## Package ‘o2plsda’

August 12, 2022

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<tr>
<td>Title</td>
<td>Multiomics Data Integration</td>
</tr>
<tr>
<td>Version</td>
<td>0.0.18</td>
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<tr>
<td>Description</td>
<td>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 <a href="">doi:10.1002/cem.775</a>. '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 <a href="">doi:10.1002/cem.1388</a>; Löfstedt et al., 2012 <a href="">doi:10.1016/j.aca.2013.06.026</a>) from the systematic sources of variance being specific for each data set separately.</td>
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<td>License</td>
<td>GPL-3</td>
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<td>Rcpp (&gt;= 1.0.7), dplyr, magrittr, parallel, ggplot2, ggrepel, methods, stats</td>
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<td>RoxygenNote</td>
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<td>Repository</td>
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<tr>
<td>Author</td>
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<td>Kai Guo <a href="mailto:guokai8@gmail.com">guokai8@gmail.com</a></td>
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loadings  Extract the loadings from an O2PLS fit

Description
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"
loadings.o2plsda

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
- `PXosc`: Orthogonal X loadings
- `WYosc`: Orthogonal X weights
- `UXosc`: Orthogonal Y scores
- `PYosc`: Orthogonal Y loadings
- `PXosc`: Orthogonal Y loadings
**CXosc**  
Orthogonal $Y$ weights

**BU**  
Regression coefficient in $T_t \sim U$

**BT**  
Regression coefficient in $U \sim T_t$

**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**

```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)
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**

```r
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 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**: 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.
plot.O2pls

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.02pls

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),
```
plot.O2pls

    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

```r
## 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
)
```

Arguments

- `x`: an o2plsda object
- `type`: score, vip 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

```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))
```

plot.plsda

Score, VIP or loading plot for the plsda results

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

ind     which components to be used for score plot or loading plot

top     the number of largest loading value to plot

type    score, vip or loading

Color

group   color used for score plot

color   color used for score or loading plot

color     color used for score plot

top     the number of largest loading value to plot

Value

a ggplot2 object

Author(s)

Kai Guo

Examples

X <- matrix(rnorm(500), 10, 50)
Y <- rep(c("a", "b"), each = 5)
fit0 <- plsda(X, Y, 2)
plot(fit0, type = "score", group = factor(Y))

Description

Perform a PLS discriminant analysis

Usage

plsda(X, Y, nc, scale = TRUE, center = TRUE, cv = TRUE, nr_folds = 5)
**Arguments**

- **X**: a matrix of predictor variables.
- **Y**: a single vector indicating 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).
- **cv**: logical indicating whether cross-validation will be performed or not (suggest TRUE).
- **nr_folds**: Integer to indicate the folds for cross validation.

**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 of X by each single component.
- **R2Y**: variance explained of Y by each single component.
- **codePRESS**: The residual sum of squares for the samples which were not used to fit the model.
- **codeQ2**: quality of cross-validation.

**Author(s)**

Kai Guo

**Examples**

```r
X <- matrix(rnorm(500),10,50)
Y <- rep(c("a","b"),each=5)
fit <- plsda(X,Y,2)
```
print.02pls

Print the summary of O2PLS results.

Description
Print the summary of O2PLS results.

Usage

## S3 method for class '02pls'
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)

print.plsda

Print the summary of plsda results.

Description
Print the summary of plsda results.

Usage

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

Arguments

x      An plsda object
...

For consistency
**scores**

**Author(s)**

Kai Guo

**Examples**

```r
X <- matrix(rnorm(500),10,50)
Y <- rep(c("a","b"),each=5)
fit <- plsda(X,Y,2)
print(fit)
```

**scores**

*Extract the scores from an O2PLS fit*

**Description**

This function extracts score matrices from an O2PLS fit

**Usage**

```r
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**

```r
## 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.plsda

Value

score matrix

scores.o2plsda  Extract the scores from an O2PLS DA analysis

Description

Extract the scores from an O2PLS DA analysis

Usage

## S3 method for class 'o2plsda'
scores(x, ...)

Arguments

x          Object of class o2plsda
...
Other arguments

Value

score matrix

Author(s)

Kai Guo

scores.plsda  Extract the scores PLSDA analysis

Description

Extract the scores PLSDA analysis

Usage

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

Arguments

x          Object of class plsda
...
Other arguments
**Summary of an O2PLS object**

**Value**

score matrix

**Author(s)**

Kai Guo

---

```r
# 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)
```
**summary.plsda**  
*Summary of an plsda object*

### Description

Summary of an plsda object

### Usage

```r
## S3 method for class 'plsda'
summary(object, ...)
```

### Arguments

- **object**  
  a plsda object

- **...**  
  For consistency

### Value

Detail of plsda results

### Author(s)

Kai Guo

### Examples

```r
X <- matrix(rnorm(500),10,50)
Y <- rep(c("a","b"),each=5)
fit <- plsda(X,Y,2)
summary(fit)
```

---

**vip**  
*Extract the VIP values from the O2PLS-DA object*

### Description

Extract the VIP values from the O2PLS-DA object

### Usage

```r
vip(x)
```

### Arguments

- **x**  
  the o2plssda object or plsda object
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**Value**
- a data frame
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