Package ‘o2plsda’

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Type Package

Title Multiomics Data Integration

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Description Provides functions to do 'O2PLS-DA' analysis for multiple omics data integration. The algorithm came from ``O2-PLS, a two-block (X±Y) latent variable regression (LVR) method with an integral OSC filter'' which published by Johan Trygg and Svante Wold at 2003 <doi:10.1002/cem.775>. 'O2PLS' is a bidirectional multivariate regression method that aims to separate the covariance between two data sets (it was recently extended to multiple data sets) (Löfstedt and Trygg, 2011 <doi:10.1002/cem.1388>; Löfstedt et al., 2012 <doi:10.1016/j.aca.2013.06.026>) from the systematic sources of variance being specific for each data set separately.

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Imports Rcpp (>= 1.0.7), dplyr, magrittr, parallel, ggplot2, ggrepel, methods, stats

Depends

Encoding UTF-8

Suggests knitr, markdown, rmarkdown

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LinkingTo Rcpp, RcppArmadillo, RcppEigen

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NeedsCompilation yes

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loadings

Extract the loadings from an O2PLS fit

Description

This function extracts loading parameters from an O2PLS fit
This function extracts loading parameters from an O2PLS fit

Usage

loadings(x, ...)

## S3 method for class 'o2pls'
loadings(x, loading = c("Xjoint", "Yjoint", "Xorth", "Yorth"), ...)

Arguments

  x               Object of class o2pls
  ...             For consistency
  loading         the loadings for one of "Xjoint", "Yjoint", "Xorth", "Yorth"

Value

Loading matrix
Loading matrix
loadings.o2plsda

extract the loading value from the O2PLSDA analysis

Description
extract the loading value from the O2PLSDA analysis

Usage
## S3 method for class 'o2plsda'
loadings(x, loading = "Xloading", ...)

Arguments
x Object of class o2plsda
loading the loadings for one of "Xjoint", "Yjoint", "Xorth", "Yorth"
... For consistency

loadings.plsda

extract the loading value from the PLSDA analysis

Description
extract the loading value from the PLSDA analysis

Usage
## S3 method for class 'plsda'
loadings(x, ...)

Arguments
x Object of class plsda
... For consistency
Cross validation for O2PLS

Usage

```r
o2cv(
  X, 
  Y, 
  nc, 
  nx, 
  ny, 
  group = NULL, 
  nr_folds = 5, 
  ncores = 1, 
  scale = FALSE, 
  center = FALSE
)
```

Arguments

- **X**: a Numeric matrix (input)
- **Y**: a Numeric matrix (input)
- **nc**: Integer. Number of joint PLS components.
- **nx**: Integer. Number of orthogonal components in X
- **ny**: Integer. Number of orthogonal components in Y
- **group**: a vector to indicate the group for Y
- **nr_folds**: Integer to indicate the folds for cross validation
- **ncores**: Integer. Number of CPUs to use for cross validation
- **scale**: boolean values determining if data should be scaled or not
- **center**: boolean values determining if data should be centered or not

Value

a data frame with the Q and RMSE values

Author(s)

Kai Guo
Examples

```r
set.seed(123)
X = matrix(rnorm(500),50,10)
Y = matrix(rnorm(500),50,10)
X = scale(X, scale = TRUE)
Y = scale(Y, scale = TRUE)
# group factor could be omitted if you don't have any group
group <- rep(c("Ctrl","Treat"), each = 25)
cv <- o2cv(X, Y, 1:2, 1:2, 1:2, group=group, nr_folds = 2, ncores=1)
```

Description

fit O2PLS model with best nc, nx, ny

Usage

```r
o2pls(X, Y, nc, nx, ny, scale = FALSE, center = FALSE)
```

Arguments

- `X`: a Numeric matrix (input)
- `Y`: a Numeric matrix (input)
- `nc`: Integer. Number of joint PLS components.
- `nx`: Integer. Number of orthogonal components in X
- `ny`: Integer. Number of orthogonal components in Y
- `scale`: boolean values determining if data should be scaled or not
- `center`: boolean values determining if data should be centered or not

Value

An object containing

- `Xscore` Joint X scores
- `Xloading` Joint X loadings
- `Yscore` Joint Y scores
- `Yloading` Joint Y loadings
- `TYosc` Orthogonal X scores
- `PYosc` Orthogonal X loadings
- `WYosc` Orthogonal X weights
- `UXosc` Orthogonal Y scores
- `PXosc` Orthogonal Y loadings
CXosc Orthogonal Y weights
BU Regression coefficient in Tt ~ U
BT Regression coefficient in U ~ Tt
R2Xhat Prediction of X with Y
R2Yhat Prediction of Y with X
R2X Variation of the modeled part in X (defined by Joint + Orthogonal variation) as proportion of total variation in X
R2Y Variation of the modeled part in Y (defined by Joint + Orthogonal variation) as proportion of total variation in Y
R2Xcorr Variation of the joint part in X
R2Ycorr Variation of the joint part in Y
R2Xo Variation of the orthogonal part in X as proportion of variation in X
R2Yo Variation of the orthogonal part in Y as proportion of variation in Y
R2Xp Variation in X joint part predicted by Y Joint part
R2Yp Variation in Y joint part predicted by X Joint part
varXj Variation in each Latent Variable (LV) in X Joint part
varYj Variation in each Latent Variable (LV) in Y Joint part
varXorth Variation in each Latent Variable (LV) in X Orthogonal part
varYorth Variation in each Latent Variable (LV) in Y Orthogonal part
Exy Residuals in X
Fxy Residuals in Y

Author(s)
Kai Guo

Examples

set.seed(123)
X = matrix(rnorm(500),50,10)
Y = matrix(rnorm(500),50,10)
X = scale(X, scale = TRUE)
Y = scale(Y, scale = TRUE)
fit <- o2pls(X, Y, 1, 2, 2)
summary(fit)
**O2pls-class**

Class "O2pls" This class represents the Annotation information

**Slots**

- **X** a Numeric matrix (input)
- **Y** a Numeric matrix (input)
- **params** parameters used in o2pls analysis
- **results** list of o2pls results

**Author(s)**

Kai Guo

---

**oplsda**

Orthogonal partial least squares discriminant analysis

**Description**

Computes orthogonal scores partial least squares regressions with the NIPALS algorithm. It returns a comprehensive set of pls outputs (e.g. scores and vip).

**Usage**

```
oplsda(X, Y, nc, scale = FALSE, center = TRUE, maxiter = 100, tol = 1e-05)
```

**Arguments**

- **X** a O2pls object or a matrix of predictor variables.
- **Y** a single vector indicating the group
- **nc** the number of pls components (the number of orthogonal components).
- **scale** logical indicating whether X must be scaled (suggest TRUE).
- **center** boolean values determining if data should be centered or not
- **maxiter** maximum number of iterations.
- **tol** limit for convergence of the algorithm in the nipals algorithm.
Value

a list containing the following elements:

- `nc` the number of components used (one joint components + number of orthogonal components)
- `scores` a matrix of scores corresponding to the observations in X. The components retrieved correspond to the ones optimized or specified.
- `Xloadings` a matrix of loadings corresponding to the explanatory variables. The components retrieved correspond to the ones optimized or specified.
- `Yloadings` a matrix of partial least squares loadings corresponding to Y
- `vip` the VIP matrix.
- `xvar` a matrix indicating the standard deviation of each component (sd), the variance explained by each single component (explained_var) and the cumulative explained variance (cumulative_explained_var). These values are computed based on the data used to create the projection matrices.
- `projection_matrix` the matrix of projection matrix
- `weight` a matrix of partial least squares ("pls") weights.

Author(s)

Kai Guo

Examples

```r
X <- matrix(rnorm(50),10,5)
Y <- matrix(rnorm(50),10,5)
fit <- o2pls(X,Y,2,1,1)
yy <- rep(c(0,1),5)
fit0 <- oplsda(fit,yy,2)
```

---

**plot.O2pls**

Score or loading plot for the O2PLS results

**Description**

Score or loading plot for the O2PLS results

**Usage**

```r
## S3 method for class 'O2pls'
plot(
  x,
  type = "score",
  var = "Xjoint",
  group = NULL,
  ind = c(1, 2),
)```
color = NULL,
top = 20,
ellipse = TRUE,
order = FALSE,
pt.size = 3,
label = TRUE,
label.size = 4,
repel = TRUE,
rotation = FALSE,
...

Arguments

x an O2pls object
type score or loading
var specify Xjoint
group color used for score plot
ind which components to be used for score plot or loading plot
color color used for score or loading plot
top the number of largest loading value to plot
ellipse TRUE/FALSE
order order by the value or not
pt.size point size
label plot label or not (TRUE/FALSE)
label.size label size
repel use ggrepel to show the label or not
rotation flip the figure or not (TRUE/FALSE)
... For consistency

Value

a ggplot2 object

Author(s)

Kai Guo

Examples

X <- matrix(rnorm(50),10,5)
Y <- matrix(rnorm(50),10,5)
fit <- o2pls(X,Y,2,1,1)
plot(fit, type="score")
plot.o2plsda

Score, VIP or loading plot for the O2PLS results

Description

Score, VIP or loading plot for the O2PLS results

Usage

## S3 method for class 'o2plsda'
plot(
  x,                     # an o2plsda object
  type = "score",        # score, vip or loading
  var = "Xjoint",       # specify Xjoint
  group = NULL,          # color used for score plot
  ind = c(1, 2),         # which components to be used for score plot or loading plot
  color = NULL,          # color used for score or loading plot
  top = 20,              # the number of largest loading value to plot
  ellipse = TRUE,        # TRUE/FALSE
  order = FALSE,         # order by the value or not
  pt.size = 3,           # point size
  label = TRUE,          # plot label or not (TRUE/FALSE)
  label.size = 4,        # label size
  repel = FALSE,         # use ggrepel to show the label or not
  rotation = FALSE,      # flip the figure or not (TRUE/FALSE)
  ...                    # For consistency
)
**Value**

a ggplot2 object

**Author(s)**

Kai Guo

**Examples**

```r
X <- matrix(rnorm(50),10,5)
Y <- matrix(rnorm(50),10,5)
fit <- o2pls(X,Y,2,1,1)
yy <- rep(c(0,1),5)
fit0 <- oplsda(fit,yy,2)
plot(fit0, type="score", group = factor(yy))
```

---

**Description**

Score, VIP or loading plot for the plsda results

**Usage**

```r
## S3 method for class 'plsda'
plot(
  x,
  type = "score",
  group = NULL,
  ind = c(1, 2),
  color = NULL,
  top = 20,
  ellipse = TRUE,
  order = FALSE,
  pt.size = 3,
  label = TRUE,
  label.size = 4,
  repel = FALSE,
  rotation = FALSE,
  ...
)
```
Arguments

- **x**: an plsda object
- **type**: score, vip or loading
- **group**: color used for score plot
- **ind**: which components to be used for score plot or loading plot
- **color**: color used for score or loading plot
- **top**: the number of largest loading value to plot
- **ellipse**: TRUE/FALSE
- **order**: order by the value or not
- **pt.size**: point size
- **label**: plot label or not (TRUE/FALSE)
- **label.size**: label size
- **repel**: use ggrepel to show the label or not
- **rotation**: flip the figure or not (TRUE/FALSE)

... For consistency

Value

- a ggplot2 object

Author(s)

Kai Guo

Examples

```r
X <- matrix(rnorm(50), 10, 5)
yy <- rep(c(0, 1), 5)
fit0 <- plsda(x = X, y = yy)
plot(fit0, type = "score", group = factor(yy))
```

---

### plsda

**Partial least squares discriminant analysis**

**Description**

Perform a PLS discriminant analysis

**Usage**

```r
plsda(X, Y, nc, scale, center)
```
Arguments

X  a matrix of predictor variables.
Y  a single vector indicate the group
nc the number of pls components (the one joint components + number of orthogonal components).
scale logical indicating whether X must be scaled (suggest TRUE).
center logical indicating whether X must be centered (suggest TRUE).

Value

a list containing the following elements:

- nc the number of components used (one joint components + number of orthogonal components)
- scores a matrix of scores corresponding to the observations in X. The components retrieved correspond to the ones optimized or specified.
- Xloadings a matrix of loadings corresponding to the explanatory variables. The components retrieved correspond to the ones optimized or specified.
- vip the VIP matrix.
- xvar variance explained by each single component

Author(s)

Kai Guo

Examples

X <- matrix(rnorm(50),10,5)
Y <- rep(c(0,1),each=5)
fit <- plsda(X,Y,2)

print.O2pls

Print the summary of O2PLS results.

Description

Print the summary of O2PLS results.

Usage

## S3 method for class 'O2pls'
print(x, ...)

Arguments

x  An O2pls object
... For consistency
Author(s)
Kai Guo

Examples

X <- matrix(rnorm(50), 10, 5)
Y <- matrix(rnorm(50), 10, 5)
object <- o2pls(X, Y, 1, 1, 1)
print(object)

scores
Extract the scores from an O2PLS fit

Description
This function extracts score matrices from an O2PLS fit

Usage

scores(x, ...)

Arguments

x Object of class O2pls
... For consistency

Value
Scores matrix

scores.O2pls
Extract the scores from an O2PLS fit

Description
This function extracts scores parameters from an O2PLS fit

Usage

## S3 method for class 'O2pls'
scores(x, score = c("Xjoint", "Yjoint", "Xorth", "Yorth"), ...)

Arguments

x Object of class O2pls
score the scores matrix for one of "Xjoint", "Yjoint", "Xorth", "Yorth"
... Other arguments
### scores.o2plsla

**Value**

score matrix

---

**scores.o2plsla** *Extract the scores from an O2PLS DA analysis*

**Description**

Extract the scores from an O2PLS DA analysis

**Usage**

```r
## S3 method for class 'o2plsla'
scores(x, ...)
```

**Arguments**

- `x` Object of class `o2plsla`
- `...` Other arguments

**Value**

score matrix

**Author(s)**

Kai Guo

---

### scores.plsda

**Description**

Extract the scores PLSDA analysis

**Usage**

```r
## S3 method for class 'plsda'
scores(x, ...)
```

**Arguments**

- `x` Object of class `plsda`
- `...` Other arguments
Value

score matrix

Author(s)

Kai Guo

## S3 method for class 'O2pls'

`summary(object, ...)`

Arguments

- `object`: a O2pls object
- `...`: For consistency

Value

Detail of O2PLS results

Author(s)

Kai Guo

Examples

```r
X <- matrix(rnorm(50),10,5)
Y <- matrix(rnorm(50),10,5)
object <- o2pls(X,Y,1,1,1)
summary(object)
```
vip

Extract the VIP values from the O2PLS-DA object

Description
Extract the VIP values from the O2PLS-DA object

Usage
vip(x)

Arguments
x
the o2plsd object or plsda object

Value
a data frame
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