Package: o2plsda (via r-universe)

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Type Package

Title Multiomics Data Integration

Version 0.0.26

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

Encoding UTF-8

Suggests knitr, markdown, rmarkdown, MASS

VignetteBuilder knitr

LinkingTo Rcpp, RcppArmadillo

RoxygenNote 7.3.3

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

o2cv *Cross validation for O2PLS*

Description

Cross validation for O2PLS

Usage

```
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

```
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)
```

`o2pls` *fit O2PLS model with best nc, nx, ny*

Description

fit O2PLS model with best nc, nx, ny

Usage

```
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
Xhat	Prediction of X with Y
Yhat	Prediction of Y with X
R2Xhat	Variation of the predicted X as proportion of variation in X
R2Yhat	Variation of the predicted Y as proportion of variation in Y
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*

Description

Class "O2pls" This class represents the Annotation information

Slots

`X` a Numeric matrix (input)

`Y` a Numeric matrix (input)

`params` paramaters ysed 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 return 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 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.

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

```
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

```
## 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,
  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 o2plsda 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

```
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

```
## 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

```
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

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

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).
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.
- PRESS The residual sum of squares for the samples which were not used to fit the model
- Q2 quality of cross-validation

Author(s)

Kai Guo

Examples

```
X <- matrix(rnorm(500),10,50)
Y <- rep(c("a","b"),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)
```

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

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

```
## 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

Value

score matrix

Author(s)

Kai Guo

`summary.O2pls` *Summary of an O2PLS object*

Description

Summary of an O2PLS object

Usage

```
## S3 method for class 'O2pls'
summary(object, ...)
```

Arguments

`object`	a O2pls object
`...`	For consistency

Value

Detail of O2PLS results

Author(s)

Kai Guo

Examples

```
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

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

Arguments

object	a plsda object
...	For consistency

Value

Detail of plsda results

Author(s)

Kai Guo

Examples

```
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

```
vip(x)
```

Arguments

x	the o2plsda object or plsda object

Value

a data frame

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