttt{Display}  
      what to display
    \item \texttt{OutputFcn}  
      the array of output functions
    \item \texttt{PlotFcns}  
      the array of plot functions
    \end{itemize}
\end{itemize}

\section*{Value}

This function does not return any data, but execute the output function(s).

\section*{Author(s)}

Author of Scilab neldermead module: Michael Baudin (INRIA - Digiteo)
Author of R adaptation: Sebastien Bihorel (\texttt{<sb.pmlab@gmail.com>})

\section*{See Also}

fminbnd, neldermead, neldermead.set,
Description

This function searches for the unconstrained minimum of a given cost function. The provided algorithm is a direct search algorithm, i.e. an algorithm which does not use the derivative of the cost function. It is based on the update of a simplex, which is a set of \(k \geq n+1\) vertices, where each vertex is associated with one point and one function value. This algorithm is the Nelder-Mead algorithm. This function is based on a specialized use of the more general neldermead function bundle. Users who want to have a more flexible solution based on direct search algorithms should consider using the neldermead functions instead of the fminsearch function.

Usage

```r
fminsearch(fun = NULL, x0 = NULL, options = NULL, verbose=FALSE)
```

Arguments

- **fun**: A cost function return a numeric scalar.
- **x0**: A numerical vector of initial guesses (length n).
- **options**: A list of optimization options, which drives the behaviour of fminsearch. These options must be set with the optimset function (see ?optimset) which returns a list with the following elements:
  - **MaxIter**: The maximum number of iterations. The default is \(200 \times n\).
  - **MaxFunEvals**: The maximum number of evaluations of the cost function. The default is \(200 \times n\).
  - **TolFun**: The absolute tolerance on function value. The default value is \(1.e-4\).
  - **TolX**: The absolute tolerance on simplex size. The default value is \(1.e-4\).
  - **Display**: The verbose level.
  - **OutputFcn**: The output function, or a list of output functions called at the end of each iteration. The default value is NULL.
  - **PlotFcns**: The plot function, or a list of plotput functions called at the end of each iteration. The default value is empty.
- **verbose**: The verbose option, controlling the amount of messages.

Details

**Termination criteria**

In this section, we describe the termination criteria used by fminsearch. The criteria is based on the following variables:

- **ssize** the current simplex size,
\textbf{shiftfv} the absolute value of the difference of function value between the highest and lowest vertices.

If both \texttt{ssize} < \texttt{options}\$TolX and \texttt{shiftfv} < \texttt{options}\$TolFun conditions are true, then the iterations stop. The size of the simplex is computed using the 'sigmamplus' method of the \texttt{optim-simplex} package. The 'sigmamplus' size is the maximum length of the vector from each vertex to the first vertex. It requires one loop over the vertices of the simplex.

\textbf{The initial simplex}

The \texttt{fminsearch} algorithm uses a special initial simplex, which is an heuristic depending on the initial guess. The strategy chosen by \texttt{fminsearch} corresponds to the content of \texttt{simplex0method} element of the neldermead object (set to 'pfeffer'). It is applied using the content of the \texttt{simplex0deltausual} (0.05) and \texttt{simplex0deltazero} (0.0075) elements. Pfeffer’s method is an heuristic which is presented in 'Global Optimization Of Lennard-Jones Atomic Clusters' by Ellen Fan. It is due to L. Pfeffer at Stanford. See in the help of optimsimplex for more details.

\textbf{The number of iterations}

In this section, we present the default values for the number of iterations in \texttt{fminsearch}.

The \texttt{options} input argument is an optional list which can contain the \texttt{MaxIter} field, which stores the maximum number of iterations. The default value is 200\texttt{n}, where \texttt{n} is the number of variables. The factor 200 has not been chosen by chance, but is the result of experiments performed against quadratic functions with increasing space dimension. This result is presented in 'Effect of dimensionality on the Nelder-mead simplex method' by Lixing Han and Michael Neumann. This paper is based on Lixing Han’s PhD, 'Algorithms in Unconstrained Optimization'. The study is based on numerical experiments with a quadratic function where the number of terms depends on the dimension of the space (i.e. the number of variables). Their study showed that the number of iterations required to reach the tolerance criteria is roughly 100\texttt{n}. Most iterations are based on inside contractions. Since each step of the Nelder-Mead algorithm only require one or two function evaluations, the number of required function evaluations in this experiment is also roughly 100\texttt{n}.

\textbf{Output and plot functions}

The \texttt{optimset} function can be used to configure one or more output and plot functions. The output or plot function is expected to have the following definition:

\texttt{myfun <- function(x , optimValues , state)}

The input arguments \texttt{x}, \texttt{optimValues} and \texttt{state} are described in detail in the \texttt{optimset} help page. The \texttt{optimValues}\$\texttt{procedure} field represents the type of step performed at the current iteration and can be equal to one of the following strings:

- " (the empty string),
- 'initial simplex',
- 'expand',
- 'reflect',
- 'contract inside',
- 'contract outside'.

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Value

Return a object of class neldermead. Use the neldermead.get to extract the following element from the returned object:

- **xopt** The vector of n numeric values, minimizing the cost function.
- **fopt** The minimum value of the cost function.
- **exitflag** The flag associated with exist status of the algorithm. The following values are available:
  - -1 The maximum number of iterations has been reached.
  - 0 The maximum number of function evaluations has been reached.
  - 1 The tolerance on the simplex size and function value delta has been reached. This signifies that the algorithm has converged, probably to a solution of the problem.
- **output** A list which stores detailed information about the exit of the algorithm. This list contains the following fields:
  - **algorithm** A string containing the definition of the algorithm used, i.e. 'Nelder-Mead simplex direct search'.
  - **funcCount** The number of function evaluations.
  - **iterations** The number of iterations.
  - **message** A string containing a termination message.

Author(s)

Author of Scilab neldermead module: Michael Baudin (INRIA - Digiteo)
Author of R adaptation: Sebastien Bihorel (<sb.pmlab@gmail.com>)

References


See Also

optimset neldermead
Examples

#In the following example, we use the fminsearch function to compute the minimum #of the Rosenbrock function. We first define the function 'banana', and then use #the fminsearch function to search the minimum, starting with the initial guess #(1.2, 1.0). In this particular case, 85 iterations are performed with 159 #function evaluations

banana <- function(x){
  y <- 100*(x[2]-x[1]^2)^2 + (1-x[1])^2
}
sol <- fminsearch(banana, c(-1.2,1))
sol

#In the following example, we configure the absolute tolerance on the size of #the simplex to a larger value, so that the algorithm performs less iterations. #Since the default value of 'TolX' for the fminsearch function is 1.e-4, we #decide to use 1.e-2. The optimset function is used to create an optimization #option list and the field 'TolX' is set to 1.e-2. The options list is then #passed to the fminsearch function as the third input argument. In this #particular case, the number of iterations is 70 with 130 function evaluations.

opt <- optimset(TolX=1.e-2)
sol <- fminsearch(banana, c(-1.2,1), opt)
sol

#In the following example, we want to produce intermediate outputs of the #algorithm. We define the outfun function, which takes the current point x as #input argument. The function plots the current point into the current graphic #window with the plot function. We use the 'OutputFcn' feature of the optimset #function and set it to the output function. Then the option list is passed #to the fminsearch function. At each iteration, the output function is called #back, which creates and update a plot. While this example creates a 2D plot, #the user may customized the output function so that it writes a message in #the console, write some data into a data file, etc... The user can distinguish #between the output function (associated with the 'OutputFcn' option) and the #plot function (associated with the 'PlotFcns' option). See the optimset for #more details on this feature.

outfun <- function(x, optimValues, state){
  plot(x[1],x[2],xlim=c(-1.5,1.5),ylim=c(-1.5,1.5))
  par(new=TRUE)
}

opt <- optimset(OutputFcn=outfun)
sol <- fminsearch(banana, c(-1.2,1), opt)
sol

#The 'Display' option allows to get some input about the intermediate steps of #the algorithm as well as to be warned in case of a convergence problem. #In the following example, we present what happens in case of a convergence #problem. We set the number of iterations to 10, instead of the default 400 #iterations. We know that 85 iterations are required to reach the convergence #criteria. Therefore, the convergence criteria is not met and the maximum number #of iterations is reached.
opt <- optimset(MaxIter=10)
sol <- fminsearch(banana, c(-1.2,1), opt)

#Since the default value of the 'Display' option is 'notify', a message is
#generated, which warns the user about a possible convergence problem. The
#previous script produces the following output.
# Exiting: Maximum number of iterations has been exceeded
# - increase MaxIter option.
# Current function value: 4.1355598

#In the following example, we present how to display intermediate steps used by
#the algorithm. We simply set the 'Display' option to the 'iter' value. This
#option allows to see the number of function evaluations, the minimum function
#value and which type of simplex step is used for the iteration.

opt <- optimset(Display='iter')
sol <- fminsearch(banana, c(-1.2,1), opt)
sol

neldermead.algo  
Nelder-Mead Algorithm

Description

neldermead.algo performs an optimization without restart using the method associated with
the method element of the neldermead object; neldermead.fixed, neldermead.variable, neldermead.box,
boxlinesearch, neldermead.storehistory, neldermead.termination, and neldermead.interpolate
are utility functions for neldermead.algo.

Usage

neldermead.algo(this = NULL)
neldermead.fixed(this = NULL)
neldermead.variable(this = NULL)
neldermead.box(this = this)
boxlinesearch(this = NULL, n = NULL, xbar = NULL, xhigh = NULL, fhigh = NULL,
rho = NULL)
neldermead.storehistory(this = NULL, n = NULL, fopt = NULL, xopt = NULL,
fv = NULL, xcoords = NULL)
neldermead.termination(this = NULL, finitial = NULL, oldfmean = NULL,
newfmean = NULL, previousxopt = NULL,
currentxopt = NULL, simplex = NULL)
neldermead.interpolate(x1 = NULL, x2 = NULL, fac = NULL)

Arguments

this  A neldermead object.
n  Number of variables.
xbar The centroid.
xhigh The high point.
fhigh The value of the cost function at xhigh.
rho The reflection factor.
fopt The current value of the function at the current optimum point estimate.
xopt The current optimum point estimate.
fv The function values, with size nbve x 1.
xcoords Matrix of size n x n+1, coordinates of the n+1 vertices
fvinitial The initial cost function value.
oldfvmean The old cost function value average on the simplex.
newfvmean The new cost function value average on the simplex.
previousxopt The previous point estimate.
currentxopt The current point estimate.
simplex The simplex. The best point estimate in the simplex is expected to be stored at 1, while the worst point estimate in the simplex is expected to be stored at n+1.
x1 The first reference point estimate to perform the interpolation.
x2 The second reference point estimate to perform the interpolation.
fac A factor to perform the interpolation.

Details

neldermead.fixed The simplex algorithm with fixed size simplex. We implement the following ‘rules’ of the method of Spendley et al.

- Rule 1 is strictly applied, but the reflection is done by reflection of the high point, since we minimize a function instead of maximizing it, like Spendley.
- Rule 2 is NOT implemented, as we expect that the function evaluation is not subject to errors.
- Rule 3 is applied, i.e. reflection with respect to next to high point. A shrink step is included, with shrinkage factor sigma.

Rule 1. Ascertain the lowest reading y, of yi ... Yk+1 Complete a new simplex Sp by excluding the point Vp corresponding to y, and replacing it by V* defined as above.

Rule 2. If a result has occurred in (k + 1) successive simplexes, and is not then eliminated by application of Rule 1, do not move in the direction indicated by Rule 1, or at all, but discard the result and replace it by a new observation at the same point.

Rule 3. If y is the lowest reading in So , and if the next observation made, y* , is the lowest reading in the new simplex S , do not apply Rule 1 and return to So from Sp . Move out of S , by rejecting the second lowest reading (which is also the second lowest reading in So).

neldermead.variable The original Nelder-Mead algorithm, with variable-size simplex.

neldermead.box The Nelder-Mead algorithm, with variable-size simplex and modifications by Box for bounds and inequality constraints.
boxlinesearch Called by neldermead.box, i.e. Box’s method. Perform a line search from xbar, on the line \((x_{\text{high}}, x_{\text{bar}})\). The reflected point estimate satisfies the following constraints:
  - \(fr < f_{\text{high}}\)
  - \(xr\) satisfies the bounds constraints
  - \(xr\) satisfies the nonlinear positive inequality constraints
  - \(xr\) satisfies the linear positive inequality constraints

The method is based on projection and scaling toward the centroid.

neldermead.storehistory Store the optimization history into the neldermead object.

neldermead.termination Determine if the algorithm must continue or terminate. The function uses the cost function average in the simplex instead of the best cost function value. This is because the function average changes at each iteration. Instead, the best function value has a step-by-step evolution and may not change between two successive iterations, leading to a stop of the algorithm.

neldermead.interpolate Compute the point estimate \(xi\) as an interpolation between \(x_1\) and \(x_2\), as follows: \(xi = (1+fac)x_1 - fac^*x_2\)

Value

neldermead.fixed, neldermead.variable, and neldermead.box Return the updated neldermead object, containing the optimum point estimate.

boxlinesearch Return a list with the following elements:
  - \(\text{this}\) The updated neldermead object.
  - \(\text{status}\) TRUE if the search is successful, FALSE otherwise.
  - \(\text{xr}\) The reflected point estimate.
  - \(\text{fr}\) The value of the cost function at \(\text{xr}\).

neldermead.storehistory Return the updated neldermead object.

neldermead.termination Return a list with the following elements:
  - \(\text{this}\) The updated neldermead object
  - \(\text{terminate}\) TRUE if the algorithm terminates, FALSE if the algorithm must continue.
  - \(\text{status}\) The termination status: 'continue', 'maxiter', 'maxfuneval', 'tolf', 'tolx', 'tolsize', 'tolsizedeltafv', 'kelleystagnation', 'tolboxf', 'tolvariance' or the user-defined termination status.

neldermead.interpolate Return a new point estimate, i.e. a column vector.

Author(s)

Author of Scilab neldermead module: Michael Baudin (INRIA - Digiteo)
Author of R adaptation: Sebastien Bihorel (<sb.pmlab@gmail.com>)
neldermead.destroy  *Erase a neldermead object.*

Description
neldermead.destroy calls optimbase.destroy and optimsimplex.destroy to erase the content of this$optbase and this$simplex0.

Usage
neldermead.destroy(this = NULL)

Arguments
this  A neldermead object.

Value
Return an updated neldermead object.

Author(s)
Author of Scilab neldermead module: Michael Baudin (INRIA - Digiteo)
Author of R adaptation: Sebastien Bihorel (<sb.pmlab@gmail.com>)

See Also
optimbase.destroy, optimsimplex.destroy

neldermead.get  *Get the value for the given element*

Description
Get the value for the given element in a neldermead object.

Usage
neldermead.get(this = NULL, key = NULL)

Arguments
this  A neldermead object.
key  The name of the key to query.
Value

Return the value of the list element `key`, or an error message if `key` does not exist in the `neldermead` object `this`.

Author(s)

Author of Scilab neldermead module: Michael Baudin (INRIA - Digiteo)
Author of R adaptation: Sebastien Bihorel (<sb.pmlab@gmail.com>)

See Also

`neldermead.set`, `optimbase.get`

---

**neldermead**  
*S3 neldermead object*

Description

These functions support the S3 class 'neldermead' and are intended to either create objects of this class or check if an object is of this class.

Usage

```r
neldermead(optbase, method, simplex0, simplex0method,  
simplex0length, simplexsize0, simplexopt, historysimplex, coords0, rho, chi,  
gamma, sigma, tolfstdeviation, tolfstdeviationmethod, tolsimplexizeabsolute,  
tolsimplexizerelative, tolsimplexizemethod, toldeltafv, tolssizedeltafvmethod,  
simplex0deltausual, simplex0deltazero, restartsimplexmethod, restartmax,  
restarteps, restartstep, restartnb, restartflag, restartdetection,  
kelleystagnationflag, kelleynormalizationflag, kelleystagnationalpha0,  
kellyalpha, startupflag, boxnbpoints, boxnbpointseff, boxineqscaling,  
checkcostfunction, scalingsimplex0, guinalphamin, boxboundsalpha,  
boxtermination, boxtolf, boxnbmatch, boxkount, boxreflect, tolvarianceflag,  
tolabsolutevariance, tolrelativevariance, variancesimplex0, mymethod,  
myterminate, myterminateflag, greedy, output, exitflag)
```

```r
## S3 method for class 'neldermead'
print(x,verbose,...)
```

```r
## S3 method for class 'neldermead'
summary(object,showhistory,...)
```

```r
## S3 method for class 'neldermead'
is(x=NULL)
```

## S3 method for class 'neldermead'
print(x,verbose,...)

## S3 method for class 'neldermead'
summary(object,showhistory,...)

## S3 method for class 'neldermead'
is(x=NULL)
Arguments

optbase

An object of class 'optimbase', i.e. a list created by `optimbase()` and containing the following elements:

verbose  The verbose option, controlling the amount of messages.
x0  The initial guess.
fx0  The value of the function for the initial guess.
xopt  The optimum parameter.
fopt  The optimum function value.
tolfunabsolute  The absolute tolerance on function value.
tolfunrelative  The relative tolerance on function value.
tolfunmethod  Logical flag for the tolerance on function value in the termination criteria. This criteria is suitable for functions which minimum is associated with a function value equal to 0.
tolxabsolute  The absolute tolerance on x.
tolxrelative  The relative tolerance on x.
tolxmethod  Possible values: FALSE, TRUE.
funevals  The number of function evaluations.
maxfunevals  The maximum number of function evaluations.
maxiter  The maximum number of iterations.
iterations  The number of iterations.
fun  The cost function.
status  The status of the optimization.
historyfopt  The vector to store the history for fopt. The values of the cost function will be stored at each iteration in a new element, so the length of `historyfopt` at the end of the optimization should be the number of iterations.
historyxopt  The list to store the history for xopt. The vectors of estimates will be stored on separated levels of the list, so the length of `historyfopt` at the end of the optimization should be the number of iterations.
verbosetermination  The verbose option for termination criteria.
outputcommand  The command called back for output.
outputcommandarg  The outputcommand argument is initialized as a string. If the user configure this element, it is expected that a matrix of values or a list is passed so that the argument is appended to the name of the function.
numberofvariables  The number of variables to optimize.
storehistory  The flag which enables/disables the storing of the history.
costfargument  The costf argument is initialized as a string. If the user configure this element, it is expected that a matrix of values or a list is passed so that the argument is appended to the name of the function.
boundsmin  Minimum bounds for the parameters.
boundsmax  Maximum bounds for the parameters.
nbineqconst  The number of nonlinear inequality constraints.
logfile The name of the log file.
logfilehandle The handle for the log file.
logstartup Set to TRUE when the logging is started up.
withderivatives Set to TRUE when the method uses derivatives.

method The name of the algorithm to use.
simplex0 An object of class 'simplex', i.e. a list created by optimsimplex(), and containing the following elements:
  verbose The verbose option, controlling the amount of messages.
  x The coordinates of the vertices, with size nbve x n.
  n The dimension of the space.
  fv The function values, with size nbve x 1.
  nbve The number of vertices.
simplex0method The method to use to compute the initial simplex.
simplex0length The length to use when the initial simplex is computed with the 'axes' or 'spendley' methods.
 rho The reflection coefficient. This parameter is used when the method element is set to 'fixed' or 'variable'.
 chi The expansion coefficient. This parameter is used when the method element is set to 'variable'.
 gamma The contraction coefficient. This parameter is used when the method element is set to 'variable'.
 sigma The shrinkage coefficient. This parameter is used when the method element is set to 'fixed' or 'variable'.
tolfstdeviation The tolerance for the standard deviation.
tolfstdeviationmethod Set to FALSE.
tolsimplexizeabsolute The absolute tolerance on the simplex size.
tolsimplexizerelative The relative tolerance on the simplex size.
tolsimplexizemethod Logical flag to enable/disable the tolerance on the simplex size. When this criteria is enabled, the values of the tolsimplexizeabsolute and tolsimplexizerelative elements are used in the termination criteria. The method to compute the size is the 'sigmaplus' method.
simplexsize0 Initial size of the simplex, for the tolerance on the simplex size.
toldeltafv The absolute tolerance on the difference between the highest and the lowest function values.
tolssizedeltafvmethod Logical flag to enable/disable the termination criteria based on the size of the simplex and the difference of function value in the simplex. If this criteria is
triggered, the status of the optimization is set to 'tolsizedeltafv'. This termination criteria uses the values of the tolsimplexizeabsolute and toldeltafv elements. This criteria is identical to Scilab's fminsearch.

**historysimplex**

The list to store the history for simplex. The simplex will be stored on a new level of the list at each iteration, so the length of historyfopt at the end of the optimization should be the number of iterations.

**coords0**

The coordinates of the vertices of the initial simplex. If the simplex0method element is set to 'given', these coordinates are used to compute the initial simplex. This matrix is expected to have shape nbve x n where nbve is the number of vertices and n is the number of variables.

**simplex0deltausual**

The relative delta for non-zero parameters in 'pfeffer' method.

**simplex0deltazero**

The absolute delta for non-zero parameters in 'pfeffer' method.

**simplexopt**

The optimum simplex, after one optimization process.

**restartsimplexmethod**

The method to compute the initial simplex after a restart.

**restartmax**

The maximum number of restarts, when automatic restart is enabled via the restartflag element.

**restarteps**

The absolute epsilon value used to check for optimality in the factorial O'Neill restart detection.

**restartstep**

The absolute step length used to check for optimality in the factorial O'Neill restart detection.

**kelleystagnationflag**

Logical flag to enable/disable the termination criteria using Kelley's stagnation detection, based on sufficient decrease condition. If this criteria is triggered, the status of the optimization is set to 'kelleystagnation'.

**kelleynormalizationflag**

Logical flag to enable/disable the normalization of the alpha coefficient in Kelley's stagnation detection, i.e. use the value of the kelleystagnationalpha0 element as is.

**kelleystagnationalpha0**

The parameter used in Kelley's stagnation detection.

**kelleyalpha**

The current value of Kelley's alpha, after normalization, if required.

**restartnb**

Number of restarts performed.

**restartflag**

Logical flag to enable/disable the automatic restart of the algorithm.

**restartdetection**

The method to detect if the automatic restart must be performed.

**startupflag**

Set to TRUE when the startup has been performed.

**boxbounds**

The number of points in the initial simplex, when the simplex0method is set to 'randbounds'. The value of this element is also use to update the simplex when a restart is performed and the restartsimplexmethod element is set to 'randbounds'. The default value is so that the number of points is twice the number of variables of the problem.
boxnbpointseff
   The effective number of points required in the simplex for Box’s algorithm.

boxineqscaling
   The scaling coefficient used to scale the trial point for function improvement or into the constraints of Box’s algorithm.

checkcostfunction
   Logical flag to enable/disable the checking of the connection of the cost function.

scalingsimplex0
   The algorithm used to scale the initial simplex into the nonlinear constraints. The following two algorithms are provided:
   'tox0’ scales the vertices toward the initial guess.
   'tocentroid’ scales the vertices toward the centroid, as recommended by Box.
   If the centroid happens to be unfeasible, because the constraints are not convex, the scaling of the initial simplex toward the centroid may fail. Since the initial guess is always feasible, scaling toward the initial guess cannot fail.

guinalphamin
   The minimum value of alpha when scaling the vertices of the simplex into nonlinear constraints in Box’s algorithm.

boxboundsalpha
   The parameter used to project the vertices into the bounds in Box’s algorithm.

boxtermination
   Logical flag to enable/disable Box’s termination criteria.

boxtolf
   The absolute tolerance on difference of function values in the simplex, suggested by Box. This tolerance is used if the boxtermination element is set to TRUE.

boxnbmatch
   The number of consecutive match of Box’s termination criteria.

boxkount
   Current number of consecutive match.

boxreflect
   The reflection factor in Box’s algorithm.

tolvarianceflag
   Logical flag to enable/disable the termination criteria based on the variance of the function value. If this criteria is triggered, the status of the optimization is set to ’tolvariance’. This criteria is suggested by Nelder and Mead.

tolabsolutevariance
   The absolute tolerance on the variance of the function values of the simplex.

tolrelativevariance
   The relative tolerance on the variance of the function values of the simplex.

variancesimplex0
   Relative tolerance on variance.

mymethod
   A user-derived simplex algorithm.

myterminate
   A user-defined terminate function.

myterminateflag
   Logical flag to enable/disable the user-defined terminate function.

greedy
   Logical flag to enable/disable greedy Nelder-Mead.

output
   The command to call back for user-defined output of specialized function.
- **exitflag**: Logical flag to enable/disable the user-defined output of specialized function.
- **x**: An object of class 'neldermead'.
- **verbose**: A logical flag, controlling the amount of data printed.
- **...**: optional arguments to 'print' or 'plot' methods.
- **object**: An object of class 'neldermead'.
- **showhistory**: Optional logical flag, to define whether optimization history must be summarized or not.

**Value**

The `neldermead` function returns a new object of class 'neldermead', with the following default content:

- **optbase**: An object of class 'optimbase' with the following default content:
  - **verbose**: Default is FALSE.
  - **x0**: Default is NULL.
  - **fx0**: Default is NULL.
  - **xopt**: Default is 0.
  - **fopt**: Default is 0.
  - **tolfunabsolute**: Default is 0.
  - **tolfunrelative**: Default is .Machine$double.eps.
  - **tolfunmethod**: Default is FALSE.
  - **tolxabsolute**: Default is 0.
  - **tolxrelative**: Default is .Machine$double.eps.
  - **tolxmethod**: Default is TRUE.
  - **funevals**: Default is 0.
  - **maxfunevals**: Default is 100.
  - **maxiter**: Default is 100.
  - **iterations**: Default is 0.
  - **fun**: Default is ".
  - **status**: Default is ".
  - **historyfopt**: Default is NULL.
  - **historyxopt**: Default is NULL.
  - **verbosemetermination**: Default is FALSE.
  - **outputcommand**: Default is ".
  - **outputcommandarg**: Default is ". If the user configures this element, it is expected to be an object of class 'optimbase.outputargs' or will be coerced to an object of class 'optimbase.outputargs'.
  - **numberofvariables**: Default is 0.
  - **storehistory**: Default is FALSE.
  - **costfargument**: Default is ". If the user configures this element, it is expected to be an object of class 'optimbase.functionargs' or will be coerced to an object of class 'optimbase.functionargs'.

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boundsmin Default is NULL.
boundsmax Default is NULL.
bineqconst Default is 0.
logfile Default is ".
logfilehandle Default is 0.
logstartup Default is FALSE.
withderivatives Default is FALSE.
method Default is 'variable'.
simplex0 Default is an object of class 'simplex', with the following content:
  verbose Default is 0.
  x Default is NULL.
  n Default is 0.
  fv Default is NULL.
  nbve Default is 0.
simplex0method Default is 'axes'.
simplex0length Default is 1.
rho Default is 1.
chi Default is 2.
gamma Default is 0.5.
sigma Default is 0.5.
tolfstdeviation Default is 0.
tolfstdeviationmethod Default is FALSE.
tolsimplexizeabsolute Default is 0.
tolsimplexizerelative Default is .Machine$double.eps.
tolsimplexizemethod Default is FALSE.
simplexsize0 Default is 0.
toldeltafv Default is .Machine$double.eps.
tolssizedeltafvmethod Default is FALSE.
historysimplex Default is NULL.
coords0 Default is NULL.
simplex0deltausual Default is 0.05.
simplex0deltazero Default is 0.0075.
simplexopt Default is NULL.
restartsimplexmethod Default is 'oriented'.
restartmax Default is 3.
restarteps Default is .Machine$double.eps.
restartstep Default is 1.
kelleystagnationflag Default is FALSE.,
**kelleynormalizationflag** Default is TRUE, i.e. the simplex gradient of the initial simplex is taken into account in the stagnation detection.

**kelleystagnationalpha0** Default is 1.e-4.

**kelleyalpha** Default is 1.e-4.

**restartnb** Default is 0.

**restartflag** Default is FALSE.

**restartdetection** Default is 'oneill'.

**startupflag** Default is FALSE.

**boxnbpoints** Default is '2n'.

**boxnbpointseff** Default is 0.

**boxineqscaling** Default is 0.

**checkcostfunction** Default is TRUE.

**scalingsimplex0** Default is 'tox0'.

**guinalphamin** Default is 1.e-6.

**boxtermination** Default is FALSE.

**boxtolf** Default is 1.e-5.

**boxnbmatch** Default is 5.

**boxkount** Default is 0.

**boxreflect** Default is 1.3.

**tolvarianceflag** Default is FALSE.

**tolabsolutevariance** Default is 0.

**tolrelativevariance** Default is .Machine$double.eps.

**variancesimplex0** Default is .Machine$double.eps.

**mymethod** Default is NULL.

**myterminate** Default is NULL.

**myterminateflag** Default is FALSE.

**greedy** Default is FALSE.

**output** Default is list().

**exitflag** Default is FALSE.

---

**Author(s)**

Author of Scilab neldermead module: Michael Baudin (INRIA - Digiteo)

Author of R adaptation: Sebastien Bihorel (<sb.pmlab@gmail.com>)

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**See Also**

optimbase, optimsimplex
neldermead.restart  
*Restart neldermead search.*

**Description**

Update the simplex with `neldermead.updatesimp` and restart the search with `neldermead.search`.

**Usage**

```
neldermead.restart(this = NULL)
```

**Arguments**

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>this</code></td>
<td>A neldermead object.</td>
</tr>
</tbody>
</table>

**Value**

Returns an updated neldermead object.

**Author(s)**

- Author of Scilab neldermead module: Michael Baudin (INRIA - Digiteo)
- Author of R adaptation: Sebastien Bihorel (`<sb.pmlab@gmail.com>`)

**See Also**

`neldermead.updatesimp`, `neldermead.search`.

neldermead.search  
*Starts the optimization*

**Description**

Performs the optimization associated with the method associated with the `method` element of the `neldermead` object and find the optimum. If the `restartflag` element is enabled, automatic restarts are performed, based on the `restartdetection` element.

**Usage**

```
neldermead.search(this = NULL)
```

**Arguments**

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>this</code></td>
<td>A neldermead object.</td>
</tr>
</tbody>
</table>

**Value**

Return an updated neldermead object.

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Author(s)

Author of Scilab neldermead module: Michael Baudin (INRIA - Digiteo)
Author of R adaptation: Sebastien Bihorel (<sb.pmlab@gmail.com>)

See Also

fminsearch, neldermead, neldermead.set,

neldermead.set  Neldermead Object Configuration

Description

Configure the current neldermead object with the given value for the given key.

Usage

neldermead.set(this = NULL, key = NULL, value = NULL)

Arguments

this  The current neldermead object.
key  The key to configure. See details for the list of possible keys.
value  The value to assign to the key.

Details

neldermead.set sets the content of the key element of the neldermead object this to value.
If key is a sub-element of this$optbase, value is assigned by optimbase.set.
The main available keys are the following:

' -verbose' Set to 1 to enable verbose logging.
' -verbosetermination' Set to 1 to enable verbose termination logging.
' -x0' The initial guess, as a n x 1 column vector, where n is the number of variables.
' -maxfunevals' The maximum number of function evaluations. If this criteria is triggered during optimization, the status of the optimization is set to 'maxfuneval'.
' -maxiter' The maximum number of iterations. If this criteria is triggered during optimization, the status of the optimization is set to 'maxiter'.option
' -tolfunabsolute' The absolute tolerance for the function value.
' -tolfunrelative' The relative tolerance for the function value.
' -tolfunmethod' The method used for the tolerance on function value in the termination criteria. The following values are available: TRUE, FALSE. If this criteria is triggered, the status of the optimization is set to 'tolf'.
' -tolxabsolute' The absolute tolerance on x.
'tolxrelative’ The relative tolerance on x.

'tolxmethod’ The method used for the tolerance on x in the termination criteria. The following values are available: TRUE, FALSE. If this criteria is triggered during optimization, the status of the optimization is set to ‘tolx’.

'function’ The objective function, which computes the value of the cost and the non linear constraints, if any. See vignette(‘neldermead’,package=‘neldermead’) for the details of the communication between the optimization system and the cost function.

'costfargument’ An additional argument, passed to the cost function.

'outputcommand’ A command which is called back for output. See vignette(‘neldermead’,package=‘neldermead’) for the details of the communication between the optimization system and the output command function.

'outputcommandarg’ An additional argument, passed to the output command option.

'numberofvariables’ The number of variables to optimize.

'storehistory’ Set to TRUE to enable the history storing.

'boundsmin’ The minimum bounds for the parameters.

'boundsmax’ The maximum bounds for the parameters.

'nbineqconst’ The number of inequality constraints.

'method’ The name of the algorithm to use. The following methods are available:

'fixed’ the fixed simplex shape algorithm of Spendley et al. This algorithm is for unconstrained problems (i.e. bounds and non linear constraints are not taken into account)

'variable’ the variable simplex shape algorithm of Nelder and Mead. This algorithm is for unconstrained problems (i.e. bounds and non linear constraints are not taken into account)

'box’ Box’s complex algorithm. This algorithm takes into account bounds and nonlinear inequality constraints.

'mine’ the user-defined algorithm, associated with the mymethod element. See vignette(‘neldermead’,package=‘neldermead’) for details.

'simplex0method’ The method to use to compute the initial simplex. The first vertex in the simplex is always the initial guess associated with the x0 element. The following methods are available:

'given’ The coordinates associated with the coords0 element are used to compute the initial simplex, with arbitrary number of vertices. This allows the user to setup the initial simplex by a specific method which is not provided by the current package (for example with a simplex computed from a design of experiments). This allows also to configure the initial simplex so that a specific behaviour of the algorithm is to be reproduced (for example the Mac Kinnon test case). The given matrix is expected to have nbve rows and n columns, where n is the dimension of the problem and nbve is the number of vertices.

'axes’ The simplex is computed from the coordinate axes and the length associated with the simplex0length element.

'spendley’ The simplex is computed so that it is regular with the length associated with the simplex0length element (i.e. all the edges have the same length).

'pfeffer’ The simplex is computed from an heuristic, in the neighborhood of the initial guess. This initial simplex depends on the -simplex0deltausual and -simplex0deltazero.
'randbounds' The simplex is computed from the bounds and a random number. This option is available only if bounds are available; if bounds are not available, an error is generated. This method is usually associated with Box's algorithm. The number of vertices in the simplex is taken from the boxnbpoints element.

'-coords0' The coordinates of the vertices of the initial simplex. If the simplex0method element is set to 'given', these coordinates are used to compute the initial simplex. This matrix is expected to have shape nbve x n, where nbve is the number of vertices and n is the number of variables.

'-simplex0length' The length to use when the initial simplex is computed with the 'axes' or 'spendley' methods. If the initial simplex is computed from 'spendley' method, the length is expected to be a scalar value. If the initial simplex is computed from 'axes' method, it may be either a scalar value or a vector of values, of length n, where n is the number of variables.

'-simplex0deltausual' The relative delta for non-zero parameters in 'pfeffer' method.

'-simplex0deltazero' The absolute delta for non-zero parameters in 'pfeffer' method.

'-rho' The reflection coefficient. This parameter is used when the method element is set to 'fixed' or 'variable'.

'-chi' The expansion coefficient. This parameter is used when the method element is set to 'variable'.

'-gamma' The contraction coefficient. This parameter is used when the method element is set to 'variable'.

'-sigma' The shrinkage coefficient. This parameter is used when the method element is set to 'fixed' or 'variable'.

'-tolsimplexizemethod' Set to FALSE to disable the tolerance on the simplex size. If this criteria is triggered, the status of the optimization is set to 'tolsizedeltafv'. When this criteria is enabled, the values of the tolsimplexizeabsolute and tolsimplexizerelative elements are used in the termination criteria. The method to compute the size is the 'sigmaplus' method.

'-tolsimplexizeabsolute' The absolute tolerance on the simplex size.

'-tolsimplexizerelative' The relative tolerance on the simplex size.

'-tolssizedeltafvmethod' Set to TRUE to enable the termination criteria based on the size of the simplex and the difference of function value in the simplex. If this criteria is triggered, the status of the optimization is set to 'tolsizedeltafv'. This termination criteria uses the values of the tolsimplexizeabsolute and toldeltafv elements.

'-toldeltafv' The absolute tolerance on the difference between the highest and the lowest function values.

'-tolvarianceflag' Set to TRUE to enable the termination criteria based on the variance of the function value. If this criteria is triggered, the status of the optimization is set to 'tolvariance'. This criteria is suggested by Nelder and Mead.

'-tolabsolutevariance' The absolute tolerance on the variance of the function values of the simplex.

'-tolrelativevariance' The relative tolerance on the variance of the function values of the simplex.
`-kelleystagnationflag` Set to TRUE to enable the termination criteria using Kelley’s stagnation detection, based on sufficient decrease condition. If this criteria is triggered, the status of the optimization is set to ‘kelleystagnation’.

`-kelleynormalizationflag` Set to FALSE to disable the normalization of the alpha coefficient in Kelley’s stagnation detection, i.e. use the value of the `kelleystagnationalpha0` element as is. Default value is TRUE, i.e. the simplex gradient of the initial simplex is takeoptionn into account in the stagnation detection.

`-kelleystagnationalpha0` The parameter used in Kelley’s stagnation detection.

`-restartflag` Set to TRUE to enable the automatic restart of the algorithm.

`-restartdetection` The method to detect if the automatic restart must be performed. The following methods are available:

  - `'oneill'` The factorial local optimality test by O’Neill is used. If the test finds a local point which is better than the computed optimum, a restart is performed.
  - `'kelley'` The sufficient decrease condition by O’Neill is used. If the test finds that the status of the optimization is ‘kelleystagnation’, a restart is performed. This status may be generated if the `-kelleystagnationflag` option is set to TRUE.

`-restartmax` The maximum number of restarts, when automatic restart is enabled via the `-restartflag` option.

`-restarteps` The absolute epsilon value used to check for optimality in the factorial O’Neill restart detection.

`-restartstep` The absolute step length used to check for optimality in the factorial O’Neill restart detection.

`-restartsimplexmethod` The method to compute the initial simplex after a restart. The following methods are available.

  - `'given'` The coordinates associated with the `coords0` element are used to compute the initial simplex, with arbitrary number of vertices. This allow the user to setup the initial simplex by a specific method which is not provided by the current package (for example with a simplex computed from a design of experiments). This allows also to configure the initial simplex so that a specific behaviour of the algorithm is to be reproduced (for example the Mc Kinnon test case). The given matrix is expected to have `nbve` rows and `n` columns, where `n` is the dimension of the problem and `nbve` is the number of vertices.
  - `'axes'` The simplex is computed from the coordinate axes and the length associated with the `-simplex0length` option.
  - `'spendley'` The simplex is computed so that it is regular with the length associated with the `-simplex0length` option (i.e. all the edges have the same length).
  - `'pfeffer'` The simplex is computed from an heuristic, in the neighborhood of the initial guess. This initial simplex depends on the `-simplex0deltausual` and `-simplex0deltazero`.
  - `'randbounds'` The simplex is computed from the bounds and a random number. This option is available only if bounds are available: if bounds are not available, an error is generated. This method is usually associated with Box’s algorithm. The number of vertices in the simplex is taken from the `-boxnbpoints` option.
  - `'oriented'` The simplex is computed so that it is oriented, as suggested by Kelley.

`-scalingsimplex0` The algorithm used to scale the initial simplex into the nonlinear constraints. The following two algorithms are provided:
'tox0' scales the vertices toward the initial guess.
'tocentroid' scales the vertices toward the centroid, as recommended by Box.

If the centroid happens to be unfeasible, because the constraints are not convex, the scaling
of the initial simplex toward the centroid may fail. Since the initial guess is always feasible,
scaling toward the initial guess cannot fail.

'-boxnbpoints' The number of points in the initial simplex, when the -simplex0method is set
to 'randbounds'. The value of this option is also use to update the simplex when a restart is
performed and the -restartsimpllexmethod option is set to 'randbounds'. The default value
is so that the number of points is twice the number of variables of the problem.

'-boxineqscaling' The scaling coefficient used to scale the trial point for function improvement
or into the constraints of Box’s algorithm.

'-guinalphamin' The minimum value of alpha when scaling the vertices of the simplex into
nonlinear constraints in Box’s algorithm.

'-boxreflect' The reflection factor in Box’s algorithm.

'-boxtermination' Set to TRUE to enable Box’s termination criteria.

'-boxtolf' The absolute tolerance on difference of function values in the simplex, suggested by
Box. This tolerance is used if the -boxtermination element is set to TRUE.

'-boxnbmatch' The number of consecutive match of Box’s termination criteria.

'-boxboundsalpha' The parameter used to project the vertices into the bounds in Box’s algo-
rithm.

'-mymethod' A user-defined simplex algorithm. See vignette('neldermead',package='neldermead')
for details.

'-myterminate' A user-defined terminate function. See vignette('neldermead',package='neldermead')
for details.

'-myterminateflag' Set to TRUE to enable the user-defined terminate function.

Value
An updated neldermead object.

Author(s)
Author of Scilab neldermead module: Michael Baudin (INRIA - Digiteo)
Author of R adaptation: Sebastien Bihorel (<sb.pmlab@gmail.com>)

See Also
neldermead
Secondary search functions
Secondary functions for neldermead.search

Description
Utility functions for neldermead.search and dependent functions.

Usage
neldermead.startup(this = NULL)
neldermead.log(this = NULL, msg = NULL)
neldermead.scaletox0(this = NULL, simplex0 = NULL)
neldermead.scaletocenter(this = NULL, simplex0 = NULL, x0 = NULL)
neldermead.termstartup(this = NULL)
neldermead.outputcmd(this = NULL, state = NULL, simplex = NULL, step = NULL)
neldermead.autorestart(this = NULL)
neldermead.istorestart(this = NULL)
neldermead.isrkelley(this = this)
neldermead.istorexelley(this = NULL)
neldermead.updatesimp(this = NULL)
scaleinconstraints(this = NULL, x = NULL, xref = NULL)
neldermead.costf(x = NULL, this = NULL)

Arguments
this A neldermead object.
msg A character string.
simplex0 The initial simplex object.
x0 A column matrix of initial parameters.
state The state of the algorithm, either 'init', 'done' or 'iter'.
simplex The current simplex object.
step The type of step performed during the iteration: 'init', 'done', 'reflection', 'expansion', 'insidecontraction', 'outsidecontraction', 'reflectionnext' or 'shrink'.
x The point estimate to scale.
xref The reference point estimate.

Details
neldermead.startup Startup the algorithm. Compute the initial simplex, depending on the content of the simplex0method element of the neldermead object ('given', 'axes', 'spendley', 'pfeffer' or 'randbounds').
neldermead.log Print a message to the log file using optimbase.log.
neldermead.scaletox0 Scale the simplex into the nonlinear inequality constraints, if any. Scale toward x0, which is feasible.
**neldermead.scaletocenter** Scale the simplex into the nonlinear inequality constraints, if any. Scale to the centroid of the points which satisfy the constraints. This is Box’s method for scaling. It is unsure, since the centroid of the points which satisfy the constraints may not be feasible.

**neldermead.termstartup** Initialize Kelley’s stagnation detection system when normalization is required, by computing kelleyalpha. If the simplex gradient is zero, then use alpha0 as alpha.

**neldermead.outputcmd** Call the array of user-defined output functions

**neldermead.autorestart** Perform an optimization with automatic restart. The loop processes for i = 1 to restartmax + 1. This is because a RE-start is performed after one simulation has been performed, hence the ‘RE’.

**neldermead.istorestart** Determine if the optimization is to restart using neldermead.isroneill or neldermead.isrkelley depending on the content of the restartdetection element.

**neldermead.isroneill** Determine if the optimization is to restart. Use O’Neill method as a criteria for restart. It is an axis-by-axis search for optimality.

**neldermead.isrkelley** Determine if the optimization is to restart. Use kelleystagnation as a criteria for restart.

**neldermead.updatesimp** Update the initial simplex simplex0 for a restart.

**scaleinconstraints** Given a point reference to scale and a reference point which satisfies the constraints, scale the point towards the reference point estimate until it satisfies all the constraints.

**neldermead.costf** Call the cost function and return the value. This function is given to the simplex function class as a callback. Input/Output arguments are swapped w.r.t. optimbase.function, so that it matches the requirements of simplex methods.

---

**Value**

**neldermead.startup** Return an updated neldermead object this.

**neldermead.log** Return the neldermead object this.

**neldermead.scaletox0** Return an updated simplex.

**neldermead.scaletocenter** Return an updated simplex.

**neldermead.termstartup** Return an updated neldermead object this.

**neldermead.outputcmd** Do not return any data, but execute the output function(s).

**neldermead.autorestart** Return an updated neldermead object this.

**neldermead.istorestart** Return a list with the following elements:

- **this** The input neldermead object.
- **istorestart** Set to TRUE if the optimization is to restart, to FALSE otherwise.

**neldermead.isroneill** Return a list with the following elements:

- **this** The input neldermead object.
- **istorestart** Set to TRUE if the optimization is to restart, to FALSE otherwise.

**neldermead.isrkelley** Return a list with the following elements:

- **this** The input neldermead object.
**istorestart** Set to TRUE if the optimization is to restart, to FALSE otherwise.

**neldermead.updatesimp** Return an updated neldermead object **this**.

**scaleinconstraints** Return a list with the following elements:
   - **this** The updated neldermead object.
   - **isscaled** TRUE if the procedure has succeeded before **boxnbloops**, FALSE if it has failed.
   - **p** The scaled parameters.

**neldermead.costf** Return a list with the following elements:
   - **f** The value of the cost function.
   - **this** The updated neldermead object.

**Author(s)**

Author of Scilab neldermead module: Michael Baudin (INRIA - Digiteo)

Author of R adaptation: Sebastien Bihorel (<sb.pmlab@gmail.com>)

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**optimget**

*Queries an optimization option list*

**Description**

This function allows to make queries on an existing optimization option list. This list must have been created and updated by the **optimset** function. The **optimget** allows to retrieve the value associated with a given key.

**Usage**

```r
optimget(options = NULL, key = NULL, value = NULL)
```

**Arguments**

- **options** A list created or modifies by **optimset**.
- **key** A single character string, which should be the name of the field in **options** to query (case insensitive).
- **value** A default value.

**Details**

**key** is matched against the field names of **options** using **grep** and a case-insensitive regular expression. If **key** is not found in **options**, the function returns NULL. If several matches are found, **optimget** is stopped.

**Value**

Return **options$**key if **key** is found in **options**. Return **value**, otherwise.
Author(s)
Author of Scilab neldermead module: Michael Baudin (INRIA - Digiteo)
Author of R adaptation: Sebastien Bihorel (<sb.pmlab@gmail.com>)

See Also
optimset

Examples
```r
opt <- optimset(method='fminsearch')
optimget(opt,'Display')
optimget(opt,'abc','!@')
```

**optimset.method**

*Default set of optimization options*

Description
This function returns a default set of optimization options for defined 'methods'; `optimset.method` is called by `optimset` when a `method` was provided as input. Currently, the only valid `method` is 'fminsearch'.

Usage
```r
optimset.method(method = NULL)
```

Arguments
- **method** A character string.

Value
Returns a list with the following fields: Display, FunValCheck, MaxFunEvals, MaxIter, Output-Fcn, PlotFcns, TolFun, and TolX.

Author(s)
Author of Scilab neldermead module: Michael Baudin (INRIA - Digiteo)
Author of R adaptation: Sebastien Bihorel (<sb.pmlab@gmail.com>)

See Also
optimset

Examples
```r
optimset.method('fminsearch')
## Not run: optimset.method('abc')
```
**optimset**

Configures and returns an optimization data structure.

**Description**

This function creates or updates a list which can be used to modify the behaviour of optimization methods. The goal of this function is to manage the options list with a set of fields (for example, 'MaxFunEvals', 'MaxIter', etc...). The user can create a new list with empty fields or create a new structure with default fields which correspond to a particular algorithm. The user can also configure each field and set it to a particular value. Finally, the user passes the list to an optimization function so that the algorithm uses the options configured by the user.

**Usage**

```r
optimset(method = NULL,...)
```

**Arguments**

- `method` If provided, the method calls the `optimset.method` function. If the content of method is recognized, a default set of options are returned. The only current recognized character strings are 'fminsearch' and 'fminbnd'.
- `...` Additional arguments which would be included in the options output if the method argument is not used. See Details.

**Details**

Most optimization algorithms require many algorithmic parameters such as the number of iterations or the number of function evaluations. If these parameters are given to the optimization function as input parameters, this forces both the user and the developer to manage many input parameters. The goal of the `optimset` function is to simplify the management of input arguments, by gathering all the parameters into a single list.

While the current implementation of the `optimset` function only supports the `fminsearch` and `fminbnd` function, it is designed to be extended to as many optimization function as required. Because all optimization algorithms do not require the same parameters, the data structure aims at remaining flexible. But, most of the time, most parameters are the same from algorithm to algorithm, for example, the tolerance parameters which drive the termination criteria are often the same, even if the termination criteria itself is not the same.

Optimization parameters that are returned by the `optimset` function and that can be defined in ... are the following:

**Display** The verbose level. The default value is 'notify'. The following is a list of available verbose levels.
- 'off' The algorithm displays no message at all.
- 'notify' The algorithm displays message if the termination criteria is not reached at the end of the optimization. This may happen if the maximum number or iterations of the maximum number of function evaluations is reached and warns the user of a convergence problem.
'final'  The algorithm displays a message at the end of the optimization, showing the num-
ber of iterations, the number of function evaluations and the status of the optimization.
This option includes the messages generated by the 'notify' option i.e. warns in case of
a convergence problem.

'iter'  The algorithm displays a one-line message at each iteration. This option includes the
messages generated by the 'notify' option i.e. warns in case of a convergence problem.
It also includes the message generated by the 'final' option.

FunValCheck  A logical flag to enable the checking of function values.
MaxFunEvals  The maximum number of evaluations of the cost function.
MaxIter   The maximum number of iterations.
OutputFcn  A function which is called at each iteration to print out intermediate state of the
optimization algorithm (for example into a log file).
PlotFcns  A function which is called at each iteration to plot the intermediate state of the
optimization algorithm (for example into a 2D graphic).
TolFun   The absolute tolerance on function value.
TolX      The absolute tolerance on the variable x.

nbMatch  Specific to Box method: the number of consecutive times the TolFun criteria must
be met to terminate the optimization.

boundsAlpha  Specific to Box method: the parameter used to project the vertices into the
bounds in Box’s algorithm

boxScaling  Specific to Box method: the scaling coefficient used to scale the trial point for
function improvement or into the constraints of Box’s algorithm

alphaMin  Specific to Box method: the minimum value of alpha when scaling the vertices of
the simplex into nonlinear constraints in Box’s algorithm

Output and plot functions The 'OutputFcn' and 'PlotFcns' options accept as argument a func-
tion (or a list of functions). In the client optimization algorithm, this output or plot function is
called back once per iteration. It can be used by the user to display a message in the console,
write into a file, etc... The output or plot function is expected to have the following definition:
myfun <- function(x, optimValues, state)
where the input parameters are:

x  The current point estimate.

optimValues  A list which contains the following fields:
    funcCount  The number of function evaluations.
    fval  The best function value.
    iteration  The current iteration number.
    procedure  The type of step performed. This string depends on the specific algorithm (see
                fminsearch for details).
    state  the state of the algorithm. The following states are available:
        'init' when the algorithm is initializing,
        'iter' when the algorithm is performing iterations,
        'done' when the algorithm is terminated.
Value

Return a list with the following fields: Display, FunValCheck, MaxFunEvals, MaxIter, OutputFcn, PlotFcns, TolFun, TolX, nbMatch, boundsAlpha, boxScaling, and alphaMin.

Author(s)

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See Also

optimset.method.fminsearch, fminbnd

Examples

optimset()
optimset(Display='iter')
optimset(method='fminbnd')

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Version 2.0 dated 2006-09-05.