Package ‘blackbox’

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Description Performs prediction of a response function from simulated response values, allowing black-box optimization of functions estimated with some error. Includes a simple user interface for such applications, as well as more specialized functions designed to be called by the Migraine software (Rousset and Leblois, 2012 <doi:10.1093/molbev/MSR262>; Leblois et al., 2014 <doi:10.1093/molbev/msu212>; and see URL). The latter functions are used for prediction of likelihood surfaces and implied likelihood ratio confidence intervals, and for exploration of predictor space of the surface. Prediction of the response is based on ordinary Kriging (with residual error) of the input. Estimation of smoothing parameters is performed by generalized cross-validation.
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**Description**

`bbob` implements optimization of a black-box function, possibly estimated with error, using prediction of the function by smoothing of its values in a given set of points, followed by a call to `optim` for optimization of the predicted function. `rbb` samples the parameter space of the function using a crude implementation of Expected Improvement (e.g., Bingham et al., 2014) methods: points with the highest predicted probability of improvement of the response value among a set of candidates sampled uniformly are retained.

**Usage**

```r
bbob(data, ParameterNames = NULL, respName = NULL, control = list(),
      force = FALSE, optimizers = blackbox.getOption("optimizers"), precision=1e-03)
```

```r
rbb(object,n=NULL,from=NULL,focus=0.75)
```

**Arguments**

- **data**
  A data frame including both function parameters and function values (or “response” values).

- **ParameterNames**
  A character vector, identifying the columns of the data that correspond to the function parameters. If NULL, all columns except the last are assumed to hold parameter values.
**respName**  
A character string, identifying the column of the data that corresponds to the function values. If NULL, the last column is assumed to hold function values.

**control**  
A list passed to the control argument of the optim function; e.g., list(fnscale=-1) for maximization.

**force**  
Boolean, passed to calcGCV. TRUE forces the analysis of data without pairs of response values for given parameter values. This is not recommended as there should be such pairs. If the response is estimated with error, this is required for good smoothing. If it is deterministic, bboptim will learn it from the information provided by the pairs.

**optimizers**  
(A vector of) character strings, from which the optimization methods are selected. Default are that of calcGCV for the smoothing step, and nloptr with its own "NLOPT_LN_BOBYQA" method for the smoothed function maximization. See the source of the function for other possible methods (the latter being subject to change with little notice).

**object**  
An object of class bboptim

**n**  
Number of distinct points to be returned. n+1 points will be returned (see Details). If NULL, the following default value is used: \( \min(2^{*(np+1)}, \text{floor}(10*(1+3*\log(np)))) \), where \( np \) is the number of function parameters.

**from**  
A larger (>2n) number of points from which n are selected by an expected improvement criterion. If NULL, a default value computed as \( n*\text{floor}(10*(1+3*\log(np))) \), where \( np \) is the number of function parameters, is used.

**focus**  
A number between 0 and 1. Determines the proportion of points that are sampled closer to the currently inferred maximum (see Details).

**precision**  
target value of prediction variance in inferred optimum.

### Details

rbb selects a proportion 1-focus of the returned points according to expected improvement, from points sampled uniformly in a space defined by a tessellation of the fitted object’s parameter points. They are completed to n-1 points, by points similarly selected but within a space defined by a selection of fitted points with the best predicted response values. Finally, two replicates of the predicted optimum (the optim $par result contained in the object) are included. A total of n+1 points (n distinct) is thus returned.

Global optimization cannot be proven, but it is tested by the following criteria: (1) the predicted optimum is close enough to the optimum among assessed parameter points (i.e. either the optimum parameters are well approached or the function is flat in some way), and (2) the prediction variance at the inferred optimum is low enough (so that the predictions used in the first criterion can be trusted). Accordingly, conv_crits has elements (1) objective that indicates whether optr$value betters optr_fitted$value by more than control$reltol, if given, or else by more than sqrt(.Machine$double.eps); and (2) precision that indicates whether variance of prediction error at the inferred optimum is lower than the target precision. This variance is computed as described for predict.HLfit, with variances=list(linPred=TRUE,dispVar=TRUE).

### Value

bboptim returns an object of class bboptim, a list which includes
optr the result of the optim call
RMSE the root meant square prediction error of response at the optimum optr$par
optr_fitted the best of the fitted points, with its fitted response value and prediction RMSE
fit the predictor of the response (an HLfit object as returned by corrHLfit, with a predict method, etc.)
conv_crits Indicators of convergence (see Details)

and some other elements.
rbb returns a data frame.

References


Examples

# Classical toy example with optional noise
fr <- function(v,sd) {  ## Rosenbrock Banana function
  10 * (v["y"] - v["x"]^2)^2 + (1 - v["x"])*2 + rnorm(1,sd=sd)
}
set.seed(123)

# Initial parameter values, including duplicates. See ?init_grid.
parsp <- init_grid(lower=c(x=0,y=0),upper=c(x=2,y=2),nUnique=25)

#### Without noise
# add function values
simuls <- cbind(parsp,bb=apply(parsp,1,"fr",sd=0))

# optimization
bbresu <- bboptim(simuls)
print(bbresu)

# refine with additional points
if (blackbox.getOption("example_maxtime")>4) {
  while ( any(! bbresu$converge) ) {
    print(unlist(bbresu$optr["par","value"]))
    candidates <- rbb(bbresu)
    newsimuls <- cbind(candidates,bb=apply(candidates,1,"fr",sd=0))
    bbresu <- bboptim(rbind(bbresu$fit$data,newsimuls))
  }
  print(bbresu)
}

#### With noise
if (blackbox.getOption("example_maxtime")>78) {
  set.seed(123)
  simuls <- cbind(parsp,bb=apply(parsp,1,"fr",sd=0.1))
}
bbresu <- bboptim(simuls, precision=0.02)

while ( any( ! bbresu$conv_crits) ) {
  print(unlist(bbresu$optr[c("par","value")]))
  candidates <- rbb(bbresu)
  newsimuls <- cbind(candidates, bb=apply(candidates, 1, "fr", sd=0.1))
  bbresu <- bboptim(rbind(bbresu$fit$data, newsimuls), precision=0.02)
}
print(bbresu)

# basic plot
## Not run:
require(spaMM)
opt <- bbresu$optr$par
mapMM(bbresu$fit, decorations=points(opt[1], opt[2], cex=2, pch="+"))

## End(Not run)

---

**blackbox**

*Black box optimization and response surface exploration*

**Description**

blackbox allows prediction and optimization of a response function from simulated response values. It also includes procedures designed mainly or only to be called, in a completely automated way without any input by users, by other R packages such as the Infusion package (under development) or by R code automatically generated by the Migraine software (see Details). For prediction, blackbox interfaces a C++ library for “ordinary Kriging” (which is jargon for: prediction in a linear mixed model with a constant term as fixed effect). It uses generalized cross validation (GCV) by default to estimate smoothing parameters.

**Details**

Beyond the usage illustrated below, this package is used in particular for smoothing the output of the Migraine software for likelihood analysis of population genetic data (http://kimura.univ-montp2.fr/~rousset/Migraine.htm). In the latter application the response function is a simulated log-likelihood surface and the procedures generate plots of the (profile) log-likelihood, compute (profile) likelihood ratio confidence intervals, and design new parameter points where the likelihood should be simulated. This package provides documentation for all user-level functions in the R script written by Migraine. Control from Migraine uses many variables stored globally in the list of options accessible through blackbox.options().

The C++ DLL was originally a C++ reimplementation of some of the internal functions of the fields package, circa 2005-2006. To estimate smoothing parameters, it requires pairs of responses values for some values of the predictor variables, but will not allow more than pairs.
Author(s)

François Rousset, with contributions by Raphaël Leblois.

References


Examples

fr <- function(v) { ## Rosenbrock Banana function with noise
  10 * (v["y"] - v["x"]^2)^2 + (1 - v["x"])^2 + rnorm(1,sd=0.1)
}  
set.seed(123)

# Initial parameter values, including duplicates. See ?init_grid.
parsp <- init_grid(lower=c(x=0,y=0),upper=c(x=2,y=2))

# add function values
simuls <- cbind(parsp,bb=apply(parsp,1,"fr"))

## The following shows the backbone of the 'bboptim' code:

sorted_etc <- prepareData(data=simuls)
# Then smoothing using GCV (beware of implicit 'decreasing=FALSE' argument)
gcvres <- calcGCV(sorted_etc)

## The results can be used as input to functions from other packages, 
## e.g. corrHLfit from spaMM:
## Not run:
require(spam)
corrHLfit(bb ~ 1+Matern(1|x+y),data=sorted_etc, 
  ranFix=list(rho=1/gcvres$CovFnParam[c("x", "y")],
  # note '1/...'
  nu=gcvres$CovFnParam["smoothness"],
  phi=gcvres$pureRMSE^2,
  # note distinct meaning of lambda notation in spaMM and blackbox
  lambda=with(gcvres,(pureRMSE^2/lambdaEst)))

## GCV is distinct from an REML fit:
corrHLfit(bb ~ 1+Matern(1|x+y),data=sorted_etc, 
  init.corrHLfit=list(rho=c(1,1)))

## End(Not run)
**buildFONKgpointls**  
Prepare data for smoothing

**Description**  
From a data frame, builds another data frame. The input data frame must contain values of the canonical parameters of the model and the variables required to construct the smoothed response. Which of the (output) parameters are variable is also determined for later use.

**Usage**

```r
buildFONKgpointls(pointls)
```

**Arguments**

- `pointls`: A data frame obtained as return value from `buildPointls`

**Details**

With controls set by the Migraine software, this can operate transformations of parameter space as well as transformations in logarithmic scale (see `islogscale`). The output frame will then contain values of transformed parameters.

**Value**

A data frame.

---

**buildPointls**  
Read a data file

**Description**

This reads a data file into a data frame, performs various checks, assign namesto columns, and can select rows.

**Usage**

```r
buildPointls(dataFile = blackbox.getOption("dataFile"), respCols = NULL,
             subsetRows = NULL, ycolname, cleanResu = "")
```
calc1DCIs

Compute 1D confidence intervals

description

This computes 1D confidence intervals from an inferred likelihood surface by profile likelihood ratio methods

Usage

calc1DCIs(oneDimCIvars, FONKgNames, fittedNames, CIlevel = blackbox.getOption("CIlevel"),
          nextBounds = blackbox.getOption("nextBounds"),
          NextBoundsLevel = blackbox.getOption("NextBoundsLevel"),
          boundsOutfile = "", dataString = "", cleanResu = "")
calc1Dprofiles

Arguments

- **oneDimCIvars**: The names of parameters for which confidence intervals are computed.
- **FONKgNames**: The names of “Fitted Or Not” parameters (see Details in `blackbox.options` for this concept).
- **fittedNames**: The names of fitted parameters (see Details in `blackbox.options` for this concept).
- **CIlevel**: Level (1-coverage) of the confidence intervals. Default is 0.05.
- **nextBounds**: For development purposes, not documented.
- **NextBoundsLevel**: For development purposes, not documented.
- **boundsOutfile**: For development purposes, not documented.
- **dataString**: A prefix string in some outputs.
- **cleanResu**: A connection, or a character string naming a file for some nicely formated output. If "" (the default), print to the standard output connection.

Value

Returns invisibly a list of profile points that met the CI level for each parameter.

Usage

```
calc1Dprofiles(varNames=blackbox.getOption("spec1DProfiles"))
calcProfileLR(varNames=blackbox.getOption("fittedNames"),
               pairlist=list(),
               cleanResu="")
calc2D3Dplots(plotFile=NULL,pairlist=list())
```

Description

Assuming that `calcPredictorOK` and `maximizeOK` have been first run: `calc1Dprofiles` plots 1D profiles of a predicted likelihood surface for each of the parameters. Poor profiles may result when only local optima are found for some parameter values. The next function provides an improvement over this. `calcProfileLR` plots 2D profiles of the predicted response surface relative to its maximum for pairs of parameters. It also plots 1D profiles taking benefit of the computation effort for the 2D profiles. `calc2D3Dplots` plots the predicted response surface (no profile) in different ways depending on the number of parameters.

These functions have almost no arguments, as almost all control is through global controls. See in particular `gridStepsNbr` (for profile plots) and `graphicPars` in `blackbox.options`.
Arguments

plotFile If a character string, the name of the file where plots are written. Otherwise, plots are output to the screen.

varNames A character vector specifying the names of predictor variables to be considered. For calc1Dprofiles (used in conjunction with the Migraine software), if the default argument is NULL, all variable canonical parameters plus some composite ones may be considered (see the source code for details).

pairlist A list of character vectors. Each vector describes a pair of predictor variables. With the default value list(), a default non-empty list may be constructed when calc2D3Dplots or calcProfileLR is typically used in conjunction with the Migraine software (see the source code for details).

cleanResu A connection, or a character string naming a file for some nicely formatted output. If it is "" (the default), print to the standard output connection.

Details

If there is only one parameter, calc2D3Dplots plots the predicted response as function of this parameter.

If there are two parameters, calc2D3Dplots plots the response surface both as a 2D surface plot and as a 3D perspective plot, and calcProfileLR also produces a plot of the response surface (no profiling is needed) relative to its maximum (hence, a likelihood ratio, if the response is a likelihood).

If there are more parameters, calc2D3Dplots plots a “slice” of the predicted surface, both as a 2D surface plot and as a 3D perspective plot, for each pair of parameters. A slice plot for a pair of parameters fixes all other parameters to values maximizing the response (hence, maximum likelihood estimates, if the response is a likelihood). calcProfileLR plots the profile response surface relative to its maximum (hence, a profile likelihood ratio, if the response is a likelihood) for pairs of parameters in varNames.

Two dimensional profile plots not only require many numerical maximizations, but will look ugly whenever one of these maximizations fails to find the right maximum, hence additional intensive computations are performed to minimize this problem. As a result, they are quite slow to compute, unless a low gridStepsNbr (say < 16) is used, in which case they do not look smooth.

Value

Returns NULL invisibly

calcGCV Estimate smoothing parameters by generalized cross-validation (GCV)
calcGCV

Description
Smoothing is based on prediction in a linear mixed model ("Kriging") with non-zero residual variance. The correlation function for the random effect is the Matern function with argument the Euclidian distance between scaled coordinates (x/scale). The Matern function also has a smoothness parameter. These parameters are by default estimated by GCV. For large data sets (say >2000 rows), it is strongly recommended to select a subset of the data using GCVptnbr, as GCV will otherwise be very slow.

Usage
calcGCV(sorted_data=data, data, CovFnParam = NULL, GCVptnbr = Inf,
  topmode = FALSE, verbose = FALSE, cleanResu = "",
  force=FALSE, decreasing=FALSE,
  verbosity = blackbox.getOption("verbosity"),
  optimizers = blackbox.getOption("optimizers"))

Arguments
sorted_data A data frame with both predictor and response variance, sorted and with attributes, as produced by prepareData
data Obsolete, for Migraine back-compatibility, should not be used.
CovFnParam Optional fixed values of scale factors for each predictor variable. Smoothness should not be included in this argument.
GCVptnbr Maximum number of rows selected for GCV.
topmode Controls the way rows are selected. For development purposes, should not be modified
verbose Whether to print some messages or not. Distinct from verbosity
verbosity Distinct from verbose. See verbosity in blackbox.options
cleanResu A connection, or a character string naming a file for some nicely formated output. If "" (the default), print to the standard output connection.
force Boolean. Forces the analysis of data without pairs of response values for given parameter values.
optimizers A vector of) character strings, from which the optimization method is selected. Default is nloptr with its own "NLOPT_LN_BOBYQA" method. See the source of the function for other methods (the latter being subject to change with little notice).
decreasing Boolean. Use TRUE if you want the result to be used in function maximization rather than minimization.

Value
A list with the following elements
CovFnParam Scale parameters and smoothness parameter of the Matern correlation function
lambdaEst Ratio of residual variance over random effect variance
calcLRTs

Compute (profile) likelihood ratio tests

Description

Assuming that calcPredictorOK and maximizeOK have been first run and that the predicted response surface is a likelihood surface, this performs likelihood ratio (LR) tests for a list of parameter points. Profiles are computed if appropriate, i.e. the point is lower-dimensional than the the parameter space.

Usage

calcLRTs(testPointList, cleanResu = "")

Arguments

testPointList A list of points in predictor (parameter) space. Each point is a numeric vector or list with named elements, the names being those of some parameters.
cleanResu A connection, or a character string naming a file for some nicely formatted output. If "" (the default), print to the standard output connection.

Value

Return a list with information about each LR test, except for tests that could not be performed (e.g. if the tested point is outside of the convex envelope of the parameter points from which the predictor has been built). The names of this list’s elements are constructed from the tested points. Each element is itself a list with elements

LRT The LR statistics (twice the difference in log-likelihood between maximized likelihood and profile for the input parameters)
pval Associated Pvalue by standard chi-square approximation
profpt Information about the profile point for the input parameters
maxpt Information about the maximum likelihood point

and other elements, not documented here.

References

calcPredictorOK

Generate smoothing predictor given smoothing parameters

Description

Assuming that calcGCV has been first run to estimate smoothing parameter, this produces a “Kriging” predictor of the response.

Usage

calcPredictorOK(FONKgpointls, minKrigPtNbr = blackbox.getOption("minKrigPtNbr"),
                 krigmax = NULL, topmode = FALSE, rawPlots = TRUE, cleanResu = "")

Arguments

FONKgpointls Input data frame as produced by buildFONKgpointls
minKrigPtNbr NULL or numeric. At least this many rows (if available) should be selected for Kriging. The default value depends on the number p of predictor variables and is 90, 159, 500, 1307, 3050, 6560 for p from 1 to 6 (beyond which it is strongly advised to use a non-default value).
krigmax NULL or Numeric. For large data sets the selected points are not “Kriged” all together. Rather, overlapping blocks of rows are selected and are Kriged separately. This sets the size of the blocks. Default depends on the operating system (see source code).
topmode Controls the way rows are selected. For development purposes, should not be modified
rawPlots Boolean. Whether to plot one-dimensional “profiles” of the raw data.
cleanResu A connection, or a character string naming a file for some nicely formated output. If "" (the default), print to the standard output connection.

Value

Returns invisibly a list with many undocumented elements. This list is also stored as a global option “fitobject”.

init_grid

Define starting points in parameter space.

Description

This function samples the space of estimated parameters. Also handles other fixed arguments that need to be passed to the function simulating the summary statistics (sample size is likely to be one such argument). The current sampling strategy is crude but achieves three desirable effects: It tries to sample the space uniformly, avoiding large gaps; it is not exactly a regular grid; and it includes replicates of some parameter points, required for good smoothing of the likelihood surface.
Usage

```
init_grid(lower=c(par=0), upper=c(par=1), steps=NULL,
  nUnique=NULL, nRepl=min(10L,nUnique),
  jitterFac=0.5
)
```

Arguments

- **lower**: A vector of lower bounds for the parameters, as well as fixed arguments to be passed to the function simulating the summary statistics. Elements must be named.
- **upper**: A vector of upper bounds for the parameters, as well as fixed parameters. Elements must be named and match those of `lower`.
- **steps**: Number of steps of the grid, in each dimension of estimated parameters. If NULL, a default value is defined from the other arguments. If a single value is given, it is applied to all dimensions. Otherwise, this must have the same length as `lower` and `upper` and named in the same way as the variable parameters in these arguments.
- **nUnique**: Number of distinct values of parameter vectors in output. Default is an heuristic guess for good start from not too many points, computed as `floor(50^((v/3)^^{1/3}))` where `v` is the number of variable parameters.
- **nRepl**: Number of replicates of distinct values of parameter vectors in output.
- **jitterFac**: Controls the amount of jitter of the points around regular grid nodes. The default value 0.5 means that a mode can move by up to half a grid step (independently in each dimension), so that two adjacent nodes moved toward each other can (almost) meet each other.

Value

A data frame. Each row defines a list of arguments of vector of the function simulating the summary statistics.

Examples

```
set.seed(123)
init_grid()
init_grid(lower=c(mu=2.8,s2=0.5,sample.size=20),
  upper=c(mu=5.2,s2=4.5,sample.size=20),
  steps=c(mu=7,s2=9),nUnique=63)
```
isloogscale  

Test for parameter log scale

Description
This tests whether a log scale is used for a parameter.

Usage
isloogscale(string, scale = blackbox.getOption("FONKgScale"),
            extraScale = blackbox.getOption("extraScale"))

Arguments

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>string</td>
<td>Name of the parameter tested</td>
</tr>
<tr>
<td>scale</td>
<td>A vector of scales for parameters of the smoothed object (i.e. parameters in blackbox.getOption(&quot;FONKgNames&quot;), see Details in blackbox.options).</td>
</tr>
<tr>
<td>extraScale</td>
<td>A vector of scales for additional transformed parameters not in blackbox.getOption(&quot;FONKgNames&quot;).</td>
</tr>
</tbody>
</table>

Value
A boolean.

maximizeOK  

Find maximum of predicted response surface

Description
Assuming that calcPredictorOK has been first run to produce a predictor of the response surface, this finds its constrained maximum in the convex envelope of the smoothed data.

Usage
maximizeOK(fitobject = blackbox.getOption("fitobject"), cleanResu = "")

Arguments

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>fitobject</td>
<td>Return object of calcPredictorOK.</td>
</tr>
<tr>
<td>cleanResu</td>
<td>A connection, or a character string naming a file for some nicely formatted output. If &quot;&quot; (the default), print to the standard output connection.</td>
</tr>
</tbody>
</table>
options

Value

A list with element

- **par**: predictor values maximizing the predicted response (in the parameter space used for Kriging)
- **value**: maximum of the predicted response
- **canonVP**: Representation of `par` in canonical parameter space

and possibly other elements (i) returned by an optimization function such as `optim`; (ii) values of additional transformed parameters; (iii) cryptic information whether maximization occurred at some boundary of the convex envelope.

---

**options**  
*blackbox options settings*

Description

Allow the user to examine a variety of “options” (most of which are not true user options) which affect operations of the blackbox package.

Usage

- `blackbox.options(...)`
- `blackbox.getOption(x)`

Arguments

- `x`: a character string holding an option name.
- `...`: A named value or a list of named values. Most are not to be manipulated by users and are undocumented. Exceptions are:
  - **ParameterNames**: See Details
  - **FONKgNames**: See Details
  - **fittedNames**: See Details
  - **gridStepsNbr**: Number of steps of the grid of value for each parameter in profile plots.
  - **graphicPars**: Graphic parameters used for most plots.
  - **coreNbr**: Number of cores that R can use for parallel profile computations (see Details for implementation of these).
  - **verbosity=0**: Controls display of information about generalized cross-validation.  
    - 0 suppresses (most) messages. 1 displays information about estimates and progress of the procedure. Higher values display more information from the optimizer and possibly additional information.
prepareData

Details

blackbox.options() provides an interface for changing options, many of which are undocumented has they are intended to by used only in conjunction with the Migraine software, in which case the Migraine documentation should be consulted.

The package has been designed first to infer likelihood surfaces by smoothing estimated likelihood points in a model with some canonical parameters (ParameterNames). A transformed parameter space may be considered for smoothing, wherein some parameters are variable (fittedNames) and others may be constant. The transformed parameter space including constant parameters has names FONKgNames (FON for Fitted Or Not).

blackbox can perform in parallel manner the Migraine-specific computations of grids of profile log-likelihood values. See the Migraine documentation for user control of the requested number of cores; direct control through R code is possible by blackbox.options(coreNbr=.). If the doSNOW back-end is attached (by explicit request from the user), it will be used; otherwise, pbapply will be used. Both provide progress bars, but doSNOW may provide more efficient load-balancing.

Value

For blackbox.getOption, the current value set for option x, or NULL if the option is unset. For blackbox.options(), a list of all set options. For blackbox.options(name), a list of length one containing the set value, or NULL if it is unset. For uses setting one or more options, a list with the previous values of the options changed (returned invisibly).

Examples

blackbox.getOption("verbosity")
## Not run:
blackbox.options(verbosity=1)
blackbox.options()

## End(Not run)

prepareData(data, ParameterNames=NULL, respName=NULL, verbose=TRUE)

Description

This sorts the data, identifies parameters and function value (response), identifies pairs of response values for identical parameter values, and may set some global controls in blackbox.options().

Usage

prepareData(data, ParameterNames=NULL, respName=NULL, verbose=TRUE)
Arguments

- **data**: A data frame including variables in `ParameterNames` and `respName`.
- **ParameterNames**: Names of the variables to be used as predictors of the smoothed surface. If NULL, all columns except the last are assumed to hold parameter values.
- **respName**: Name of the variable to be used as response of the smoothed surface. If NULL, the last column is assumed to hold function values.
- **verbose**: Whether to print some information (in particular a message if replicate responses values are identical for given parameter values, which will be suspect in some applications).

Value

A data frame with the required variables, ordered by increasing values as in `do.call(order, data)`. This may set some global controls in `blackbox.options()` as a side effect.

Examples

```r
require(spaMM)
data(blackcap) # use dataset as template
sorted_etc <- prepareData(data=blackcap,ParameterNames=c("longitude", "latitude"),
respName="means")
```

---

**preprocessbboptions**

**Set controls for most functions in the package**

Description

Preprocesses a list of argument. The return value of this function serves as argument to `blackbox.options` (see Examples). Providing in this way the information described in the Details section of `blackbox.options` is essential for further usage of the package functions.

Usage

```r
preprocessbboptions(optionList)
```

Arguments

- **optionList**: A list, with named elements, which names will (mostly) match the names of options set by this function.

Value

A list, returned invisibly.
## Examples

```r
## Not run:
GP <- list(ParameterNames=c("theta_1","theta_2"))
p <- preprocessbboptions(GP)
do.call(blackbox.options, p) ## essential

## End(Not run)
```

---

### Description

Assuming that `calcPredictorOK` and `maximizeOK` have been first run: predictor points can be sampled in several ways: the convex hull of predictor points with predicted response higher than some threshold value can be sampled uniformly. An Expected Improvement (e.g. Bingham et al., 2014) strategy can be used; whereby points with the highest predicted probability of improvement of the response value among a set of candidates sampled uniformly are retained. An expanded convex hull allowing further exploration of predictor space can also be considered. This function performs various combinations of these methods and (if the response was treated as a likelihood surface) can further use information from any previous likelihood ratio test of confidence interval computations.

### Usage

```r
sampleByResp(size = blackbox.getOption("nextPointNumber"), outfile = NULL, useEI,
             NextBoundsLevel = 0.001,
             threshold = qchisq(1 - NextBoundsLevel, 1)/2,
             rnd.seed = NULL, verbose = FALSE)
```

### Arguments

- **size**: sample size
- **outfile**: If not NULL, the name of an ASCII file where to print the result as a table.
- **useEI**: Whether to use an expected improvement criterion
- **NextBoundsLevel**: Controls threshold in a way meaningful for log-likelihood surfaces
- **threshold**: Controls the threshold for selection of the vertices of the convex hull to be sampled, and for inclusion of candidate predictor points in the sample. This threshold corresponds to a difference between predicted value and maximum predicted value. The actual maximal difference for inclusion of vertices additionally depends on the residual error of the predictor.
- **rnd.seed**: NULL (in which case nothing is done) or an integer (in which case `set.seed(seed=rnd.seed)` is called).
- **verbose**: To print information about evaluation, for development purposes.
saveOldFile

Details

The sampling procedure is designed to balance exploration of new regions of the predictor space and filling the top of a likelihood surface, or accurately locating the maximum and bounds of one-dimensional profile likelihood confidence interval. Details are yet to be documented.

Value

Returns the predictor points invisibly.

References


saveOldFile

Description

This checks if a file of given name already exists in the current directory, and if so saves a copy of it under an automatically generated name (see below).

Usage

saveOldFile(filename)

Arguments

filename Name of file to be saved.

Details

This function copies the file named “first names”.ext under a name created by inserting a string of the form .old_n between “first names” and .ext, where n is one more than the highest value for any file, matching the first names and extension, already in the current directory, and 0 if no file matches. For example, if filename is my.beautiful.pdf, it is copied as my.beautiful.old_0.pdf if no my.beautiful.old_n.pdf file exists, and is is copied as my.beautiful.old_4.pdf if my.beautiful.old_3.pdf (and any lower n) file exists.

Value

Returns "" if no file with given name was present on disk, FALSE if it failed to copy an existing old file, and the name of the copy if it successfully copied such a file.
Examples

## Not run:
saveOldFile("same.story")

## End(Not run)

writeFinalInfo

Pretty output, and management of output files

Description

Final code of the R script written by the Migraine software (http://kimura.univ-montp2.fr/~rousset/Migraine.htm; see main documentation page for the package, for the context). This prints some information, close output files, and beeps to warn that a possibly long computation is finished.

Usage

writeFinalInfo(cleanResu = "")

Arguments

cleanResu A connection, or a character string naming a file for some nicely formatted output. If "" (the default), print to the standard output connection.

Value

returns NULL invisibly.
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