Package ‘profExtrema’
October 14, 2022

Type Package
Title Compute and Visualize Profile Extrema Functions
Version 0.2.1
Maintainer Dario Azzimonti <dario.azzimonti@gmail.com>
Date 2020-03-20
Description Computes profile extrema functions for arbitrary functions. If the function is expensive-
to-evaluate it computes profile extrema by emulating the function with a Gaussian process (us-
ing package ‘DiceKriging’). In this case uncertainty quantification on the profile ex-
trema can also be computed. The different plotting functions for profile ex-
trema give the user a tool to better locate excursion sets.
License GPL-3
Encoding UTF-8
LazyData true
Depends R (>= 2.10), DiceKriging, KrigInv, pGpX
Imports microbenchmark, quantreg, lhs, splines, methods, RColorBrewer,
utils, MASS, rcdd
RoxygenNote 6.1.1
NeedsCompilation no
Author Dario Azzimonti [aut, cre, cph]
  (<https://orcid.org/0000-0001-5080-3061>)
Repository CRAN
Date/Publication 2020-03-21 17:10:02 UTC

R topics documented:

approxMaxMin .................................................. 2
approxProfileExtrema .................................... 4
bound_profiles ............................................. 7
cleanProfileResults ...................................... 8
coastal_flooding .......................................... 9
coordinateProfiles ..................................... 12
approxMaxMin

Approximate coordinate profile functions

Description

Evaluate profile extrema over other variables with approximations at few values

Usage

approxMaxMin(f, fprime = NULL, d, opts = NULL)
approxMaxMin

Arguments

- **f**: the function to be evaluated
- **fprime**: derivative of the function
- **d**: dimension of the input domain
- **opts**: a list containing the options for this function and the subfunctions getMax, getMin or getMaxMinMC, see documentation of getMax, getMin, getMaxMinMC for details. The options only for approxMaxMin are:
  - **limits**: an optional list with the upper and lower limits of each dimension, if NULL then for each dimension limits are 0,1
  - **smoother**: Select which smoother to use: a string that selects which smoother to use:
    - "1order": first order interpolation with gradient
    - "splineSmooth": smoothing spline with default degrees of freedom (DEFAULT OPTION)
    - "quantSpline": profile inf and profile sup approximated with quantile spline regression at levels 0.1 and 0.9 respectively
  - **heavyReturn**: If TRUE returns also all minimizers, default is FALSE.
  - **initDesign**: The design of few points where the expensive sup is evaluated.
  - **fullDesignSize**: The full design where the function is approximated.
  - **multistart**: number of multistarts for optim procedure.
  - **MonteCarlo**: if TRUE, computes sup with Monte Carlo procedure.
  - **numMCsamples**: number of MC samples for the sup.
  - **plts**: If TRUE, plots the max/min functions at each coordinate, default is FALSE.
  - **verb**: If TRUE, outputs intermediate results, default is FALSE.

Value

A list of two data frames (min, max) of the evaluations of \( f_{\text{up}}(x_i) = \sup_{x_j \neq i} f(x_1, \ldots, x_d) \) and \( f_{\text{inf}}(x_i) = \inf_{x_j \neq i} f(x_1, \ldots, x_d) \) for each i at the design Design. By default Design is a 100 equally spaced points for each dimension. It can be changed by defining it in options$Design

Author(s)

Dario Azzimonti

Examples

```r
if (!requireNamespace("DiceKriging", quietly = TRUE)) {
  stop("DiceKriging needed for this example to work. Please install it.",
       call. = FALSE)
}
# Compute the coordinate profile extrema with full optimization on 2d example

# Define the function
```
\[ g(x) = \frac{1}{2} x_1^2 - x_1 x_2 + \frac{1}{4} x_2^2 - \frac{1}{\pi^2} \sin(x_1) \]

# Define the gradient
\[ g'(x) = \begin{bmatrix} -f_1' & -f_2' \end{bmatrix} \]

# generic approximation options
\begin{verbatim}
init_des <- lhs::maximinLHS(15, 2)
options_approx <- list(multistart = 4, heavyReturn = TRUE, initDesign = init_des, fullDesignSize = 100)
\end{verbatim}

# 1order approximation
\begin{verbatim}
options_approx$smoother <- "1order"
coordProf_approx_1order <- approxMaxMin(f = g, fprime = gprime, d = 2, opts = options_approx)
\end{verbatim}

# quantile regression
\begin{verbatim}
options_approx$smoother <- "quantSpline"
coordProf_approx_quantReg <- approxMaxMin(f = g, fprime = gprime, d = 2, opts = options_approx)
\end{verbatim}

# Consider threshold = -10
threshold <- -10
# obtain the points where the profiles take the threshold value
pp_change <- getChangePoints(threshold = threshold, allRes = coordProf_approx_quantReg)
# evaluate g at a grid and plot the image
x <- seq(0, 1, , 100)
g_evals <- apply(X = grid, MARGIN = 1, FUN = g)
image(x = x, y = x, z = matrix(g_evals, nrow = 100)), col = grey.colors(20))
contour(x = x, y = x, z = matrix(g_evals, nrow = 100)), add = TRUE, nlevels = 20)
abline(h = pp_change$neverEx$[-10], col = "darkgreen", lwd = 2)
abline(v = pp_change$neverEx$[-10], col = "darkgreen", lwd = 2)
# Plot the coordinate profiles and a threshold
plotMaxMin(allRes = coordProf_approx_1order, threshold = threshold, changes = TRUE)
plotMaxMin(allRes = coordProf_approx_quantReg, threshold = threshold, changes = TRUE)

**approxProfileExtrema**  
**Approximate profile extrema functions**

**Description**

Evaluate profile extrema for a set of Psi with approximations at few values.
approxProfileExtrema

Usage

approxProfileExtrema(f, fprime = NULL, d, allPsi, opts = NULL)

Arguments

f the function to be evaluated
fprime derivative of the function
d dimension of the input domain
allPsi a list containing the matrices Psi (dim pxd) for which to compute the profile extrema
opts a list containing the options for this function and the subfunctions getProfileSup_optim, getProfileInf_optim or getProfileExtrema. The options only for approxProfileExtrema are
  • limits: an optional list with the upper and lower limits of input space dimension, if NULL then limits=list(upper=rep(1,d),lower=rep(0,d))
  • smoother: Select which smoother to use: a string that selects which smoother to use:
    – "1order": first order interpolation with gradient
    – "splineSmooth": smoothing spline with default degrees of freedom (DEFAULT OPTION)
    – "quantSpline": profile inf and profile sup approximated with quantile spline regression at levels 0.1 and 0.9 respectively
  • heavyReturn: If TRUE returns also all minimizers, default is FALSE.
  • initDesign: A list of the same length as allPsi containing the designs of few points where the expensive sup is evaluated. If Null it is automatically initialized
  • fullDesignSize: The full design where the function is approximated.
  • multistart: number of multistarts for optim procedure.
  • numMCsamples: number of MC samples for the sup.
  • plts: If TRUE, plots the max/min functions at each coordinate, default is FALSE.
  • verb: If TRUE, outputs intermediate results, default is FALSE.

Value

a list of two data frames (min, max) of the evaluations of $f_{sup}(x_i) = sup_{x_i \neq i} f(x_1, \ldots, x_d)$ and $f_{inf}(x_i) = inf_{x_i \neq i} f(x_1, \ldots, x_d)$ for each i at the design Design. By default Design is a 100 equally spaced points for each dimension. It can be changed by defining it in options$Design

Author(s)

Dario Azzimonti
Examples

# Compute the oblique profile extrema with approximate optimization on 2d example

# Define the function
testF <- function(x, params, v1 = c(1, 0), v2 = c(0, 1)) {
  return(sin(crossprod(v1, x) * params[1] + params[2]) + cos(crossprod(v2, x) * params[3] + params[4]) - 1.5)
}

testFprime <- function(x, params, v1 = c(1, 0), v2 = c(0, 1)) {
  return(matrix(c(params[1] * v1[1] * cos(crossprod(v1, x) * params[1] + params[2]) -
}

# Define the main directions of the function
theta = pi/6
pparams <- c(1, 0, 10, 0)
vv1 <- c(cos(theta), sin(theta))
vv2 <- c(cos(theta + pi/2), sin(theta + pi/2))

# Define optimizer friendly function
f <- function(x) {
  return(testF(x, pparams, vv1, vv2))
}
fprime <- function(x) {
  return(testFprime(x, pparams, vv1, vv2))
}

# Define list of directions where to evaluate the profile extrema
all_Psi <- list(Psi1 = vv1, Psi2 = vv2)

# Evaluate profile extrema along directions of all_Psi
allOblique <- approxProfileExtrema(f = f, fprime = fprime, d = 2, allPsi = all_Psi,
                                   opts = list(plts = FALSE, heavyReturn = TRUE))

# Consider threshold=0
threshold <- 0

# Plot oblique profile extrema functions
plotMaxMin(allOblique, allOblique$Design, threshold = threshold)

## Since the example is two dimensional we can visualize the regions excluded by the profile extrema
# evaluate the function at a grid for plots
inDes <- seq(0, 1, , 100)
inputs <- expand.grid(inDes, inDes)
outs <- apply(X = inputs, MARGIN = 1, function(x) {return(testF(x, pparams, v1 = vv1, v2 = vv2))})

# obtain the points where the profiles take the threshold value
cccObl <- getChangePoints(threshold = threshold, allRes = allOblique, Design = allOblique$Design)
# visualize the functions and the regions excluded

```r
de_image(inDes,inDes,matrix(outs,ncol=100),col=grey.colors(20),main="Example and oblique profiles")
contour(inDes,inDes,matrix(outs,ncol=100),add=TRUE,nlevels = 20)
contour(inDes,inDes,matrix(outs,ncol=100),add=TRUE,levels = c(threshold),col=4,lwd=1.5)
plotOblique(cccObl$alwaysEx$'0'[[1]],all_Psi[[1]],col=3)
plotOblique(cccObl$alwaysEx$'0'[[2]],all_Psi[[2]],col=3)
plotOblique(cccObl$neverEx$'0'[[1]],all_Psi[[1]],col=2)
plotOblique(cccObl$neverEx$'0'[[2]],all_Psi[[2]],col=2)
```

**bound_profiles**  
*Bound for profile extrema quantiles*

**Description**

The function `bound_profiles` computes the upper and lower bounds for the profile extrema quantiles of a Gaussian process model.

**Usage**

```r
bound_profiles(objectUQ, mean_var_delta = NULL, beta = 0.0124,
 alpha = 0.025, allPsi = NULL, options_approx = NULL,
 options_full_sims = NULL)
```

**Arguments**

- **objectUQ**: an object returned by `coordProf_UQ` or the object saved in `obj$res_UQ`, if `obj` is the object returned by `coordinateProfiles`.
- **mean_var_delta**: the profile extrema functions at `options_approx$design` for the mean and variance function of the difference process $Z^\Delta = Z_x - \bar{Z}_x$. Object returned by `prof_mean_var_Delta`.
- **beta**: the level of confidence for the approximate simulations.
- **alpha**: the level of confidence for the bound.
- **allPsi**: optional list of matrices (dim `pxd`) for which to compute the profile extrema. If `NULL` coordinate profiles are computed.
- **options_approx**: an optional list of options for `approxMaxMin` (or `approxProfileExtrema` if `allPsi` not `NULL`).
- **options_full_sims**: an optional list of options for `getAllMaxMin` (or `getProfileExtrema` if `allPsi` not `NULL`). If `NULL` the full computations are not executed. NOTE: this computations might be very expensive!
Value

a list containing

- `bound`: a list containing the upper/lower bound for profile sup and inf
- `approx`: a list containing the upper/lower approximate quantiles for profile sup and inf

Author(s)

Dario Azzimonti

cleanProfileResults  

Clean a profile extrema object

Description

The function `cleanProfileResults` cleans a profile extrema object to partially redo some computations.

Usage

`cleanProfileResults(object, level = 1)`

Arguments

- `object`: a list containing profile extrema results.
- `level`: an integer 1-4 denoting how much it should be removed from `object`. See Value for details.

Value

returns `object` with the deleted parts as selected by `level`. In particular

- 1: keep only `profMean_full`.
- 2: keep `profMean_full` and `profMean_approx`. Remove all UQ results.
- 3: keep `profMean_full` and `profMean_approx` and the pilot points. Remove all UQ simulations.
- 4: Remove only the bound computations.

Author(s)

Dario Azzimonti
Examples

```r
if (!requireNamespace("DiceKriging", quietly = TRUE)) {
  stop("DiceKriging needed for this example to work. Please install it.",
       call. = FALSE)
}
# Compute a kriging model from 50 evaluations of the Branin function
# Define the function
g=function(x){
  return(-branin(x))
}
gp_des<-lhs::maximinLHS(20,2)
reals<-apply(gp_des,1,g)
kmModel<-km(design = gp_des,response = reals,covtype = "matern3_2")
threshold=-10

# Compute coordinate profiles on the posterior mean
# Increase multistart and size of designs for more precise results
options_full<-list(multistart=2,heavyReturn=TRUE, Design = replicate(2,seq(0,1,,50)))
init_des<-lhs::maximinLHS(12,2)
options_approx<- list(multistart=2,heavyReturn=TRUE,initDesign=init_des,fullDesignSize=50)
cProfilesMean<-coordinateProfiles(object=kmModel,threshold=threshold,options_full=options_full,
                                   options_approx=options_approx,uq_computations=FALSE,
                                   plot_level=3,plot_options=NULL,CI_const=NULL,return_level=2)

# If we want to run again the computation of approximate coordinate profiles
# we delete that result and run again the coordinate profiles function
# cProfiles_full <- cleanProfileResults(cProfilesMean,level=1)
## Not run:
# Coordinate profiles with UQ with approximate profiles
plot_options<-list(save=FALSE, titleProf = "Coordinate profiles",
                   title2d = "Posterior mean",qq_fill=TRUE)
cProfilesUQ<-coordinateProfiles(object=cProfilesMean,threshold=threshold,options_full=options_full,
                                options_approx=options_approx,uq_computations=TRUE,
                                plot_level=3,plot_options=NULL,CI_const=NULL,return_level=2)

# If we would like to remove all UQ results
# cProf_noUQ <- cleanProfileResults(cProfilesUQ,level=2)

# If we would like to remove the simulations but keep the pilot points
# cProf_noSims <- cleanProfileResults(cProfilesUQ,level=3)
# the line above is useful, for example, if we need a more accurate UQ. In that case
# we obtain more simulations with the same pilot points and then combine the results.

## End(Not run)
```

Coastal flooding as function of offshore forcing conditions.
Description
A dataset containing the results of a numerical simulation conducted with the MARS model (Lazure and Dumas, 2008) for coastal flooding. The numerical model was adapted to the Boucholeurs area (French Atlantic coast), close to La Rochelle, and validated with data from the 2010 Xynthia storm event. See Azzimonti et al. (2017+) and Rohmer et al. (2018) for more details.

Usage
coastal_flooding

Format
A data frame with 200 rows and 6 variables:

- **Tide**: High tide level in meters;
- **Surge**: Surge peak amplitude in meters;
- **phi**: Phase difference between high tide and surge peak;
- **t-**: Duration of the increasing part of the surge temporal signal (assumed to be triangular);
- **t+**: Duration of the decreasing part of the surge temporal signal (assumed to be triangular);
- **Area**: Flooded area in m$^2$.

Details
The data frame contains 5 input variables: Tide, Surge, phi, t-, t+ detailing the offshore forcing conditions for the model. All input variables are normalized in [0, 1]. The response is Area, the area flooded in m$^2$.

References


Examples

```r
# Define inputs
inputs<-data.frame(coastal_flooding[,-6])
colnames(inputs)<-colnames(coastal_flooding[,-6])
colnames(inputs)[4:5]<-c("tPlus","tMinus")

# put response in areaFlooded variable
areaFlooded<-data.frame(coastal_flooding[,6])
colnames(areaFlooded)<-colnames(coastal_flooding)[6]
response = sqrt(areaFlooded)
```
model <- km(formula=~Tide+Surge+I(phi^2)+tMinus+tPlus,
    design = inputs,response = response,covtype="matern3_2")

# Fix threshold
threshold<-sqrt(c(1.2e6,1.9e6,3.1e6,6.5e6))

# use the coordinateProfile function
## set up plot options
options_plots <- list(save=FALSE, folderPlots = "/",
    titleProf = "Coordinate profiles",
    title2d = "Posterior mean",qq_fill=TRUE)

# set up full profiles options
options_full<-list(multistart=15,heavyReturn=TRUE)

# set up approximation options
init_des<-maximinLHS(5*d, d)
options_approx<- list(multistart=2,heavyReturn=TRUE, initDesign=init_des, fullDesignSize=100, smoother="quantSpline")

# run the coordinate profile extrema on the mean
CF_CoordProf_mean<- coordinateProfiles(object = model, threshold = threshold,
    uq_computations = FALSE, options_approx = options_approx,
    plot_level=3, plot_options= options_plots, return_level=3,
    options_full=options_full)

## Not run:
## UQ computations might require a long time

# set up simulation options
## reduce nsims and batchsize for faster/less accurate UQ
nsims=200
opts_sims<-list(algorithm="B", lower=rep(0,d),
    upper=rep(1,d), batchsize=150,
    optimcontrol=list(method="genoud", pop.size=100,print.level=0),
    integcontrol = list(distrib="sobol",n.points=2000),nsim=nsims)

opts_sims$integration.param <- integration_design(opts_sims$integcontrol,
    d, opts_sims$lower,
    opts_sims$upper,
    model,threshold)

opts_sims$integration.param$alpha <- 0.5

# run UQ computations
CF_CoordProf_UQ<- coordinateProfiles(object = CF_CoordProf_mean, threshold = threshold,
    uq_computations = TRUE, options_approx = options_approx,
    plot_level=3, plot_options= options_plots, return_level=3,
    options_sims=opts_sims,options_full=options_full,
    options_bound = list(beta=0.024, alpha=0.05))

## End(Not run)
coordinateProfiles  

**Coordinate profiles starting from a kriging model**

**Description**

The function coordinateProfiles computes the profile extrema functions for the posterior mean of a Gaussian process and its confidence bounds.

**Usage**

```r
coordinateProfiles(object, threshold, options_full = NULL,
                   options_approx = NULL, uq_computations = FALSE, plot_level = 0,
                   plot_options = NULL, CI_const = NULL, return_level = 1, ...)
```

**Arguments**

- `object`: either a km model or a list containing partial results. If `object` is a km model then all computations are carried out. If `object` is a list, then the function carries out all computations to complete the list results.
- `threshold`: the threshold of interest
- `options_full`: an optional list of options for `getAllMaxMin`, see `getAllMaxMin` for details.
- `options_approx`: an optional list of options for `approxMaxMin`, see `approxMaxMin` for details.
- `uq_computations`: boolean, if TRUE the uq computations for the profile mean are computed.
- `plot_level`: an integer to select the plots to return (0=no plots, 1=basic plots, 2=all plots)
- `plot_options`: an optional list of parameters for plots. See `setPlotOptions` for currently available options.
- `CI_const`: an optional vector containing the constants for the CI. If not NULL, then profiles extrem for \( m_n(x) \pm CI_{const}[i] \ast s_n(x, x) \) are computed.
- `return_level`: an integer to select the amount of details returned
- `...`: additional parameters to be passed to `coordProf_UQ`.

**Value**

If `return_level`=1 a list containing

- `profMean_full`: the results of `getAllMaxMin` for the posterior mean
- `profMean_approx`: the results of `approxMaxMin` for the posterior mean
- `res_UQ`: the results of `coordProf_UQ` for the posterior mean

If `return_level`=2 the same list as above but also including

- `abs_err`: the vector of maximum absolute approximation errors for the profile inf /sup on posterior mean for the chosen approximation
- `times`: a list containing
  - `full`: computational time for the full computation of profile extrema
  - `approx`: computational time for the approximate computation of profile extrema
Author(s)
Dario Azzimonti

Examples

```r
if (!requireNamespace("DiceKriging", quietly = TRUE)) {
  stop("DiceKriging needed for this example to work. Please install it.",
       call. = FALSE)
}
# Compute a kriging model from 50 evaluations of the Branin function
# Define the function
g <- function(x){
  return(-branin(x))
}
gp_des <- lhs::maximinLHS(20, 2)
reals <- apply(gp_des, 1, g)
kmModel <- km(design = gp_des, response = reals, covtype = "matern3_2")
threshold <- -10
# Compute coordinate profiles on the posterior mean
# Increase multistart and size of designs for more precise results
options_full <- list(multistart=2, heavyReturn=TRUE, Design = replicate(2, seq(0, 1, , 50)))
init_des <- lhs::maximinLHS(12, 2)
options_approx <- list(multistart=2, heavyReturn=TRUE, initDesign=init_des, fullDesignSize=50)
cProfilesMean <- coordinateProfiles(object=kmModel, threshold=threshold, options_full=options_full,
                                  options_approx=options_approx, uq_computations=FALSE,
                                  plot_level=3, plot_options=NULL, CI_const=NULL, return_level=2)
## Not run:
# Coordinate profiles with UQ with approximate profiles
plot_options <- list(save=FALSE, titleProf = "Coordinate profiles",
                     title2d = "Posterior mean", qq_fill=TRUE)
cProfilesUQ <- coordinateProfiles(object=cProfilesMean, threshold=threshold, options_full=options_full,
                                  options_approx=options_approx, uq_computations=TRUE,
                                  plot_level=3, plot_options=NULL, CI_const=NULL, return_level=2)
# Coordinate profiles with UQ with fully optim profiles
options_full_sims <- list(multistart=4, heavyReturn=TRUE, Design = replicate(2, seq(0, 1, , 60)))
cProfilesUQ <- coordinateProfiles(object=cProfilesMean, threshold=threshold, options_full=options_full,
                                  options_approx=options_approx, uq_computations=TRUE,
                                  plot_level=3, plot_options=NULL, CI_const=NULL, return_level=2,
                                  options_full_sims=options_full_sims)
## End(Not run)
```

coordProf_UQ
Coordinate profiles UQ from a kriging model
Description

The function coordProf_UQ computes the profile extrema functions for posterior realizations of a Gaussian process and its confidence bounds.

Usage

coordProf_UQ(object, threshold, allResMean = NULL,
             quantiles_uq = c(0.05, 0.95),
             options_approx = NULL,
             options_full_sims = NULL,
             options_bound = NULL,
             plot_level = 0,
             plot_options = NULL,
             return_level = 1)

Arguments

object: either a km model or a list containing partial results. If object is a km model then all computations are carried out. If object is a list, then the function carries out all computations to complete the results list.

threshold: the threshold of interest

allResMean: a list resulting from getAllMaxMin or approxMaxMin for the profile extrema on the mean. If NULL the median from the observations is plotted

quantiles_uq: a vector containing the quantiles to be computed

options_approx: an optional list of options for approxMaxMin, see approxMaxMin for details.

options_full_sims: an optional list of options for getAllMaxMin, see getAllMaxMin for details. If NULL the full computations are not executed. NOTE: this computations might be very expensive!

options_sims: an optional list of options for the posterior simulations.

  • algorithm: string choice of the algorithm to select the pilot points ("A" or "B", default "B");
  • lower: d dimensional vector with lower bounds for pilot points, default rep(0,d);
  • upper: d dimensional vector with upper bounds for pilot points, default rep(1,d);
  • batchsize: number of pilot points, default 120;
  • optimcontrol: list containing the options for optimization, see optim_dist_measure;
  • integcontrol: list containing the options for numerical integration of the criterion, see optim_dist_measure;
  • integration.param: list containing the integration design, obtained with the function integration_design;
  • nsim: number of approximate GP simulations, default 300.

options_bound: an optional list containing beta the confidence level for the approximation and alpha the confidence level for the bound. Note that alpha > 2*beta. If NULL, the bound is not computed.

plot_level: an integer to select the plots to return (0=no plots, 1=basic plots, 2=all plots)
plot_options

an optional list of parameters for plots. See setPlotOptions for currently available options.

return_level

an integer to select the amount of details returned

Value

If return_level=1 a list containing

• profSups: an array dxfullDesignSizexnsims containing the profile sup for each coordinate for each realization.
• profInfs: an array dxfullDesignSizexnsims containing the profile inf for each coordinate for each realization.
• prof_quantiles_approx: a list containing the quantiles (levels set by quantiles_uq) of the profile extrema functions.

if return_level=2 the same list as above but also including more: a list containing

• times: a list containing
  – tSpts: computational time for selecting pilot points.
  – tApprox1ord: vector containing the computational time required for profile extrema computation for each realization
• simuls: a matrix containing the value of the field simulated at the pilot points
• sPts: the pilot points

Author(s)

Dario Azzimonti

Examples

```r
if (!requireNamespace("DiceKriging", quietly = TRUE)) {
  stop("DiceKriging needed for this example to work. Please install it.",
       call. = FALSE)
}
# Compute a kriging model from 50 evaluations of the Branin function
# Define the function
g <- function(x){
  return(-branin(x))
}
# Compute a kriging model from 50 evaluations of the Branin function
gp_des<-lhs::maximinLHS(20,2)
reals<-apply(gp_des,1,g)
kmModel<-km(design = gp_des,response = reals,covtype = "matern3_2")
threshold=-10
d<-2
# Compute coordinate profiles UQ starting from GP model
# define simulation options
options_sims<-list(algorithm="B", lower=rep(0,d), upper=rep(1,d),
                   batchsize=80, optimcontrol = list(method="genoud", pop.size=100, print.level=0),
                   return_level=1)
```
integcontrol = list(distrib="sobol", n.points=1000), nsim=150)
# define 1 order approximation options
init_des<- lhs::maximinLHS(15,d)
options_approx<- list(multistart=4, heavyReturn=TRUE,
    initDesign=init_des, fullDesignSize=100,
    smoother="1order")

# define plot options
options_plots<-list(save=FALSE, titleProf = "Coordinate profiles",
    title2d = "Posterior mean", qq_fill=TRUE)
## Not run:
# profile UQ on approximate coordinate profiles
cProfiles_UQ<- coordProf_UQ(object = kmModel, threshold = threshold, allResMean = NULL,
    quantiles_uq = c(0.05, 0.95), options_approx = options_approx,
    options_full_sims = NULL, options_sims = options_sims,
    options_bound = NULL, plot_level = 3,
    plot_options = options_plots, return_level = 3)

# profile UQ on full optim coordinate profiles
cProfiles_UQ_full<- coordProf_UQ(object = cProfiles_UQ, threshold = threshold, allResMean = NULL,
    quantiles_uq = c(0.05, 0.95), options_approx = options_approx,
    options_full_sims = options_full_sims, options_sims = options_sims,
    options_bound = NULL, plot_level = 3,
    plot_options = options_plots, return_level = 3)

# profile UQ on full optim coordinate profiles with bound
cProfiles_UQ_full_bound<- coordProf_UQ(object = cProfiles_UQ_full, threshold = threshold,
    allResMean = NULL, quantiles_uq = c(0.05, 0.95),
    options_approx = options_approx,
    options_full_sims = options_full_sims,
    options_sims = options_sims,
    options_bound = list(beta=0.024, alpha=0.05),
    plot_level = 3, plot_options = options_plots,
    return_level = 3)
## End(Not run)

getAllMaxMin

getAllMaxMin

Coordinate profile extrema with BFGS optimization

description

Evaluate coordinate profile extrema with full optimization.

Usage

getAllMaxMin(f, fprime = NULL, d, options = NULL)
getAllMaxMin

Arguments

- **f**: the function to be evaluated
- **fprime**: derivative of the function
- **d**: dimension of the input domain
- **options**: a list containing the options for this function and the subfunctions getMax, getMin see documentation of getMax, getMin for details. The options only for getAllMaxMin are
  - **Design**: an optional design matrix with the discretization of each dimension, if NULL then for each dimension Design[,coord] = seq(0,1,length.out=100)
  - **heavyReturn**: If TRUE returns also all minimizers, default is FALSE.
  - **plts**: If TRUE, plots the max/min functions at each coordinate, default is FALSE.
  - **verb**: If TRUE, outputs intermediate results, default is FALSE.
  - **MonteCarlo**: If TRUE, use the MC optimizer otherwise use standard optim.

Value

a list of two data frames (min, max) of the evaluations of \( f_{\sup}(x_i) = \sup_{x_{ij} \neq i} f(x_1, \ldots, x_d) \) and \( f_{\inf}(x_i) = \inf_{x_{ij} \neq i} f(x_1, \ldots, x_d) \) for each \( i \) at the design Design. By default Design is a 100 equally spaced points for each dimension. It can be changed by defining it in options$Design

Author(s)

Dario Azzimonti

Examples

```r
if (!requireNamespace("DiceKriging", quietly = TRUE)) {
  stop("DiceKriging needed for this example to work. Please install it.
       call. = FALSE")
}

# Compute the coordinate profile extrema with full optimization on 2d example

# Define the function
g=function(x){
  return(-branin(x))
}

# Define the gradient
gprime = function(x){
  x1 = x[1]*15-5
  x2 = x[2]*15
  f1prime = (15*25)/(4*pi^4)*x1^3 - (15*75)/(2*pi^3)*x1^2 + (80*15)/(pi^2)*x1 - (5*15)/(pi^2)*x2*x1 + 10*15/pi*x2 - 60*15/pi - 10*15*(1 - 1/(8*pi))*sin(x1)
  f2prime = 2*15*(x2-5/(4*pi^2)*x1^2 + 5/pi*x1-6)
  return(c(-f1prime,-f2prime))
}

# set up dimension
coordProf<-(getAllMaxMin(f = g,fprime = gprime,d=2,options = list(multistart=4,heavyReturn=TRUE))
```
# Consider threshold=-10
threshold<- -10
# obtain the points where the profiles take the threshold value
pp_change<-getChangePoints(threshold = threshold, allRes = coordProf)
# evaluate g at a grid and plot the image
x<-seq(0,1,,100)
grid<-expand.grid(x,x)
g_evals<- apply(X = grid,MARGIN = 1,FUN = g)
image(x = x,y = x,z = matrix(g_evals,nrow = 100),col = grey.colors(20))
contour(x=x,y=x,z=matrix(g_evals,nrow = 100), add=TRUE, nlevels = 20)
contour(x=x,y=x,z=matrix(g_evals,nrow = 100), add=TRUE, levels = threshold,col=2)
abline(h = pp_change$neverEx$[2],col="darkgreen",lwd=2)
abline(v = pp_change$neverEx$[1],col="darkgreen",lwd=2)
# Plot the coordinate profiles and a threshold
plotMaxMin(allRes = coordProf,threshold = threshold,changes = TRUE)

---

**getChangePoints**

*Coordinate profiles crossing points*

**Description**

Obtain the points where the coordinate profile extrema functions cross the threshold

**Usage**

```r
getChangePoints(threshold, Design = NULL, allRes)
```

**Arguments**

- `threshold`: if not null plots the level
- `Design`: a d dimensional design corresponding to the points
- `allRes`: list containing the list `res` which contains the computed minima and maxima. The object returned by the function `getAllMaxMin`.

**Value**

returns a list containing two lists with d components where

- `alwaysEx`: each component is a numerical vector indicating the points \( x_i \) where \( \inf_{x ightarrow x_i} f(x) > \) threshold;
- `neverEx`: each component is a numerical vector indicating the points \( x_i \) where \( \sup_{x ightarrow x_i} f(x) < \) threshold.

**Author(s)**

Dario Azzimonti
**getClosePoints**

*Find close points*

**Description**

Obtain points close in one specific dimension

**Usage**

```r
getClosePoints(x, allPts, whichDim)
```

**Arguments**

- `x` one dimensional point
- `allPts` dataframe containing a list of d dimensional points
- `whichDim` integer defining the dimension of `x`

**Value**

the index in `allPts` (row number) of the closest point in `allPts` to `x` along the `whichDim` dimension

**Author(s)**

Dario Azzimonti

**getMax**

*Coordinate profile sup function*

**Description**

Compute coordinate profile sup functions

**Usage**

```r
getMax(x, f, fprime, coord, d, options = NULL)
```

**Arguments**

- `x` one dimensional point where the function is to be evaluated
- `f` function to be optimized (takes a vector `y` of dimension `d` and returns a real number)
- `fprime` derivative of `f` (same format)
- `coord` integer selecting the dimension that is fixed, the other ones are optimized over
- `d` dimension of the input for `f`
getMaxMinMC

options a list containing the options to be passed to optim:

- par: contains the starting point (a point in dimension d-1)
- method: is the string denoting the chosen method for the optimization (see optim for details)
- lower: the lower bounds for the optimization domain (see optim for details)
- upper: the upper bounds for the optimization domain (see optim for details)

Value

a real value corresponding to $\max_{x_1,\ldots,x_{\text{coord}-1},x_{\text{coord}+1},\ldots,x_d} f(x_1,\ldots,x_d)$

Author(s)

Dario Azzimonti

getMaxMinMC Coordinate profile extrema with MC

Description

Compute coordinate profile extrema with MC

Usage

getMaxMinMC(x, f, fprime, coord, d, options = NULL)

Arguments

- x one dimensional point where the function is to be evaluated
- f function to be optimized (takes a vector y of dimension d and returns a real number)
- fprime derivative of f (same format)
- coord integer selecting the dimension that is fixed, the other ones are optimized over
- d dimension of the input for f
- options a list containing the options to be passed to the MC optimizer:
  - par: contains the starting point (a point in dimension d-1)
  - numMCsamples: number of MC samples
  - randstring that chooses the type of randomness in MC: "unif" (uniform in [lower, upper]), "norm" (independent normal with mean 0 and variance 1)
  - lower: the lower bounds for the optimization domain (see optim for details)
  - upper: the upper bounds for the optimization domain (see optim for details)
**getMin**

**Value**

a real value corresponding to \( \max_{x_1, \ldots, x_{\text{coord}-1}, x_{\text{coord}+1}, \ldots, x_d} f(x_1, \ldots, x_d) \)

**Author(s)**

Dario Azzimonti

---

**getMin**  \hspace{1cm}  *Coordinate profile inf function*

**Description**

Compute coordinate profile inf functions

**Usage**

```r
getMin(x, f, fprime, coord, d, options = NULL)
```

**Arguments**

- \( x \)  
  one dimensional point where the function is to be evaluated
- \( f \)  
  function to be optimized (takes a vector \( y \) of dimension \( d \) and returns a real number)
- \( fprime \)  
  derivative of \( f \) (same format)
- \( coord \)  
  integer selecting the dimension that is fixed, the other ones are optimized over
- \( d \)  
  dimension of the input for \( f \)
- \( options \)  
  a list containing the options to be passed to optim:
  - \( \text{par} \): contains the starting point (a point in dimension \( d-1 \))
  - \( \text{method} \): is the string denoting the chosen method for the optimization (see optim for details)
  - \( \text{lower} \): the lower bounds for the optimization domain (see optim for details)
  - \( \text{upper} \): the upper bounds for the optimization domain (see optim for details)

**Value**

a real value corresponding to \( \min_{x_1, \ldots, x_{\text{coord}-1}, x_{\text{coord}+1}, \ldots, x_d} f(x_1, \ldots, x_d) \)

**Author(s)**

Dario Azzimonti
getPointProportion  Obtain proportion of true observations in excursion set

Description

Computes the proportion of observations in the excursion set from true function evaluations, binned by the grid determined with xBins, yBins.

Usage

gpointProportion(pp, xBins, yBins, whichAbove, plt = FALSE)

Arguments

pp  a matrix of dimension nPts x 2 with the true points locations in 2 dimensions.
xBins  numerical vector with the ordered breaks of the grid along the x axis
yBins  numerical vector with the ordered breaks of the grid along the y axis
whichAbove  boolean vector of dimension nPts, selects the points above
plt  if not TRUE plots the grid, the points and the counts for each cell.

Value

a list containing above, the counts of points in excursion, full the counts per cell of all points, freq, the relative frequency.

Author(s)

Dario Azzimonti

getProfileExtrema  Profile extrema with BFGS optimization

Description

Evaluate profile extrema for a set of matrices allPsi with full optimization.

Usage

gprofileExtrema(f, fprime = NULL, d, allPsi, opts = NULL)
**getProfileExtrema**

**Arguments**

- **f**
  - the function to be evaluated
- **fprime**
  - derivative of the function
- **d**
  - dimension of the input domain
- **allPsi**
  - a list containing the matrices Psi (dim pxd) for which to compute the profile extrema
- **opts**
  - a list containing the options for this function and the subfunctions `getProfileSup_optim`, `getProfileInf_optim`. The options only for `getProfileExtrema` are
  - `limits`: an optional list containing `lower` and `upper`, two vectors with the limits of the input space. If NULL then limits=list(upper=rep(1,d),lower=rep(0,d))
  - `discretization`: an optional integer representing the discretization size for the profile computation for each dimension of eta. Pay attention that this leads to a grid of size `discretization^p`.
  - `heavyReturn`: If TRUE returns also all minimizers, default is FALSE.
  - `plts`: If TRUE and p==1 for all Psi in allPsi, plots the profile functions at each Psi, default is FALSE.
  - `verb`: If TRUE, outputs intermediate results, default is FALSE.

**Value**

a list of two data frames (min, max) of the evaluations of $P^*_{sup}psi(f(eta)) = sup_{psix=eta} f(x)$ and $P^*_{inf}psi(f(eta)) = inf_{psix=eta} f(x)$ discretized over 50 equally spaced points for each dimension for each Psi in allPsi. This number can be changed by defining it in `options$discretization`.

**Author(s)**

Dario Azzimonti

**Examples**

# Compute the oblique profile extrema with full optimization on 2d example

# Define the function
testF <- function(x,params,v1=c(1,0),v2=c(0,1)){
  return(sin(crossprod(v1,x)*params[1]+params[2])+cos(crossprod(v2,x)*params[3]+params[4])-1.5)
}
testFprime <- function(x,params,v1=c(1,0),v2=c(0,1)){
  return(matrix(c(params[1]*v1[1]*cos(crossprod(v1,x)*params[1]+params[2])-
               params[3]*v2[1]*sin(crossprod(v2,x)*params[3]+params[4]),
               params[1]*v1[2]*cos(crossprod(v1,x)*params[1]+params[2])-
               params[3]*v2[2]*sin(crossprod(v2,x)*params[3]+params[4])),ncol=1))
}

# Define the main directions of the function
theta=pi/6
pparams<-c(1,0,10,0)
vv1 <- c(cos(theta), sin(theta))
vv2 <- c(cos(theta + pi/2), sin(theta + pi/2))

# Define optimizer friendly function
f <- function(x){
  return(testF(x, pparams, vv1, vv2))
}
fprime <- function(x){
  return(testFprime(x, pparams, vv1, vv2))
}

# Define list of directions where to evaluate the profile extrema
all_Psi <- list(Psi1 = vv1, Psi2 = vv2)

# Evaluate profile extrema along directions of all_Psi
allOblique <- getProfileExtrema(f = f, fprime = fprime, d = 2, allPsi = all_Psi,
                               opts = list(plts = FALSE, discretization = 100, multistart = 8))

# Consider threshold = 0
threshold <- 0

# Plot oblique profile extrema functions
plotMaxMin(allOblique, allOblique$Design, threshold = threshold)

## Since the example is two dimensional we can visualize the regions excluded by the profile extrema
# evaluate the function at a grid for plots
inDes <- seq(0, 1, , 100)
inputs <- expand.grid(inDes, inDes)
outs <- apply(X = inputs, MARGIN = 1, function(x){return(testF(x, pparams, v1 = vv1, v2 = vv2))})

# obtain the points where the profiles take the threshold value
cccObl <- getChangePoints(threshold = threshold, allRes = allOblique, Design = allOblique$Design)

# visualize the functions and the regions excluded
image(inDes, inDes, matrix(outs, ncol = 100), col = grey.colors(20), main = "Example and oblique profiles")
contour(inDes, inDes, matrix(outs, ncol = 100), add = TRUE, nlevels = 20)
contour(inDes, inDes, matrix(outs, ncol = 100), add = TRUE, levels = c(threshold), col = 4, lwd = 1.5)
plotOblique(cccObl$alwaysEx$0[[1]], all_Psi[[1]], col = 3)
plotOblique(cccObl$alwaysEx$0[[2]], all_Psi[[2]], col = 3)
plotOblique(cccObl$neverEx$0[[1]], all_Psi[[1]], col = 2)
plotOblique(cccObl$neverEx$0[[2]], all_Psi[[2]], col = 2)
Description

Compute profile inf function for an arbitrary matrix \( \Psi \) with the L-BFGS-B algorithm of \texttt{optim}. Here the linear equality constraint is eliminated by using the Null space of \( \Psi \).

Usage

\[
\text{getProfileInf\_optim}(\eta, \Psi, f, fprime, d, \text{options} = \text{NULL})
\]

Arguments

- \( \eta \): \( p \) dimensional point where the function is to be evaluated
- \( \Psi \): projection matrix of dimension \( p \times d \)
- \( f \): function to be optimized (takes a vector \( y \) of dimension \( d \) and returns a real number)
- \( fprime \): derivative of \( f \) (same format, returning a \( d \) dimensional vector)
- \( d \): dimension of the input for \( f \)
- \( \text{options} \): a list containing the options to be passed to \texttt{optim}:
  - \( \text{par} \): contains the starting point (a point in dimension \( d \))
  - \( \text{lower} \): the lower bounds for the optimization domain (see \texttt{optim} for details)
  - \( \text{upper} \): the upper bounds for the optimization domain (see \texttt{optim} for details)

Value

A real value corresponding to \( \min_{x \in D_{\Psi}} f(x) \)

Author(s)

Dario Azzimonti

See Also

\texttt{getProfileSup\_optim, plotMaxMin}

---

\texttt{getProfileSup\_optim} \hspace{1cm} Generic profile sup function computation with \texttt{optim}

Description

Compute profile sup function for an arbitrary matrix \( \Psi \) with the L-BFGS-B algorithm of \texttt{optim}.

Usage

\[
\text{getProfileSup\_optim}(\eta, \Psi, f, fprime, d, \text{options} = \text{NULL})
\]
getSegments

Arguments

- **eta**: \( p \) dimensional point where the function is to be evaluated
- **Psi**: projection matrix of dimensions \( p \times d \)
- **f**: function to be optimized (takes a vector \( y \) of dimension \( d \) and returns a real number)
- **fprime**: derivative of \( f \) (same format, returning a \( d \) dimensional vector)
- **d**: dimension of the input for \( f \)
- **options**: a list containing the options to be passed to `optim`:
  - `par`: contains the starting point (a point in dimension \( d-1 \))
  - `lower`: the lower bounds for the optimization domain (see `optim` for details)
  - `upper`: the upper bounds for the optimization domain (see `optim` for details)

Value

A real value corresponding to \( \max_{x \in D_P \Psi} f(x) \)

Author(s)

Dario Azzimonti

See Also

`getProfileInf_optim`, `plotMaxMin`

Description

Auxiliary function for `getChangePoints`

Usage

`getSegments(y)`

Arguments

- **y**: a vector

Value

Plots the sup and inf of the function for each dimension. If threshold is not NULL.

Author(s)

Dario Azzimonti
Description

Computes the gradient of the posterior mean and variance of the kriging model in object at the points newdata.

Usage

gradKm_dnewdata(object, newdata, type, se.compute = TRUE, light.return = FALSE, bias.correct = FALSE)

Arguments

object
  a km object
newdata
  a vector, matrix or data frame containing the points where to perform predictions.
type
  a character corresponding to the type of kriging family ("SK" or "UK").
se.compute
  an optional boolean indicating whether to compute the posterior variance or not. Default is TRUE.
light.return
  an optional boolean indicating whether to return additional variables. Default is FALSE.
bias.correct
  an optional boolean to correct bias in the UK variance. Default is FALSE.

Value

Returns a list containing

- mean: the gradient of the posterior mean at newdata.
- trend: the gradient of the trend at newdata.
- s2: the gradient of the posterior variance at newdata.

Author(s)

Dario Azzimonti
**Description**

The function `grad_mean_Delta_T` computes the gradient for the mean function of the difference process $Z_x - \tilde{Z}_x$ at $x$.

**Usage**

```
grad_mean_Delta_T(x, kmModel, simupoints, T.mat, F.mat)
```

**Arguments**

- `$x$`: a matrix `rxd` containing the $r$ points where the function is to be computed.
- `$kmModel$`: the `km` model of the Gaussian process $Z$.
- `$simupoints$`: the matrix `lxd` containing the pilot points $G$.
- `$T.mat$`: the upper triangular factor of the Choleski decomposition of the covariance matrix of `rbind(kmModel@X,simupoints)`.
- `$F.mat$`: the evaluation of the trend function at `rbind(kmModel@X,simupoints)`, see `model.matrix`.

**Value**

The value of the gradient for the mean function at $x$ for the difference process $Z^\Delta = Z_x - \tilde{Z}_x$.

**Author(s)**

Dario Azzimonti

---

**Description**

The function `grad_var_Delta_T` computes the gradient for the variance function of the difference process $Z_x - \tilde{Z}_x$ at $x$.

**Usage**

```
grad_var_Delta_T(x, kmModel, simupoints, T.mat, F.mat)
```

**Value**

The value of the gradient for the variance function at $x$ for the difference process $Z^\Delta = Z_x - \tilde{Z}_x$. 
**Arguments**

- `x`: a matrix `rxd` containing the `r` points where the function is to be computed.
- `kmModel`: the `km` model of the Gaussian process `Z`.
- `simupoints`: the matrix `lxd` containing the pilot points `G`.
- `T.mat`: the upper triangular factor of the Choleski decomposition of the covariance matrix of `rbind(kmModel@X,simupoints)`
- `F.mat`: the evaluation of the trend function at `rbind(kmModel@X,simupoints)`, see `model.matrix`.

**Value**

- the value of the gradient for the variance function at `x` for the difference process \( Z^\Delta = Z_x - \tilde{Z}_x \).

**Author(s)**

- Dario Azzimonti

---

**kGradSmooth**

*First order approximation*

**Description**

Compute first order approximation of function from evaluations and gradient

**Usage**

```r
kGradSmooth(newPoints, profPoints, profEvals, profGradient)
```

**Arguments**

- `newPoints`: vector of points where to approximate the function
- `profPoints`: locations where the function was evaluated
- `profEvals`: value of the evaluation at `profPoints`
- `profGradient`: value of the gradient at `profPoints`

**Value**

- approximated values of the function at `newPoints`

**Author(s)**

- Dario Azzimonti
The function mean_Delta_T computes the mean function of the difference process \( Z_x - \bar{Z}_x \) at \( x \).

**Usage**

```r
mean_Delta_T(x, kmModel, simupoints, T.mat, F.mat)
```

**Arguments**

- **x**: a matrix \( r \times d \) containing the \( r \) points where the function is to be computed.
- **kmModel**: the \( km \) model of the Gaussian process \( Z \).
- **simupoints**: the matrix \( l \times d \) containing the pilot points \( G \).
- **T.mat**: the upper triangular factor of the Choleski decomposition of the covariance matrix of \( \text{rbind}(\text{kmModel@X, simupoints}) \).
- **F.mat**: the evaluation of the trend function at \( \text{rbind}(\text{kmModel@X, simupoints}) \), see \text{model.matrix}.

**Value**

the value of the mean function at \( x \) for the difference process \( Z^\Delta = Z_x - \bar{Z}_x \).

**Author(s)**

Dario Azzimonti

---

The function obliqueProfiles computes the (oblique) profile extrema functions for the posterior mean of a Gaussian process and its confidence bounds

**Usage**

```r
obliqueProfiles(object, allPsi, threshold, options_full = NULL, options_approx = NULL, uq_computations = FALSE, plot_level = 0, plot_options = NULL, CI_const = NULL, return_level = 1, ...)
```
Arguments

object either a km model or a list containing partial results. If object is a km model then all computations are carried out. If object is a list, then the function carries out all computations to complete the list results.

allPsi a list containing the matrices Psi (dim pxd) for which to compute the profile extrema

threshold the threshold of interest

options_full an optional list of options for getProfileExtrema, see getProfileExtrema for details.

options_approx an optional list of options for approxProfileExtrema, see approxProfileExtrema for details.

uq_computations boolean, if TRUE the uq computations for the profile mean are computed.

plot_level an integer to select the plots to return (0=no plots, 1= basic plots, 2= all plots)

plot_options an optional list of parameters for plots. See setPlotOptions for currently available options.

CI_const an optional vector containing the constants for the CI. If not NULL, then profiles extrema for \( m_n(x) \pm CI_{const[i]} s_n(x, x) \) are computed.

return_level an integer to select the amount of details returned

... additional parameters to be passed to obliqueProf_UQ.

Value

If return_level=1 a list containing

- profMean_full: the results of getProfileExtrema for the posterior mean
- profMean_approx: the results of approxProfileExtrema for the posterior mean
- res_UQ: the results of obliqueProf_UQ for the posterior mean

if return_level=2 the same list as above but also including

- abs_err: the vector of maximum absolute approximation errors for the profile inf / sup on posterior mean for the chosen approximation
- times: a list containing
  - full: computational time for the full computation of profile extrema
  - approx: computational time for the approximate computation of profile extrema

Author(s)

Dario Azzimonti
Examples

if (!requireNamespace("DiceKriging", quietly = TRUE)) {
  stop("DiceKriging needed for this example to work. Please install it.",
       call. = FALSE)
}

# Compute a kriging model from 50 evaluations of the Branin function
# Define the function
f=function(x){
  return(-branin(x))
}

gp_des<-lhs::maximinLHS(20,2)
reals<-apply(gp_des,1,f)
kmModel<-km(design = gp_des,response = reals,covtype = "matern3_2")

threshold=-10

# Compute oblique profiles on the posterior mean
# (for theta=0 it is equal to coordinateProfiles)
options_full<-list(multistart=4,heavyReturn=TRUE,discretization=100)
options_approx<- list(multistart=4,heavyReturn=TRUE,initDesign=NULL,fullDesignSize=100)
theta=pi/4
allPsi = list(Psi1=matrix(c(cos(theta),sin(theta)),ncol=2),
              Psi2=matrix(c(cos(theta+pi/2),sin(theta+pi/2)),ncol=2))

## Not run:
profMeans<-obliqueProfiles(object = kmModel,allPsi = allPsi,threshold = threshold,
                            options_full = options_full,options_approx = options_approx,
                            uq_computations = FALSE,plot_level = 3,plot_options = NULL,
                            CI_const = NULL,return_level = 2)

# Approximate oblique profiles with UQ
plot_options<-list(save=FALSE, titleProf = "Coordinate profiles",
                  title2d = "Posterior mean",qq_fill=TRUE)
options_sims<-list(nsim=150)
obProfUQ<-obliqueProfiles(object=profMeans,threshold=threshold,allPsi = allPsi,
                          options_full=options_full, options_approx=options_approx,
                          uq_computations=TRUE, plot_level=3,plot_options=NULL,
                          CI_const=NULL,return_level=2,options_sims=options_sims)

## End(Not run)

obliqueProf_UQ  Oblique profiles UQ from a kriging model

Description

The function obliqueProf_UQ computes the profile extrema functions for posterior realizations of
a Gaussian process and its confidence bounds.
Usage

```r
obliqueProf_UQ(object, allPsi, threshold, allResMean = NULL,
quantiles_uq = c(0.05, 0.95), options_approx = NULL,
options_full_sims = NULL, options_sims = NULL,
options_bound = NULL, plot_level = 0, plot_options = NULL,
return_level = 1)
```

Arguments

- **object**
  - either a `km` model or a list containing partial results. If `object` is a `km` model, then all computations are carried out. If `object` is a list, then the function carries out all computations to complete the results list.
- **allPsi**
  - a list containing the matrices $\Psi$ (dim $pxd$) for which to compute the profile extrema
- **threshold**
  - the threshold of interest
- **allResMean**
  - a list resulting from `getProfileExtrema` or `approxProfileExtrema` for the profile extrema on the mean. If NULL, the median from the observations is plotted
- **quantiles_uq**
  - a vector containing the quantiles to be computed
- **options_approx**
  - an optional list of options for `approxProfileExtrema`, see `approxProfileExtrema` for details.
- **options_full_sims**
  - an optional list of options for `getProfileExtrema`, see `getProfileExtrema` for details. If NULL, the full computations are not executed. NOTE: this computations might be very expensive!
- **options_sims**
  - an optional list of options for the posterior simulations.
    - **algorithm**: string choice of the algorithm to select the pilot points ("A" or "B");
    - **lower**: $d$ dimensional vector with lower bounds for pilot points, default `rep(0, d)`;
    - **upper**: $d$ dimensional vector with upper bounds for pilot points, default `rep(1, d)`;
    - **batchsize**: number of pilot points, default 120;
    - **optimcontrol**: list containing the options for optimization, see `optim_dist_measure`;
    - **integcontrol**: list containing the options for numerical integration of the criterion, see `optim_dist_measure`;
    - **integration.param**: list containing the integration design, obtained with the function `integration_design`;
    - **nsim**: number of approximate GP simulations, default 300.
- **options_bound**
  - an optional list containing `beta` the confidence level for the approximation and `alpha` the confidence level for the bound. Note that $\alpha > 2*\beta$. If NULL, the bound is not computed.
- **plot_level**
  - an integer to select the plots to return (0=no plots, 1=basic plots, 2=all plots)
- **plot_options**
  - an optional list of parameters for plots. See `setPlotOptions` for currently available options.
- **return_level**
  - an integer to select the amount of details returned
obliqueProf_UQ

Value

If return_level=1 a list containing

• profSups: an array dxfullDesignSizexnsims containing the profile sup for each coordinate for each realization.
• profInfs: an array dxfullDesignSizexnsims containing the profile inf for each coordinate for each realization.
• prof_quantiles_approx: a list containing the quantiles (levels set by quantiles_uq) of the profile extrema functions.

if return_level=2 the same list as above but also including more: a list containing

• times: a list containing
  – tSpts: computational time for selecting pilot points.
  – tApprox1ord: vector containing the computational time required for profile extrema computation for each realization
• simuls: a matrix containing the value of the field simulated at the pilot points
• sPts: the pilot points

Author(s)

Dario Azzimonti

Examples

if (!requireNamespace("DiceKriging", quietly = TRUE)) {
  stop("DiceKriging needed for this example to work. Please install it.", call. = FALSE)
}

# Compute a kriging model from 50 evaluations of the Branin function
# Define the function
g<-function(x){
  return(-branin(x))
}

gp_des<-lhs::maximinLHS(20,2)
reals<-apply(gp_des,1,g)
kmModel<-km(design = gp_des,response = reals,covtype = "matern3_2")

threshold<-10
d<-2

# Compute oblique profiles UQ starting from GP model
# define simulation options
options_sims<-list(algorithm="B", lower=rep(0,d), upper=rep(1,d),
  batchsize=80, optimcontrol = list(method="genoud",pop.size=100,print.level=0),
  integcontrol = list(distrib="sobol",n.points=1000), nsim=150)

# define approximation options
options_approx<- list(multistart=4,heavyReturn=TRUE,
  initDesign=NULL,FullDesignSize=100,
  smoother=NULL)
# define plot options
options_plots<-list(save=FALSE, titleProf = "Coordinate profiles",
                    title2d = "Posterior mean",qq_fill=TRUE)

# Define the oblique directions
# (for theta=0 it is equal to coordinateProfiles)
theta=pi/4
allPsi = list(Psi1=matrix(c(cos(theta),sin(theta)),ncol=2),
              Psi2=matrix(c(cos(theta+pi/2),sin(theta+pi/2)),ncol=2))

## Not run:
# here we reduce the number of simulations to speed up the example
# a higher number should be used
options_sims$nsim <- 50

# profile UQ on approximate oblique profiles
oProfiles_UQ<-obliqueProf_UQ(object = kmModel,threshold = threshold,allPsi=allPsi,
                              allResMean = NULL,quantiles_uq = c(0.05,0.95),
                              options_approx = options_approx, options_full_sims = NULL,
                              options_sims = options_sims,options_bound = NULL,
                              plot_level = 3, plot_options = options_plots,return_level = 3)

# profile UQ on full optim oblique profiles
options_full_sims<-list(multistart=4,heavyReturn=TRUE)
oProfiles_UQ_full<- obliqueProf_UQ(object = oProfiles_UQ,threshold = threshold,allPsi=allPsi,
                                   allResMean = NULL,quantiles_uq = c(0.05,0.95),
                                   options_approx = options_approx, options_full_sims = options_full_sims,
                                   options_sims = options_sims,options_bound = NULL,
                                   plot_level = 3, plot_options = options_plots,return_level = 3)

# profile UQ on full optim oblique profiles with bound
oProfiles_UQ_full_bound<-obliqueProf_UQ(object = oProfiles_UQ_full,threshold = threshold,allPsi=allPsi,
                                         allResMean = NULL,quantiles_uq = c(0.05,0.95),
                                         options_approx = options_approx, options_full_sims = options_full_sims,
                                         options_sims = options_sims,options_bound = list(beta=0.024,alpha=0.05),
                                         plot_level = 3, plot_options = options_plots,
                                         return_level = 3)

## End(Not run)

---

**plotBivariateProfiles**  
Plot bivariate profiles

**Description**

Plot bivariate profiles, for dimension up to 6.
plotMaxMin

**Description**

Plot coordinate profiles, for dimension up to 6.

**Usage**

```r
plotMaxMin(allRes, Design = NULL, threshold = NULL, changes = FALSE, trueEvals = NULL, ...)
```

**Arguments**

- `allRes` list containing the list `res` which contains the computed minima and maxima. The object returned by the function `getAllMaxMin`.
- `Design` a d dimensional design corresponding to the points
- `threshold` if not NULL plots the level as a contour.

**Author(s)**

Dario Azzimonti
**plotOblique**

- **changes**
  - boolean, if not FALSE plots the points where profile extrema take values near the threshold.
- **trueEvals**
  - if not NULL adds to each plot the data points and the observed value
- **...**
  - additional parameters to be passed to the plot function

**Value**

plots the sup and inf of the function for each dimension. If threshold is not NULL

**Author(s)**

Dario Azzimonti

---

**plotOblique**

**Description**

Auxiliary function for 2d plotting of excluded regions

**Usage**

plotOblique(changePoints, direction, ...)

**Arguments**

- **changePoints**
  - Numerical vector with the change points (usually if cp=getChangePoints(...), then this is cc$alwaysEx[[1]][[1]] for example)
- **direction**
  - The Psi vector used for the direction
- **...**
  - parameters to be passed to abline

**Value**

adds to the current plot the lines \( x \) s.t. \( \text{direction}^\top x = \text{changePoints}[i] \) for all \( i \)

**Author(s)**

Dario Azzimonti
plotOneBivProfile  
*Plot bivariate profiles*

**Description**

Plots the bivariate profiles stored in `allRes` for each `Psi` in `allPsi`.

**Usage**

```r
plotOneBivProfile(allRes, allPsi, Design = NULL, threshold = NULL,
                   trueEvals = NULL, main_addendum = "", ...)```

**Arguments**

- **allRes**: list containing the list `res` which contains the computed minima and maxima. The object returned by the function `getProfileExtrema`.
- **allPsi**: a list containing the matrices `Psi` (dim `2xd`) for which to compute the profile extrema.
- **Design**: a matrix of dimension `(2d)xnumPsi` encoding the first `(Design[1:d,])` and the second `(Design[(d+1):(2*d),])` axis values.
- **threshold**: if not NULL plots the level as a contour.
- **trueEvals**: if not NULL adds to each plot the data points and the observed value.
- **main_addendum**: additional string to add to image title. Default is empty string.
- **...** additional parameters to be passed to the plot function.

**Value**

plots the 2d maps of the profile sup and inf in `allRes` for each `Psi` in `allPsi`. If threshold is not NULL also contours the threshold level.

**Author(s)**

Dario Azzimonti

**See Also**

`plotBivariateProfiles`
Description

Function to plot the univariate profile extrema functions with UQ

Usage

plot_univariate_profiles_UQ(objectUQ, plot_options, nsims, threshold, 
nameFile = "prof_UQ", quantiles_uq = c(0.05, 0.95), 
profMean = NULL, typeProf = "approx")

Arguments

objectUQ an object returned by coordProf_UQ or the object saved in obj$res_UQ, if obj is the object returned by coordinateProfiles.
plot_options a list containing the same elements as the one passed to coordinateProfiles
nsims number of simulations
threshold threshold of interest
nameFile the central name of the plot file
quantiles_uq a vector containing the quantiles to be computed
profMean the profile coordinate extrema functions for the mean. It is saved in obj$profMean_full or obj$profMean_approx if obj is an object returned by coordinateProfiles.
typeProf a string to choose with type of profile extrema for simulations to plot
  • "approx" plots only the approximate profile extrema for simulations
  • "full" plots only the full profile extrema for simulations
  • "both" plots both the approximate and full profile extrema for simulations

Value

Plots either to the default graphical device or to pdf (according to the options passed in plot_options)
Description

Computation and plots of profile extrema functions. The package main functions are:

**Computation:**
- `coordinateProfiles`: Given a km objects computes the coordinate profile extrema function for the posterior mean and its quantiles.
- `coordProf_UQ`: UQ part of `coordinateProfiles`.
- `obliqueProfiles`: Given a km objects computes the profile extrema functions for a generic list of matrices Psi for the posterior mean and its quantiles.
- `obliqueProf_UQ`: The UQ part of `obliqueProfiles`.
- `getAllMaxMin`: computes coordinate profile extrema with full optimization for a deterministic function.
- `approxMaxMin`: approximates coordinate profile extrema for a deterministic function.
- `getProfileExtrema`: computes profile extrema given a list of matrices Psi for a deterministic function.
- `approxProfileExtrema`: approximates profile extrema given a list of matrices Psi for a deterministic function.

**Plotting:**
- `plot_univariate_profiles_UQ`: plots for the results of `coordProf_UQ` or `obliqueProf_UQ`. Note that this function only works for univariate profiles.
- `plotBivariateProfiles`: plots the bivariate maps results of a call to `obliqueProfiles` with a two dimensional projection matrix Psi.
- `plotMaxMin`: simple plotting function for univariate profile extrema.
- `plotOneBivProfile`: simple plotting function for bivariate profile extrema.

Details

Package: profExtrema
Type: Package
Version: 0.2.1
Date: 2020-03-20

Note

This work was supported in part the Hasler Foundation, grant number 16065 and by the Swiss National Science Foundation, grant number 167199. The author warmly thanks David Ginsbourger, Jérémy Rohmer and Déborah Idier for fruitful discussions and accurate, thought provoking suggestions.

Author(s)

Dario Azzimonti (dario.azzimonti@gmail.com).
References


---

**prof_mean_var_Delta**  
Profile extrema for the mean and variance functions of difference process

### Description

The function `prof_mean_var_Delta` computes the profile extrema functions for the mean and variance functions of the difference process $Z_x - \tilde{Z}_x$ at $x$.

### Usage

```r
prof_mean_var_Delta(kmModel, simupoints, allPsi = NULL, 
options_full_sims = NULL, options_approx = NULL, F.mat = NULL, 
T.mat = NULL)
```

### Arguments

- **kmModel**: the km model of the Gaussian process $Z$.
- **simupoints**: the matrix $l \times d$ containing the pilot points $G$.
- **allPsi**: optional list of matrices (dim $p \times d$) for which to compute the profile extrema. If NULL coordinate profiles are computed.
setPlotOptions

setPlotOptions(plot_options = NULL, d, num_T, kmModel = NULL)

Arguments

- **plot_options** the list of plot options to set-up
- **d** number of coordinates
- **num_T** number of thresholds of interest
- **kmModel** a km model, used to obtain the coordinates names.

Value

the properly set-up list containing the following fields

- **save**: boolean, if TRUE saves the plots in folderPlots
- **folderPlots**: a string containing the destination folder for plots, if save==TRUE default is ./
• ylim: a matrix coordx2 containing the ylim for each coordinate, if NULL in plot_options this is left NULL and automatically set at the plot time.

• titleProf: a string containing the title for the coordinate profile plots, default is "Coordinate profiles"

• title2d: a string containing the title for the 2d plots (if the input is 2d), default is "Posterior mean"

• design: a dxr matrix where d is the input dimension and r is the size of the discretization for plots at each dimension

• coord_names: a d-vector of characters naming the dimensions. If NULL and kmModel not NULL then it is the names of kmModel@X otherwise x_1,...,x_d

• id_save: a string to be added to the plot file names, useful for serial computations on HPC, left as in plot_options.

• qq_fill: if TRUE it fills the region between the first 2 quantiles in quantiles_uq and between the upper and lower bound in objectUQ$bound$bound, if NULL, it is set as FALSE.

• bound_cols: a vector of two strings containing the names of the colors for upper and lower bound plots.

• qq_fill_colors: a list containing the colors for qq_fill: approx for 2 quantiles, bound_min for bounds on the profile inf, bound_max for profile sup. Initialized only if qq_fill==TRUE.

• col_CCPthresh_nev: Color palette of dimension num_T for the colors of the vertical lines delimiting the intersections between the profiles sup and the thresholds

• col_CCPthresh_alw: Color palette of dimension num_T for the colors of the vertical lines delimiting the intersections between the profiles inf and the thresholds

• col_thresh: Color palette of dimension num_T for the colors of the thresholds

• fun_evals: integer denoting the level of plot for the true evaluations.
  – 0: default, no plots for true evaluations;
  – 1: plot the true evaluations as points in 2d plots, no true evaluation plots in 1d;
  – 2: plot true evaluations, in 2d with different color for values above threshold;
  – 3: plot true evaluations, in 2d plots in color, with background of the image colored as proportion of points inside excursion;

if all the fields are already filled then returns plot_options

Author(s)

Dario Azzimonti
var_Delta_T

Variance function of difference process

Description

The function var_Delta_T computes the gradient for the variance function of the difference process \( Z_x - \tilde{Z}_x \) at \( x \).

Usage

var_Delta_T(x, kmModel, simupoints, T.mat, F.mat)

Arguments

- \( x \): a matrix \( r \times d \) containing the \( r \) points where the function is to be computed.
- kmModel: the km model of the Gaussian process \( Z \).
- simupoints: the matrix \( l \times d \) containing the pilot points \( G \).
- T.mat: the upper triangular factor of the Choleski decomposition of the covariance matrix of \( \text{rbind}(\text{kmModel}@X, \text{simupoints}) \).
- F.mat: the evaluation of the trend function at \( \text{rbind}(\text{kmModel}@X, \text{simupoints}) \), see model.matrix.

Value

the value of the variance function at \( x \) for the difference process \( Z^\Delta = Z_x - \tilde{Z}_x \).

Author(s)

Dario Azzimonti
Index

* datasets
  coastal_flooding, 9
approxMaxMin, 2, 7, 12, 14, 40, 42
approxProfileExtrema, 4, 7, 31, 33, 40, 42
bound_profiles, 7
cleanProfileResults, 8
coastal_flooding, 9
coordinateProfiles, 7, 12, 39, 40, 42
coordProf_UQ, 7, 12, 13, 39, 40, 42
getAllMaxMin, 7, 12, 14, 16, 40, 42
getChangePoints, 18
getClosePoints, 19
getMax, 19
getMaxMinMC, 20
getMin, 21
getPointProportion, 22
getProfileExtrema, 5, 7, 22, 31, 33, 40
getProfileInf_optim, 5, 23, 24, 26
getProfileSup_optim, 5, 23, 25, 25
getSegments, 26
grad_mean_Delta_T, 28
grad_var_Delta_T, 44
integation_design, 14, 33
kGradSmooth, 29
km, 12, 14, 27–31, 33, 40–42, 44
mean_Delta_T, 30
model.matrix, 28–30, 42, 44
obliqueProf_UQ, 31, 32, 40, 42
obliqueProfiles, 30, 40, 42
optim, 25
optim_dist_measure, 14, 33
plot_univariate_profiles_UQ, 39, 40, 42
plotBivariateProfiles, 35, 40, 42
plotMaxMin, 25, 26, 36, 40
plotOblique, 37
plotOneBivProfile, 38, 40
prof.mean.var.Delta, 7, 41
profExtrema, 40
profExtrema-package (profExtrema), 40
setPlotOptions, 12, 15, 31, 33, 42
var.Delta.T, 44