

Package ‘o2plsda’

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Type Package

Title Multiomics Data Integration

Version 0.0.15

Description Provides functions to do 'O2PLS-DA' analysis for multiple omics data integration.

The algorithm came from "O2-PLS, a two-block ($X \pm Y$) 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](https://doi.org/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](https://doi.org/10.1002/cem.1388)>; Löfstedt et al., 2012 <[doi:10.1016/j.aca.2013.06.026](https://doi.org/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

VignetteBuilder knitr

LinkingTo Rcpp, RcppArmadillo

RoxygenNote 7.1.1

NeedsCompilation yes

Repository CRAN

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| | |
|----------|---|
| loadings | <i>Extract the loadings from an O2PLS fit</i> |
|----------|---|

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 | <i>extract the loading value from the O2PLSDA analysis</i> |
|------------------|--|

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 | <i>extract the loading value from the PLSDA analysis</i> |
|----------------|--|

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 |
| Yloaing | 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 $Tt \sim U$ |
| BT | Regression coefficient in $U \sim Tt$ |
| 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 |
| E _{xy} | Residuals in X |
| F _{xy} | 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

 opllda

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

```
opllda(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 <- oplstda(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 | <i>Score, VIP or loading plot for the O2PLS results</i> |
|--------------|---|

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

```
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 <- oplstda(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(50),10,5)
yy <- rep(c(0,1),5)
fit0 <- plsda(X,yy,2)
plot(fit0, type = "score", group = factor(yy))
```

plsda

Partial least squares discriminant analysis

Description

Perform a PLS discriminant analysis

Usage

```
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 |

Value

score matrix

| | |
|----------------|---|
| scores.o2plsda | <i>Extract the scores from an O2PLS DA analysis</i> |
|----------------|---|

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 | <i>Extract the scores PLSDA analysis</i> |
|--------------|--|

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)
```

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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