Package ‘scpropreg’

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Type Package

Title Simplicially Constrained Regression Models for Proportions

Version 1.0

Date 2025-11-16

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Depends R (>= 4.0)

Imports quadprog, Rfast, Rfast2

Description Simplicially constrained regression models for proportions in both sides. The constraint is always that the betas are non-negative and sum to 1. References: Iverson S.J.., Field C., Bowen W.D. and Blanchard W. (2004) ``Quantitative Fatty Acid Signature Analysis: A New Method of Estimating Predator Diets''. Ecological Monographs, 74(2): 211-235. <doi:10.1890/02-4105>.

License GPL (>= 2)

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Contents

`scpropreg-package` *Simplicially Constrained Regression Models for Proportions*

Description

Simplicially Constrained Regression Models for Proportions. The constraint is always that the betas are non-negative and sum to 1.

Details

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Maintainers

Michail Tsagris <mtsagris@uoc.gr>.

Author(s)

Michail Tsagris `<mtsagris@uoc.gr>`

References

Iverson Sara J., Field Chris, Bowen W. Don and Blanchard Wade (2004) Quantitative Fatty Acid Signature Analysis: A New Method of Estimating Predator Diets. Ecological Monographs, 74(2): 211-235.

`Positive and unit sum constrained least squares`
Positive and unit sum constrained least squares

Description

Positive and unit sum constrained least squares.

Usage

```
pcls(y, x)
mpcls(y, x)
```

Arguments

`y`	The response variable. For the pcls() a numerical vector with observations, but for the mpcls() a numerical matrix.
`x`	A matrix with independent variables, the design matrix.

Details

The constraint is that all beta coefficients are positive and sum to 1. That is $min \sum_{i=1}^n (y_i - \boldsymbol{x}_i \top \boldsymbol{\beta})^2$ such that $0 \leq \beta_j \leq 1$ and $\sum_{j=1}^d \beta_j = 1$. The pcls() function performs a single regression model, whereas the mpcls() function performs a regression for each column of y. Each regression is independent of the others.

Value

A list including:

`coefficients`	A numerical matrix with the positively constrained beta coefficients.
`value`	A numerical vector with the mean squared error.

Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <`mtsagris@uoc.gr`>.

See Also

`kld`, `mkld`

Examples

```
x <- matrix(runif(30 * 8), ncol = 30)
x <- t( x / rowSums(x) )
y <- runif(30)
y <- y / sum(y)
pcls(y, x)
```

`QFASA diet estimates for many predators using various distances`

QFASA diet estimates for many predators using various distances

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Description

QFASA diet estimates for many predators using various distances.

Usage

```
mkld(Y, x, tol = 1e-8, maxit = 50000, alpha = 0.1)
mait(Y, x, tol = 1e-8, maxit = 50000, alpha = 0.01)
mlsq(Y, x, tol = 1e-8, maxit = 50000, alpha = 0.01)
mlr(Y, x, tol = 1e-8, maxit = 100)
```

Arguments

`Y`	The response variable, a matrix with values between 0 and 1 that sum to 1. For some functions, zero values are allowed. Every column corresponds to the food composition of a predator. The column-wise sums are equal to 1.
`x`	A matrix with independent variables, values between 0 and 1. Each column contains a prey's diet. The column-wise sums are equal to 1.
`tol`	The tolerance value to terminate the algorithm.
`maxit`	The maximum iterations allowed.
`alpha`	The step-size parameter of the fixed points iteration algorithm. This is similar to the η parameter in the gradient descent algorithm.

Details

The function estimates the betas that minimize a distance. The fitted values are linear constraints of the observed xs. The constraint is that all beta coefficients are positive and sum to 1. That is $\hat{y}_i = \sum_{j=1} \boldsymbol{x}_{ij}\beta_j$ such that $0 \leq \beta_j \leq 1$ and $\sum_{j=1}^d \beta_j = 1$.

Value

A list including:

`coefficients`	A numerical matrix with the positively constrained beta coefficients.
`value`	A numerical vector with the value of the objective function.
`iters`	The number of iterations required until termination of the algorithm.

Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <`mtsagris@uoc.gr`>.

References

Iverson Sara J., Field Chris, Bowen W. Don and Blanchard Wade (2004) Quantitative Fatty Acid Signature Analysis: A New Method of Estimating Predator Diets. Ecological Monographs, 74(2): 211-235.

See Also

`kld`, `mpcls`

Examples

```
x <- matrix(runif(30 * 6), ncol = 30)
x <- t( x / rowSums(x) )
Y <- matrix(runif(30 * 10), ncol = 30)
Y <- t( Y / rowSums(Y) )
mkld(Y, x)
```

`QFASA diet estimates using various distances`

QFASA diet estimates using various distances

Description

QFASA diet estimates using various distances.

Usage

```
kld(y, x, tol = 1e-8, maxit = 50000, alpha = 0.1)
ait(y, x, tol = 1e-8, maxit = 50000, alpha = 0.01)
lsq(y, x, tol = 1e-8, maxit = 50000, alpha = 0.01)
jsd(y, x, tol = 1e-8, maxit = 300000, alpha = 0.01)
lr(y, x, tol = 1e-8, maxit = 100)
```

Arguments

`y`	The response variable. The predator's food composition. A vector with values between 0 and 1 that sum to 1. For some functions, zero values are allowed.
`x`	A matrix with independent variables, values between 0 and 1. Each column contains a prey's diet. The column-wise sums are equal to 1.
`tol`	The tolerance value to terminate the algorithm.
`maxit`	The maximum iterations allowed.
`alpha`	The step-size parameter of the fixed points iteration algorithm. This is similar to the η parameter in the gradient descent algorithm.

Details

The function estimates the betas that minimize a distance. The fitted values are linear constraints of the observed xs. The constraint is that all beta coefficients are positive and sum to 1. That is $\hat{y}_i = \sum_{j=1} \boldsymbol{x}_{ij}\beta_j$ such that $0 \leq \beta_j \leq 1$ and $\sum_{j=1}^d \beta_j = 1$.

Value

A list including:

`coefficients`	A numerical matrix with the positively constrained beta coefficients.
`value`	A numerical vector with the value of the objective function.
`iters`	The number of iterations required until termination of the algorithm.

Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <`mtsagris@uoc.gr`>.

References

Iverson Sara J., Field Chris, Bowen W. Don and Blanchard Wade (2004) Quantitative Fatty Acid Signature Analysis: A New Method of Estimating Predator Diets. Ecological Monographs, 74(2): 211-235.

See Also

`mkld`, `pcls`

Examples

```
x <- matrix(runif(30 * 8), ncol = 30)
x <- t( x / rowSums(x) )
y <- runif(30)
y <- y / sum(y)
kld(y, x)
ait(y, x)
lsq(y, x)
lr(y, x)
```

Index