Package 'OptimaRegion'

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Type Package

Title Confidence Regions for Optima

Version 0.1.0

Author Enrique del Castillo, John Hunt, and James Rapkin

Maintainer Enrique del Castillo <exd13@psu.edu>

Depends R (>= 3.2.3)

Imports fields,rsm,nloptr,DepthProc

Description Computes confidence regions on the location of response surface optima.

License GPL (>= 2)

LazyData TRUE

RoxygenNote 5.0.1

NeedsCompilation no

R topics documented:

`Drug` *Mixture-amount experiment*

Description

A pharmaceutical mixture-amount experiment in two components

Usage

```
data("Drug")
```

Format

A data frame with 360 observations on the following 3 variables.

`'Component_1'` Component 1 amount (mg)

`'Component_2'` Component 2 amount (mg)

`Percent` Percent of cells killed (response)

Examples

```
## Not run:
plot(Drug[,1:2])

## End(Not run)
```

`OptRegionQuad` *Computes Confidence Regions of Optima of Quadratic Polynomial Models*

Description

Computes an displays the confidence region on the location of the optima of a quadratic response surface in 2 factors using bootstrapping.

Usage

```
OptRegionQuad(X, y, nosim=200, alpha=0.05, LB, UB,
triangularRegion=FALSE, vertex1=NULL, vertex2=NULL,
maximization=TRUE,
xlab="Protein eaten, mg",
ylab="Carbohydrates eaten, mg",
outputPDFFile="CRplot.pdf")
```

Arguments

`X`	nx2 matrix with the values of the 2 regressors (experimental factors) in the n observations
`y`	nx1 vector of response value observations
`nosim`	number of simulations (default=200)
`alpha`	confidence level (0<alpha<1; default=0.05)
`LB,UB`	2x1 vectors of lower and upper bounds for search region where optima may lie
`triangularRegion`	logical: if TRUE it will constrain the optimum points to lie inside a triangle defined by the coordinates (0,0), and those in "vertex1", and "vertex2", see below (in addition to being constrained to lie inside the region defined by LB and UB). NOTE: use TRUE when the treatments form a triangular experimental region in shape. If FALSE, maxima will only be constrained to lie inside the rectangular region defined by LB and UB. Default is FALSE.

`vertex1,vertex2`
: 2x1 vectors with coordinates defining two of the 3 vertices of a triangular region. Must be provided if triangularRegion is TRUE (NOTE: vertices numbered clockwise, vertex0=c(0,0) always)

`maximization`
: logical: if TRUE (default) it maximizes it FALSE it minimizes

`xlab`
: text label for x axis in confidence region plot (default: "Protein eaten, mg")

`ylab`
: text label for y axis in confidence region plot (default: "Carbohydrates eaten, mg")

`outputPDFFile`
: name of the PDF file where the CR plot is saved (default: "CRplot.pdf")

Details

Computes and displays an approximated 100*(1-alpha) percent confidence region (CR) for the linear-constrained maximum of a quadratic polynomial regression model in 2 controllable factors. Grey region on output plot is the approximate CR. The CR is computed as the convex hull of the coordinates of the optima found from bootstrapping nosim quadratic polynomial regressions to the data (therefore, it is an approximate CR). The mean value of the optimum is shown as a red point, and a smoothed contour plot of the X,y data obtained via thin plate splines is shown as well.

Usage assuming all default options:

out<-OptRegionQuad(X=X,y=y,LB=LB,UB=UB)

Value

`meanPoint`
: a 2x1 vector with the coordinates of the mean optimum point

`xin`
: an mx2 matrix with the x,y coordinates of all simulated #points that belong to the confidence region (dim(m) is (1-alpha)*nosim)

Note

Upon completion, a PDF file containing the CR plot with name as set in ouputPDFFile is created.

Author(s)

Enrique del Castillo <exd13@psu.edu>, John Hunt <J.Hunt@exeter.ac.uk> and James Rapkin <jr297@exeter.ac.uk>

References

Del Castillo, E., Hunt, J., and Rapkin, J. , "Data-depth bootstrapped confidence regions for the optima of parametric and nonparametric response surfaces".

Examples

```
## Not run:
## Example 1: randomly generated 2-variable response surface data

X<-cbind(runif(100,-2,2),runif(100,-2,2))

y<-as.matrix(72-11.78*X[,1]+0.74*X[,2]-7.25*X[,1]^2-7.55*X[,2]^2-4.85*X[,1]*X[,2]+
rnorm(100,0,8))

## Find a 95 percent confidence region for the maximum of a quadratic polynomial
fitted to these data
```

```
out<-OptRegionQuad(X=X,y=y,nosim=200,LB=c(-2,-2),UB=c(2,2), xlab="X1",ylab="X2",
outputPDFFile="CR_plot.pdf")

## Example 2: a mixture-amount experiment in two components (Drug dataset) with
non-normal data. Note triangular experimental region. Resulting 95p confidence
region is pushed against the constraint and results in a "thin line"

out<-OptRegionQuad(X=Drug[,1:2],y=Drug[,3],nosim=500,LB=c(0,0),UB=c(0.08,11),
 xlab="Component 1 (mg.)",ylab="Component 2 (mg.)",triangularRegion = TRUE,
 vertex1 = c(0.02,11),vertex2 = c(0.08,1.8),outputPDFFile="Mixture_plot.pdf")

## End(Not run)
```

OptRegionTps *Computes Confidence Regions of Optima of Thin Plate Spline Models*

Description

Computes and displays the confidence region on the location of the optima of a thin plate spline surface in 2 factors using bootstrapping.

Usage

```
OptRegionTps(X, y, lambda=0.04, nosim=1000, alpha=0.05, LB, UB,
triangularRegion=FALSE, vertex1=NULL, vertex2=NULL, maximization=TRUE,
xlab="Protein eaten, mg",
ylab="Carbohydrate eaten, mg",
outputPDFFile="CRplot.pdf",outputOptimaFile="Optima.txt")
```

Arguments

X	nx2 matrix with the values of the 2 regressors (experimental factors) in the n observations
y	nx1 vector of response value observations
lambda	penalization parameter (larger values implies more smoothing). Default is 0.04
nosim	number of simulations (default=1000)
alpha	confidence level (0<alpha<1; default=0.05)
LB,UB	2x1 vectors of lower and upper bounds for search region where optima may lie
triangularRegion	logical: if TRUE it will constrain the optimum points to lie inside a triangle defined by the coordinates (0,0), and those in "vertex1", and "vertex2", see below (in addition to being constrained to lie inside the region defined by LB and UB). NOTE: use TRUE when the treatments form a triangular experimental region in shape. If FALSE, maxima will only be constrained to lie inside the rectangular region defined by LB and UB. Default is FALSE.
vertex1,vertex2	2x1 vectors with coordinates defining two of the 3 vertices of a triangular region. Must be provided if triangularRegion is TRUE (NOTE: vertices numbered clockwise, vertex0=c(0,0) always)

maximization	logical: if TRUE (default) it maximizes it FALSE it minimizes
xlab	text label for x axis in confidence region plot (default: "Protein eaten, mg")
ylab	text label for y axis in confidence region plot (default: "Carbohydrates eaten, mg")
outputPDFFile	name of the PDF file where the CR plot is saved (default: "CRplot.pdf")
outputOptimaFile	name of the text file containing the coordinates of all the optima found (same information as in output vector xin, see below)

Details

This program approximates the confidence region (CR) of the location of the optimum of a Thin Plate Spline (TPS) in 2 regressors x constrained inside a rectangular region defined by LB and UB. If triangularRegion=TRUE it will also contrain the optimum to lie inside the experimental region assumed to be well approximated by a triangle. The CR is generated pointwise by bootstrapping the residuals of a TPS fit to the given (X,y) data, refitting Tps models, and solving the corresponding constrained maximization (or minimization) problems. The confidence region is approximated by the convex hull of all the solutions (x1*,x2*) found.

Usage assuming all default options:

out<-OptRegionTps(X=X,y=y,LB=LB,UB=UB)

Value

meanPoint	a 2x1 vector with the coordinates of the mean optimum point
xin	an mx2 matrix with the x,y coordinates of all simulated #points that belong to the confidence region (dim(m) is (1-alpha)*nosim)

Note

Upon completion, a PDF file containing the CR plot with name as set in ouputPDFFile is created. A text file named as set in outputOptimaFile with all xin values is created too.

Author(s)

Enrique del Castillo, <exd13@psu.edu>

References

Del Castillo, E., Hunt, J., and Rapkin, J. , "Data-depth bootstrapped confidence regions for the optima of parametric and nonparametric response surfaces".

Examples

```
## Not run:
## Example 1: randomly generated 2-variable response surface data

X<-cbind(runif(100,-2,2),runif(100,-2,2))

y<-as.matrix(72-11.78*X[,1]+0.74*X[,2]-7.25*X[,1]^2-7.55*X[,2]^2-4.85*X[,1]*X[,2]+
rnorm(100,0,8))

## Find a 95 percent confidence region for the maximum of a Thin Plate Spline
model fitted to these data
```

```
out<-OptRegionTps(X=X,y=y,nosim=200,LB=c(-2,-2),UB=c(2,2), xlab="X1",ylab="X2",
outputPDFFile="CR_plot.pdf")

## Example 2: a mixture-amount experiment in two components (Drug dataset) with
non-normal data. Note triangular experimental region. Resulting 95p confidence
region of the maxima of a TPS model has area > 0. Contrast with region for
quadratic polynomial model. Note: 500 iterations may take a couple of minutes.

out<-OptRegionTps(X=Drug[,1:2],y=Drug[,3],nosim=500,lambda=0.05,LB=c(0,0),UB=
 c(0.08,11), xlab="Component 1 (mg.)",ylab="Component 2 (mg.)",triangularRegion
 = TRUE,vertex1 = c(0.02,11),vertex2 = c(0.08,1.8),outputPDFFile=
 "Mixture_plot.pdf")

## End(Not run)
```

`plotConvexHull` *Computes and displays the convex hull of a set of 2-dimensional points*

Description

Given a vector of 2-dimensional coordinates, computes and displays the convex hull formed by these points.

Usage

```
plotConvexHull(xin, LB, UB, xlab, ylab)
```

Arguments

`xin`	n x 2 vector of coordinate points
`LB`	2x1 vector of lower bounds for the x,y region where the convex hull is to be plot. Required.
`UB`	2x1 vector of lower bounds for the x,y region where the convex hull is to be plot. Required.
`xlab`	Label for x axis.
`ylab`	Label for y axis.

Value

An integer vector giving the indices of the unique points lying on the convex hull, in clockwise order. (The first will be returned for duplicate points.). Same as returned by chull(xin).

Note

Function also plots the convex hull upon return.

Author(s)

E. del Castillo

Examples

```
## Not run:
## Generate some random 2-dimensional point set

X<-cbind(runif(100,-2,2),runif(100,-2,2))

## Compute and plot convex hull

plotConvexHull(xin=X, LB=c(-4,-4), UB=c(4,4), xlab=X, ylab=Y)

## End(Not run)
```

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