### Package ‘o2pllda’

**October 14, 2022**

**Type**  Package  
**Title**  Multiomics Data Integration  
**Version**  0.0.18  
**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.  
**License**  GPL-3  
**Imports**  Rcpp (>= 1.0.7), dplyr, magrittr, parallel, ggplot2, ggrepel, methods, stats  
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**VignetteBuilder**  knitr  
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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)
```

---

**o2plsls**

*fit O2PLS model with best nc, nx, ny*

**Description**

fit O2PLS model with best nc, nx, ny

**Usage**

```r
o2plsls(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)
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

---

**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 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.
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
```
## S3 method for class 'o2plsda'
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 = FALSE,
  rotation = FALSE,
  ...
)
```

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))
```

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

---

### plsda

**Partial least squares discriminant analysis**

### Description

Perform a PLS discriminant analysis

### Usage

```r
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** 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**

```r
## S3 method for class '02pls'
print(x, ...)
```

**Arguments**

- `x` An O2pls object
- `...` For consistency

**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)
print(object)
```

---

print.plsda

*Print the summary of plsda results.*

**Description**

Print the summary of plsda results.

**Usage**

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

**Arguments**

- `x` An plsda object
- `...` For consistency
Author(s)
Kai Guo

Examples
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
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
Value

score matrix

---

**scores.o2plsda**

*Extract the scores from an O2PLS DA analysis*

**Description**

Extract the scores from an O2PLS DA analysis

**Usage**

```r
## 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**

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

**Arguments**

- `x`: Object of class `plsda`
- `...`: Other arguments
Summary of an O2PLS object

Description

Summary of an O2PLS object

Usage

```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 o2plsd object or plsda object
vip

Value

a data frame
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