The neldermead Package - version 1.0-10

Sébastien Bihorel

January 11, 2015

neldermead is a R port of a module originally developped 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 `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 `costfargument` element is configured. The function should be defined as described in `vignette('optimbase',package='optimbase')`:

```
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,

`index`: (optional), an integer representing the value to compute, and

`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,

`this`: must be set to `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:

```
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', 're-flection', '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 additionnal 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` $\geq$ `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` $\geq$ `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 `ssize < tolsimplexizerelative ·` `simplexsize0 + tolsimplexizeabsolute`, where `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 `ssize <` `tolsimplexizeabsolute` and `shiftfv < toldelta` are true where `ssize` is the current simplex size and `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 `newfvmean ≤ oldfvmean - alpha · t(sg) · sg` where `newfvmean` (resp. `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 `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 `shiftfv < boxtolf` and `boxkount == boxnbmatch` are true, where `shiftfv` is the difference of function value between the best and worst vertices, and `boxkount` is the number of consecutive iterations where this criteria is met, then the status is set to 'tolboxf' and terminate is set to TRUE. Here, the `boxtolf` parameter is the value associated with the `boxtolf` element of the neldermead object and is a user-defined absolute tolerance on the function value. The `boxnbmatch` parameter is the value associated with the `boxnbmatch` 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 `var < tolrelativevariance · variancesimplex0 + tolabsolutevariance`, where `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 `tolrelativevariance` parameter is the value associated with the `tolrelativevariance` 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 = alpha0 · sigma0 / nsg`, where `sigma0` 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 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).'

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 to 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 analyse 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 fe<fr, 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 `tolvarianceflag` element of the neldermead object, which is disabled by default.

1.10   Box's complex algorithm implementation notes

In this section, we analyse 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 `scalingsimplex0` element of the 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 `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 `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 developped 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:

```
>   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:

```
>   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 α 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 feasbility 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.

```
>    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)))
+   }
>   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)))
  }

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

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.

```
>   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))
```
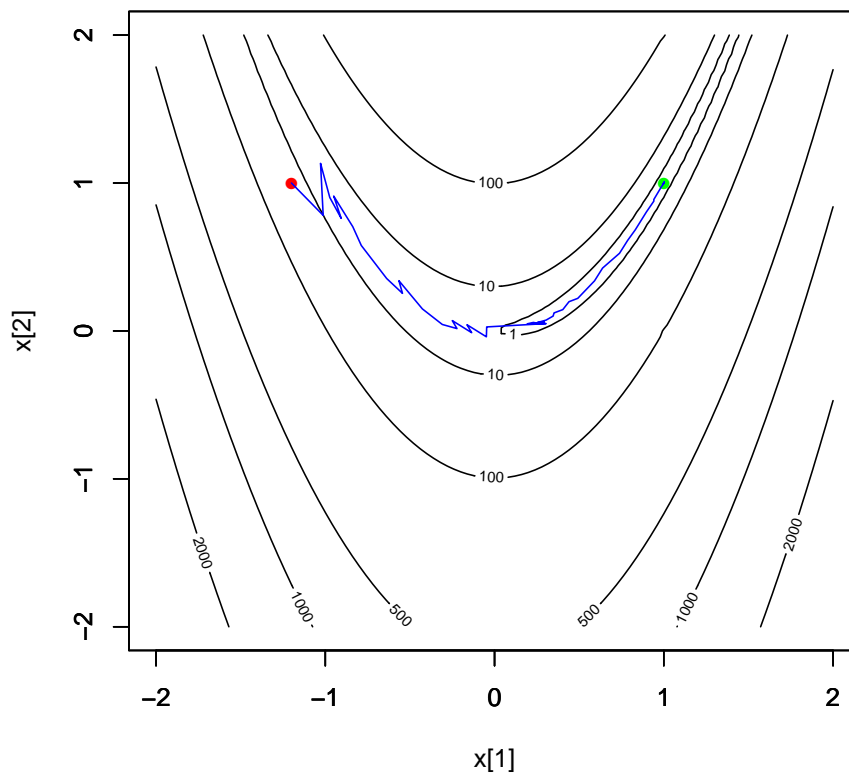

Setting the 'verbose' element of the neldermead object to 1 allows to get detailed information about the current optimization process. The following is a sample output for an optimization based on the Nelder and Mead variable-shape simplex algorithm. Only the output corresponding to the iteration #156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

12

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.

```
>    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):
  Initial    Final Lower bound Upper bound
1     1.2 1.000001           1           2
2     1.9 1.000001           1           2

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)))
  }

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] [1]. This problem consists in minimizing: $G_6(x) = (x_1 - 10)^3 + (x_2 - 20)^3$, given the nonlinear constraints:

$c1: \quad (x_1 - 5)^2 + (x_2 - 5)^2 - 100 \geq 0$
$c2: \quad -(x_1 - 6)^2 - (x_2 - 5)^2 + 82.81 \geq 0$
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.

```
>   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

```
>   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):
```
   Initial        Final Lower bound Upper bound
1   15.00 14.0950000          13          20
2    4.99  0.8429608           0          10
```

Number of Inequality Contraints: 2

Cost Function:
```
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)
  }
```

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
Number of vertices: nbve=3

```
  Vertex #1/3 : fv=-3.256755e+03, x=1.500000e+01 4.990000e+00
  Vertex #2/3 : fv=-3.276394e+03, x=1.506683e+01 4.953517e+00
  Vertex #3/3 : fv=-3.188984e+03, x=1.507561e+01 5.082317e+00

- Simplex at Optimal Point:
Dimension: n=2
Number of vertices: nbve=3
  Vertex #1/3 : fv=-6.961814e+03, x=1.409500e+01 8.429608e-01
  Vertex #2/3 : fv=-6.961814e+03, x=1.409500e+01 8.429608e-01
  Vertex #3/3 : fv=-6.961814e+03, x=1.409500e+01 8.429608e-01
```

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 modifed 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 `fmsdundata`.
`neldermead` creates a new neldermead object. Then we use `neldermead.set` to configure the pa-
rameters of the problem, including `costfargument`, set to `fmsdundata`, 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.

```
>   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)
>   nm <- neldermead.set(nm,'boundsmin',c(-100, 0))
```

---

[2]Example suggested by Mark Taper

```
>   nm <- neldermead.set(nm,'boundsmax',c(100, 100))
>   nm <- neldermead.search(this=nm)
>   summary(nm)
```

Number of Estimated Variable(s): 2

Estimated Variable(s):
  Initial   Final Lower bound Upper bound
1   45 50.164922   -100   100
2   3 1.978316   0   100

Cost Function:
```
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):
$data
  [1] 51.17106 51.41893 49.78139 49.09301 51.21177 46.36409 51.26020
  [8] 49.44763 49.43168 48.16136 49.76750 53.63462 50.74126 51.04043
 [15] 48.49894 51.63380 48.22728 49.33684 52.24143 50.59745 51.55924
 [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 50.55591
 [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 53.06191 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 46.90542
[148] 51.69931 51.79203 50.27738 46.76134 51.09680 50.39056 48.38700
[155] 49.78275 49.49811 53.39869 49.31140 50.13554 48.69886 49.02472
[162] 50.60630 49.51605 49.03653 48.01639 49.43870 51.26603 47.52036
[169] 53.52863 49.95264 50.39984 52.69439 50.07215 51.64916 46.59466

18
```

```
[176] 50.96190 54.96710 50.80273 50.43035 46.36858 48.17652 49.90191
[183] 49.18923 52.26076 51.63093 50.15284 52.90749 50.74824 49.65819
[190] 48.99557 51.08704 48.98963 51.57359 50.60190 52.62045 51.59687
[197] 51.70172 49.11286 49.10645 50.02661 47.12771 48.74148 50.48704
[204] 52.11672 51.66270 50.21042 46.51657 51.29049 50.19421 49.84653
[211] 51.98390 48.28150 49.43684 54.13249 48.77689 50.63123 51.32059
[218] 46.55560 45.73075 50.13789 51.73564 45.41991 49.69962 49.46244
[225] 53.58266 51.34454 49.58140 50.02437 53.06823 50.15458 50.15688
[232] 48.44148 50.33312 50.53065 51.78156 49.06422 51.51675 48.71653
[239] 51.25534 50.49666 48.59985 48.86520 49.47721 47.87223 49.78726
[246] 51.54221 55.49481 49.83213 51.08714 51.50572 48.38265 52.00224
[253] 50.91211 47.13150 49.46939 51.28354 49.16996 49.08085 48.41501
[260] 47.68292 51.42178 52.53520 49.71370 48.96994 52.96578 49.67482
[267] 50.08342 50.96608 47.63975 48.67285 48.73070 48.59607 51.15370
[274] 45.77384 50.52182 52.29425 50.02959 49.37652 48.08761 50.94683
[281] 46.97227 50.32856 48.25827 53.18666 51.29320 50.71474 50.20479
[288] 48.64947 51.94417 51.51174 49.14343 48.57215 49.61923 50.79973
[295] 48.04431 50.36747 45.69938 48.75407 48.46912 50.92862 51.04456
[302] 50.01959 49.11895 52.39898 49.76506 50.07642 52.38961 50.68792
[309] 49.34185 53.34172 48.16388 49.82439 52.64059 53.46157 54.32519
[316] 49.36854 48.84981 47.18729 54.53572 48.45829 50.76063 51.21027
[323] 52.03935 50.94989 45.62811 51.86638 50.95087 50.78056 48.54534
[330] 51.97311 52.84797 50.96946 50.69847 51.72025 50.80922 50.73409
[337] 46.96160 53.09961 50.99976 50.92175 54.15342 49.38470 51.90474
[344] 51.06558 49.80890 49.71587 47.63395 51.09064 44.83629 51.55780
[351] 50.58588 49.82658 47.06728 47.83364 52.11547 49.27936 50.70119
[358] 50.05652 50.94610 48.16169 49.24835 46.37433 50.57720 49.62075
[365] 50.03572 51.30086 50.62051 53.33671 51.34523 49.44496 49.70795
[372] 53.40286 50.94272 51.16340 51.33204 48.44220 52.32665 46.07091
[379] 51.53834 54.51954 49.04546 49.79484 50.73739 48.92913 51.01320
[386] 49.69889 51.80849 54.48407 47.60975 49.16295 51.59650 50.99634
[393] 50.23912 49.26559 50.52466 50.52541 51.28148 50.61418 49.93374
[400] 47.25050 51.25593 50.00429 50.56876 47.99644 48.76556 51.65639
[407] 49.83036 49.13056 47.59033 47.95863 48.05754 49.67817 52.40937
[414] 50.13349 48.23508 49.96016 50.65603 48.13874 47.73717 52.17246
[421] 51.02848 50.58634 48.87469 50.41429 52.45615 49.13997 52.66382
[428] 48.47347 52.46464 51.21812 48.35492 49.90470 50.34136 47.54986
[435] 50.77467 50.98134 54.47825 51.78442 51.59787 53.87089 50.78850
[442] 51.26504 50.20518 52.02042 52.42936 51.00174 48.18106 45.60558
[449] 50.87709 47.94117 51.42616 52.05654 48.85873 49.13198 52.01063
[456] 52.40709 52.99237 49.68680 48.12794 50.70508 47.42762 49.45495
[463] 50.31383 48.23637 49.75620 48.28950 47.98854 48.17210 45.84353
[470] 49.71871 52.59928 49.94126 45.52676 51.09006 51.66168 49.00484
[477] 48.79795 48.97560 49.99014 49.80570 49.95193 49.74522 49.73623
[484] 50.90748 47.18733 50.42186 51.50467 50.27676 50.31936 50.45687
[491] 47.67443 51.70932 49.51581 45.96801 49.54462 50.44834 48.52635
[498] 48.30658 49.77708 49.37680
```

```
attr(,"class")
[1] "optimbase.functionargs"

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.

```
>   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
Evaluating combination number: 17/30
Evaluating combination number: 18/30
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

      x1 x2      f feasible
22   1.0  1    0.0        1
15   0.0  0    1.0        1
20  -1.0  1    4.0        1
24  -1.2  1   24.2        1
30  -1.2  2   36.2        1
16   1.0  0  100.0        1
28   1.0  2  100.0        1
9    0.0 -1  101.0        1
21   0.0  1  101.0        1
14  -1.0  0  104.0        1
26  -1.0  2  104.0        1
18  -1.2  0  212.2        1
10   1.0 -1  400.0        1
3    0.0 -2  401.0        1
27   0.0  2  401.0        1
29   2.0  2  401.0        1
8   -1.0 -1  404.0        1
25  -2.0  2  409.0        1
12  -1.2 -1  600.2        1
```

```
4   1.0 -2  900.0      1
23  2.0  1  901.0      1
2  -1.0 -2  904.0      1
19 -2.0  1  909.0      1
6  -1.2 -2 1188.2      1
17  2.0  0 1601.0      1
13 -2.0  0 1609.0      1
11  2.0 -1 2501.0      1
7  -2.0 -1 2509.0      1
5   2.0 -2 3601.0      1
1  -2.0 -2 3609.0      1
```

4 References

[1] C.T. Kelley. *Iterative Methods for Optimization*. SIAM Frontiers in Applied Mathematics, Philadelphia, PA, 1999.

[2] J.A. Guin. Discussion and correspondence: modification of the complex method of constrained optimization. *The Computer Journal*, 10(4):416–417, 1968.

[3] J.A. Nelder and R. Mead. A Simplex Method for Function Minimization. *The Computer Journal*, 7(4):308–313, 1965.

[4] M.J. Box. A New Method of Constrained Optimization and a Comparison With Other Methods. *The Computer Journal*, 1(8):42–52, 1965.

[5] R. O'Neill. Algorithm AS47 - Function minimization using a simplex procedure. *Applied Statistics*, 20:338–345, 1971.

[6] W. Spendley and G.R. Hext and F.R. Himsworth. Sequential Application of Simplex Designs in Optimisation and Evolutionary Operation. *Technometrics*, 4:441–461, 1962.

[7] Z. Michalewicz and D.B. Fogel. *How to solve it: modern heuristics*, chapter Constraint-handling techniques, pages 231–270. Springer, 2004.

5 Dependencies of fminsearch

We illustrate in the figures below the network of functions of the **neldermead**, **optimbase**, and **optimsimplex** 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

Package:	neldermead
Type:	Package
Version:	1.0-10
Date:	2015-01-11
License:	CeCILL-2
LazyLoad:	yes

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

'Sequential Application of Simplex Designs in Optimisation and Evolutionary Operation', Spendley, W. and Hext, G. R. and Himsworth, F. R., American Statistical Association and American Society for Quality, 1962

'A Simplex Method for Function Minimization', Nelder, J. A. and Mead, R., The Computer Journal, 1965

'A New Method of Constrained Optimization and a Comparison With Other Methods', M. J. Box, The Computer Journal 1965 8(1):42-52, 1965 by British Computer Society

'Discussion and correspondence: modification of the complex method of constrained optimization', J. A. Guin, The Computer Journal, 1968

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

'Iterative Methods for Optimization', C. T. Kelley, SIAM Frontiers in Applied Mathematics, 1999

'Algorithm AS47 - Function minimization using a simplex procedure', O'Neill, R., Applied Statistics, 1971

See Also

optimbase optimsimplex

---

costf.transposex   *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.transposex(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 `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

`neldermead.costf`

| `fmin.gridsearch` | *Grid evaluation of an unconstrained cost function* |

Description

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

Usage

```
fmin.gridsearch(fun = NULL, x0 = NULL, xmin = NULL,
                xmax = NULL, npts = 3, alpha = 10)
```

Arguments

`fun`	An unconstrained cost function returning a numeric scalar, similar to those used in the `fminsearch` function.
`x0`	The initial point estimate, provided as a numeric vector.
`xmin`	Optional: a vector of lower bounds.
`xmax`	Optional: a vector of upper bounds.
`npts`	An integer scalar greater than 2, indicating the number of evaluation points will be used on each dimension to build the search grid.
`alpha`	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 `alpha` length is lower than that of `x0`, elements of `alpha` are recycled. If its length is higher than that of `x0`, `alpha` is truncated.

Details

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

The actual evaluation of the cost function is delegated to `optimbase.gridsearch`.

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>`)

---

fminbnd.outputfun   *fminbnd Output Function Call*

Description

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

Usage

```
fminbnd.outputfun(state = NULL, data = NULL, fmsdata = NULL)
```

Arguments

state	The current state of the algorithm either 'init', 'iter' or 'done'.
data	The data at the current state. This is an object of class 'neldermead.data', i.e. a list with the following elements:

    x The current parameter estimates.

    fval The current value of the cost function.

    simplex The current simplex object.

    iteration The number of iterations performed.

    funccount The number of function evaluations.

    step The type of step in the previous iteration.

fmsdata	This is an object of class 'optimbase.functionargs' which contains specific data of the `fminbnd` algorithm:

    Display what to display

    OutputFcn the array of output functions

    PlotFcns the array of plot functions

Value

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

Author(s)

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

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

See Also

fminbnd, neldermead, neldermead.set,

fminsearch	*Computation of the unconstrained minimum of given function with the Nelder-Mead algorithm.*

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>=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

```
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 * n.
>
> **MaxFunEvals** The maximum number of evaluations of the cost function. The default is 200 * 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,

shiftfv the absolute value of the difference of function value between the highest and lowest vertices.

If both `ssize < options$TolX` and `shiftfv < options$TolFun` conditions are true, then the iterations stop. The size of the simplex is computed using the 'sigmaplus' method of the **optimsimplex** 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.

The initial simplex

The `fminsearch` algorithm uses a special initial simplex, which is an heuristic depending on the initial guess. The strategy chosen by `fminsearch` corresponds to the content of `simplex0method` element of the neldermead object (set to 'pfeffer'). It is applied using the content of the `simplex0deltausual` (0.05) and `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.

The number of iterations

In this section, we present the default values for the number of iterations in `fminsearch`.

The `options` input argument is an optional list which can contain the `MaxIter` field, which stores the maximum number of iterations. The default value is 200n, where 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 100n. 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 100n.

Output and plot functions

The `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:

```
myfun <- function(x , optimValues , state)
```

The input arguments x, `optimValues` and `state` are described in detail in the `optimset` help page. The `optimValues$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'.

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

'Sequential Application of Simplex Designs in Optimisation and Evolutionary Operation', Spendley, W. and Hext, G. R. and Himsworth, F. R., American Statistical Association and American Society for Quality, 1962

'A Simplex Method for Function Minimization', Nelder, J. A. and Mead, R., The Computer Journal, 1965

'Iterative Methods for Optimization', C. T. Kelley, SIAM Frontiers in Applied Mathematics, 1999

'Algorithm AS47 - Function minimization using a simplex procedure', O'Neill, R., Applied Statistics, 1971

'Effect of dimensionality on the nelder-mead simplex method', Lixing Han and Michael Neumann, Optimization Methods and Software, 21, 1, 1–16, 2006.

'Algorithms in Unconstrained Optimization', Lixing Han, Ph.D., The University of Connecticut, 2000.

'Global Optimization Of Lennard-Jones Atomic Clusters' Ellen Fan, Thesis, February 26, 2002, McMaster University

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, fvinitial = NULL, oldfvmean = NULL,
                       newfvmean = 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 (xhigh,xbar). The reflected point estimate satisfies the following constraints:

- fr < fhigh
- 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 x1 and x2, as follows: xi = (1+fac)x1 - fac*x2

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:

this The updated neldermead object.

status TRUE if the search is successful, FALSE otherwise.

xr The reflected point estimate.

fr The value of the cost function at **xr**.

`neldermead.storehistory` Return the updated neldermead object.

`neldermead.termination` Return a list with the following elements:

this The updated neldermead object

terminate TRUE if the algorithm terminates, FALSE if the algorithm must continue.

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

```
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,
  kelleyalpha, startupflag, boxnbpoints, boxnbpointseff, boxineqscaling,
  checkcostfunction, scalingsimplex0, guinalphamin, boxboundsalpha,
  boxtermination, boxtolf, boxnbmatch, boxkount, boxreflect, tolvarianceflag,
  tolabsolutevariance, tolrelativevariance, variancesimplex0, mymethod,
  myterminate, myterminateflag, greedy, output, exitflag)

  ## 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.

boxnbpoints   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.

46

`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-derined 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.

verbosetermination 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'.

boundsmin Default is NULL.

boundsmax Default is NULL.

nbineqconst 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>`)

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

this   A neldermead object.

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

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

`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 additionnal argument, passed to the cost function.

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

'-outputcommandarg' An additionnal 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',pa` 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 'tolsize'. 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.option

'-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 -restartsimplexmethod 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 algorithm.

'-mymethod' A user-derined 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 functions for neldermead.search

Description

Utility functions for `neldermead.serch` 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.isroneill(this = NULL)
neldermead.isrkelley(this = this)
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 `boxnbnlloops`, 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>`)

---

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

```
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.

Examples

```
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

```
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

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

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

```
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 number 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 function (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, Output-Fcn, PlotFcns, TolFun, TolX, nbMatch, boundsAlpha, boxScaling, and alphaMin.

Author(s)

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

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

See Also

`optimset.method`,`fminsearch`, `fminbnd`

Examples

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

7   CeCILL FREE SOFTWARE LICENSE AGREEMENT

```
    Notice
```

```
This Agreement is a Free Software license agreement that is the result
of discussions between its authors in order to ensure compliance with
the two main principles guiding its drafting:

    * firstly, compliance with the principles governing the distribution
      of Free Software: access to source code, broad rights granted to
      users,
    * secondly, the election of a governing law, French law, with which
      it is conformant, both as regards the law of torts and
      intellectual property law, and the protection that it offers to
      both authors and holders of the economic rights over software.

The authors of the CeCILL (for Ce[a] C[nrs] I[nria] L[ogiciel] L[ibre])
license are:

Commissariat a l'Energie Atomique - CEA, a public scientific, technical
and industrial research establishment, having its principal place of
business at 25 rue Leblanc, immeuble Le Ponant D, 75015 Paris, France.

Centre National de la Recherche Scientifique - CNRS, a public scientific
and technological establishment, having its principal place of business
at 3 rue Michel-Ange, 75794 Paris cedex 16, France.

Institut National de Recherche en Informatique et en Automatique -
INRIA, a public scientific and technological establishment, having its
```

principal place of business at Domaine de Voluceau, Rocquencourt, BP
105, 78153 Le Chesnay cedex, France.

Preamble

The purpose of this Free Software license agreement is to grant users
the right to modify and redistribute the software governed by this
license within the framework of an open source distribution model.

The exercising of these rights is conditional upon certain obligations
for users so as to preserve this status for all subsequent redistributions.

In consideration of access to the source code and the rights to copy,
modify and redistribute granted by the license, users are provided only
with a limited warranty and the software's author, the holder of the
economic rights, and the successive licensors only have limited liability.

In this respect, the risks associated with loading, using, modifying
and/or developing or reproducing the software by the user are brought to
the user's attention, given its Free Software status, which may make it
complicated to use, with the result that its use is reserved for
developers and experienced professionals having in-depth computer
knowledge. Users are therefore encouraged to load and test the
suitability of the software as regards their requirements in conditions
enabling the security of their systems and/or data to be ensured and,
more generally, to use and operate it in the same conditions of
security. This Agreement may be freely reproduced and published,
provided it is not altered, and that no provisions are either added or
removed herefrom.

This Agreement may apply to any or all software for which the holder of
the economic rights decides to submit the use thereof to its provisions.

    Article 1 - DEFINITIONS

For the purpose of this Agreement, when the following expressions
commence with a capital letter, they shall have the following meaning:

Agreement: means this license agreement, and its possible subsequent
versions and annexes.

Software: means the software in its Object Code and/or Source Code form
and, where applicable, its documentation, "as is" when the Licensee
accepts the Agreement.

Initial Software: means the Software in its Source Code and possibly its

Object Code form and, where applicable, its documentation, "as is" when it is first distributed under the terms and conditions of the Agreement.

Modified Software: means the Software modified by at least one Contribution.

Source Code: means all the Software's instructions and program lines to which access is required so as to modify the Software.

Object Code: means the binary files originating from the compilation of the Source Code.

Holder: means the holder(s) of the economic rights over the Initial Software.

Licensee: means the Software user(s) having accepted the Agreement.

Contributor: means a Licensee having made at least one Contribution.

Licensor: means the Holder, or any other individual or legal entity, who distributes the Software under the Agreement.

Contribution: means any or all modifications, corrections, translations, adaptations and/or new functions integrated into the Software by any or all Contributors, as well as any or all Internal Modules.

Module: means a set of sources files including their documentation that enables supplementary functions or services in addition to those offered by the Software.

External Module: means any or all Modules, not derived from the Software, so that this Module and the Software run in separate address spaces, with one calling the other when they are run.

Internal Module: means any or all Module, connected to the Software so that they both execute in the same address space.

GNU GPL: means the GNU General Public License version 2 or any subsequent version, as published by the Free Software Foundation Inc.

Parties: mean both the Licensee and the Licensor.

These expressions may be used both in singular and plural form.

    Article 2 - PURPOSE

The purpose of the Agreement is the grant by the Licensor to the

Licensee of a non-exclusive, transferable and worldwide license for the Software as set forth in Article 5 hereinafter for the whole term of the protection granted by the rights over said Software.

Article 3 - ACCEPTANCE

3.1 The Licensee shall be deemed as having accepted the terms and conditions of this Agreement upon the occurrence of the first of the following events:

* (i) loading the Software by any or all means, notably, by downloading from a remote server, or by loading from a physical medium;
* (ii) the first time the Licensee exercises any of the rights granted hereunder.

3.2 One copy of the Agreement, containing a notice relating to the characteristics of the Software, to the limited warranty, and to the fact that its use is restricted to experienced users has been provided to the Licensee prior to its acceptance as set forth in Article 3.1 hereinabove, and the Licensee hereby acknowledges that it has read and understood it.

Article 4 - EFFECTIVE DATE AND TERM

4.1 EFFECTIVE DATE

The Agreement shall become effective on the date when it is accepted by the Licensee as set forth in Article 3.1.

4.2 TERM

The Agreement shall remain in force for the entire legal term of protection of the economic rights over the Software.

Article 5 - SCOPE OF RIGHTS GRANTED

The Licensor hereby grants to the Licensee, who accepts, the following rights over the Software for any or all use, and for the term of the Agreement, on the basis of the terms and conditions set forth hereinafter.

Besides, if the Licensor owns or comes to own one or more patents protecting all or part of the functions of the Software or of its

components, the Licensor undertakes not to enforce the rights granted by these patents against successive Licensees using, exploiting or modifying the Software. If these patents are transferred, the Licensor undertakes to have the transferees subscribe to the obligations set forth in this paragraph.

5.1 RIGHT OF USE

The Licensee is authorized to use the Software, without any limitation as to its fields of application, with it being hereinafter specified that this comprises:

1. permanent or temporary reproduction of all or part of the Software by any or all means and in any or all form.

2. loading, displaying, running, or storing the Software on any or all medium.

3. entitlement to observe, study or test its operation so as to determine the ideas and principles behind any or all constituent elements of said Software. This shall apply when the Licensee carries out any or all loading, displaying, running, transmission or storage operation as regards the Software, that it is entitled to carry out hereunder.

5.2 ENTITLEMENT TO MAKE CONTRIBUTIONS

The right to make Contributions includes the right to translate, adapt, arrange, or make any or all modifications to the Software, and the right to reproduce the resulting software.

The Licensee is authorized to make any or all Contributions to the Software provided that it includes an explicit notice that it is the author of said Contribution and indicates the date of the creation thereof.

5.3 RIGHT OF DISTRIBUTION

In particular, the right of distribution includes the right to publish, transmit and communicate the Software to the general public on any or all medium, and by any or all means, and the right to market, either in consideration of a fee, or free of charge, one or more copies of the Software by any means.

The Licensee is further authorized to distribute copies of the modified or unmodified Software to third parties according to the terms and

conditions set forth hereinafter.

5.3.1 DISTRIBUTION OF SOFTWARE WITHOUT MODIFICATION

The Licensee is authorized to distribute true copies of the Software in
Source Code or Object Code form, provided that said distribution
complies with all the provisions of the Agreement and is accompanied by:

1. a copy of the Agreement,

2. a notice relating to the limitation of both the Licensor's
   warranty and liability as set forth in Articles 8 and 9,

and that, in the event that only the Object Code of the Software is
redistributed, the Licensee allows future Licensees unhindered access to
the full Source Code of the Software by indicating how to access it, it
being understood that the additional cost of acquiring the Source Code
shall not exceed the cost of transferring the data.

5.3.2 DISTRIBUTION OF MODIFIED SOFTWARE

When the Licensee makes a Contribution to the Software, the terms and
conditions for the distribution of the resulting Modified Software
become subject to all the provisions of this Agreement.

The Licensee is authorized to distribute the Modified Software, in
source code or object code form, provided that said distribution
complies with all the provisions of the Agreement and is accompanied by:

1. a copy of the Agreement,

2. a notice relating to the limitation of both the Licensor's
   warranty and liability as set forth in Articles 8 and 9,

and that, in the event that only the object code of the Modified
Software is redistributed, the Licensee allows future Licensees
unhindered access to the full source code of the Modified Software by
indicating how to access it, it being understood that the additional
cost of acquiring the source code shall not exceed the cost of
transferring the data.

5.3.3 DISTRIBUTION OF EXTERNAL MODULES

When the Licensee has developed an External Module, the terms and
conditions of this Agreement do not apply to said External Module, that

may be distributed under a separate license agreement.

5.3.4 COMPATIBILITY WITH THE GNU GPL

The Licensee can include a code that is subject to the provisions of one of the versions of the GNU GPL in the Modified or unmodified Software, and distribute that entire code under the terms of the same version of the GNU GPL.

The Licensee can include the Modified or unmodified Software in a code that is subject to the provisions of one of the versions of the GNU GPL, and distribute that entire code under the terms of the same version of the GNU GPL.

Article 6 - INTELLECTUAL PROPERTY

6.1 OVER THE INITIAL SOFTWARE

The Holder owns the economic rights over the Initial Software. Any or all use of the Initial Software is subject to compliance with the terms and conditions under which the Holder has elected to distribute its work and no one shall be entitled to modify the terms and conditions for the distribution of said Initial Software.

The Holder undertakes that the Initial Software will remain ruled at least by this Agreement, for the duration set forth in Article 4.2.

6.2 OVER THE CONTRIBUTIONS

The Licensee who develops a Contribution is the owner of the intellectual property rights over this Contribution as defined by applicable law.

6.3 OVER THE EXTERNAL MODULES

The Licensee who develops an External Module is the owner of the intellectual property rights over this External Module as defined by applicable law and is free to choose the type of agreement that shall govern its distribution.

6.4 JOINT PROVISIONS

The Licensee expressly undertakes:

1. not to remove, or modify, in any manner, the intellectual property notices attached to the Software;

2. to reproduce said notices, in an identical manner, in the copies of the Software modified or not.

The Licensee undertakes not to directly or indirectly infringe the intellectual property rights of the Holder and/or Contributors on the Software and to take, where applicable, vis-a-vis its staff, any and all measures required to ensure respect of said intellectual property rights of the Holder and/or Contributors.

Article 7 - RELATED SERVICES

7.1 Under no circumstances shall the Agreement oblige the Licensor to provide technical assistance or maintenance services for the Software.

However, the Licensor is entitled to offer this type of services. The terms and conditions of such technical assistance, and/or such maintenance, shall be set forth in a separate instrument. Only the Licensor offering said maintenance and/or technical assistance services shall incur liability therefor.

7.2 Similarly, any Licensor is entitled to offer to its licensees, under its sole responsibility, a warranty, that shall only be binding upon itself, for the redistribution of the Software and/or the Modified Software, under terms and conditions that it is free to decide. Said warranty, and the financial terms and conditions of its application, shall be subject of a separate instrument executed between the Licensor and the Licensee.

Article 8 - LIABILITY

8.1 Subject to the provisions of Article 8.2, the Licensee shall be entitled to claim compensation for any direct loss it may have suffered from the Software as a result of a fault on the part of the relevant Licensor, subject to providing evidence thereof.

8.2 The Licensor's liability is limited to the commitments made under this Agreement and shall not be incurred as a result of in particular: (i) loss due the Licensee's total or partial failure to fulfill its obligations, (ii) direct or consequential loss that is suffered by the Licensee due to the use or performance of the Software, and (iii) more generally, any consequential loss. In particular the Parties expressly

agree that any or all pecuniary or business loss (i.e. loss of data, loss of profits, operating loss, loss of customers or orders, opportunity cost, any disturbance to business activities) or any or all legal proceedings instituted against the Licensee by a third party, shall constitute consequential loss and shall not provide entitlement to any or all compensation from the Licensor.

   Article 9 - WARRANTY

9.1 The Licensee acknowledges that the scientific and technical state-of-the-art when the Software was distributed did not enable all possible uses to be tested and verified, nor for the presence of possible defects to be detected. In this respect, the Licensee's attention has been drawn to the risks associated with loading, using, modifying and/or developing and reproducing the Software which are reserved for experienced users.

The Licensee shall be responsible for verifying, by any or all means, the suitability of the product for its requirements, its good working order, and for ensuring that it shall not cause damage to either persons or properties.

9.2 The Licensor hereby represents, in good faith, that it is entitled to grant all the rights over the Software (including in particular the rights set forth in Article 5).

9.3 The Licensee acknowledges that the Software is supplied "as is" by the Licensor without any other express or tacit warranty, other than that provided for in Article 9.2 and, in particular, without any warranty as to its commercial value, its secured, safe, innovative or relevant nature.

Specifically, the Licensor does not warrant that the Software is free from any error, that it will operate without interruption, that it will be compatible with the Licensee's own equipment and software configuration, nor that it will meet the Licensee's requirements.

9.4 The Licensor does not either expressly or tacitly warrant that the Software does not infringe any third party intellectual property right relating to a patent, software or any other property right. Therefore, the Licensor disclaims any and all liability towards the Licensee arising out of any or all proceedings for infringement that may be instituted in respect of the use, modification and redistribution of the Software. Nevertheless, should such proceedings be instituted against the Licensee, the Licensor shall provide it with technical and legal assistance for its defense. Such technical and legal assistance shall be decided on a case-by-case basis between the relevant Licensor and the

Licensee pursuant to a memorandum of understanding. The Licensor disclaims any and all liability as regards the Licensee's use of the name of the Software. No warranty is given as regards the existence of prior rights over the name of the Software or as regards the existence of a trademark.

Article 10 - TERMINATION

10.1 In the event of a breach by the Licensee of its obligations hereunder, the Licensor may automatically terminate this Agreement thirty (30) days after notice has been sent to the Licensee and has remained ineffective.

10.2 A Licensee whose Agreement is terminated shall no longer be authorized to use, modify or distribute the Software. However, any licenses that it may have granted prior to termination of the Agreement shall remain valid subject to their having been granted in compliance with the terms and conditions hereof.

Article 11 - MISCELLANEOUS

11.1 EXCUSABLE EVENTS

Neither Party shall be liable for any or all delay, or failure to perform the Agreement, that may be attributable to an event of force majeure, an act of God or an outside cause, such as defective functioning or interruptions of the electricity or telecommunications networks, network paralysis following a virus attack, intervention by government authorities, natural disasters, water damage, earthquakes, fire, explosions, strikes and labor unrest, war, etc.

11.2 Any failure by either Party, on one or more occasions, to invoke one or more of the provisions hereof, shall under no circumstances be interpreted as being a waiver by the interested Party of its right to invoke said provision(s) subsequently.

11.3 The Agreement cancels and replaces any or all previous agreements, whether written or oral, between the Parties and having the same purpose, and constitutes the entirety of the agreement between said Parties concerning said purpose. No supplement or modification to the terms and conditions hereof shall be effective as between the Parties unless it is made in writing and signed by their duly authorized representatives.

11.4 In the event that one or more of the provisions hereof were to

conflict with a current or future applicable act or legislative text, said act or legislative text shall prevail, and the Parties shall make the necessary amendments so as to comply with said act or legislative text. All other provisions shall remain effective. Similarly, invalidity of a provision of the Agreement, for any reason whatsoever, shall not cause the Agreement as a whole to be invalid.

11.5 LANGUAGE

The Agreement is drafted in both French and English and both versions are deemed authentic.

Article 12 - NEW VERSIONS OF THE AGREEMENT

12.1 Any person is authorized to duplicate and distribute copies of this Agreement.

12.2 So as to ensure coherence, the wording of this Agreement is protected and may only be modified by the authors of the License, who reserve the right to periodically publish updates or new versions of the Agreement, each with a separate number. These subsequent versions may address new issues encountered by Free Software.

12.3 Any Software distributed under a given version of the Agreement may only be subsequently distributed under the same version of the Agreement or a subsequent version, subject to the provisions of Article 5.3.4.

Article 13 - GOVERNING LAW AND JURISDICTION

13.1 The Agreement is governed by French law. The Parties agree to endeavor to seek an amicable solution to any disagreements or disputes that may arise during the performance of the Agreement.

13.2 Failing an amicable solution within two (2) months as from their occurrence, and unless emergency proceedings are necessary, the disagreements or disputes shall be referred to the Paris Courts having jurisdiction, by the more diligent Party.

Version 2.0 dated 2006-09-05.