Package 'loadings'

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Type Package

Title Loadings for Principal Component Analysis and Partial Least Squares

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Description Computing principal component (Yamamoto, H. et al. (2014) <doi:10.1186/1471-2105-15-51> and Yamamoto, H. et al. (2021) <doi:10.3390/metabo11030149>) and partial least squares loading (Yamamoto, H. (2017) <doi:10.1002/cem.2883>) and its statistical hypothesis testing.

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NeedsCompilation no

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R topics documented:

fasting *Metabolome analysis of mouse liver samples in fasting conditions*

Description

This data includes metabolome data of liver samples from normal and 12 hour fasted mice measured by capillary electrophoresis time-of-flight mass spectrometry. The data matrix contains 10 samples (5 samples in each groups) and 282 metabolites.

Usage

```
data(fasting)
```

Format

The list object "fasting" contains the following elements:

X : Data matrix that include metabolites in each columns.

Y : Dummy matrix that include group information 0,1 in each columns.

Source

Yamamoto H., Fujimori T., Sato H., Ishikawa G., Kami K., Ohashi Y. (2014). "Statistical hypothesis testing of factor loading in principal component analysis and its application to metabolite set enrichment analysis". BMC Bioinformatics, (2014) 15(1):51.

greentea *Metabolome analysis of Japanese green tea*

Description

This includes metabolome data of Japanese green tea measured by gas chromatgraphy mass spectrometry. The data matrix contains 30 samples and 225 metabolites.

Usage

```
data(greentea)
```

Format

The list object "greentea" contains the following elements:

X : Data matrix that include metabolites in each columns.

Y : Dummy matrix that include group information 0,1 in each columns.

D : Differential matrix (Second order).

M : Averaging matrix for repeated data.

y : Ranking of taste in competitive exhibition.

Source

Statistics in Microsoft Excel (http://prime.psc.riken.jp/compms/others/main.html#Statistics)

Pongsuwan W., Fukusaki E., Bamba T., Yonetani T., Yamahara A.T., Kobayashi A. Prediction of Japanese Green Tea Ranking by Gas Chromatography/Mass Spectrometry-Based Hydrophilic Metabolite Fingerprinting. J. Agric. Food Chem. 2007;55:231-236.

`ospca_loading` *Orthogonal smoothed principal component loading*

Description

This function computes orthogonals smoothed principal component (OS-PC) loading from the result of the "os_pca" function. This is also wrapper function of pls_loading function.

Usage

```
ospca_loading(ospca)
```

Arguments

`ospca`	The following variables (P,T,Q and U) are included in the ospca object.
	P : A matrix with OS-PC loading in each column
	T : A matrix with OS-PC score in each column
	MT : A matrix with averaging OS-PC score for repeated data in each column (If not for repeated data, the matrix MT equals to the matrix T)
	Q : A matrix with OS-PC loading for auxiliary variable in each column
	U : A matrix with OS-PC score for auxiliary variable in each column

Details

The OS-PC loading and the p-value by statistical hypothesis testing is added to the ospca object returned by the "os-pca" function.

Value

The return value is a list object that contains the following elements:

R : OS-PCA loading (Correlation coefficient between OS-PC score of auxiliary variable and each variables in data matrix.)

p.value : p-value of OS-PCA loading

Author(s)

Hiroyuki Yamamoto

References

Yamamoto H., Nakayama Y., Tsugawa H. (2021) OS-PCA: Orthogonal Smoothed Principal Component Analysis Applied to Metabolome Data, Metabolites, 11(3):149.

Examples

```
# metabolic turnover data
data(turnover)
X <- turnover$X
D <- turnover$D

ospca <- os_pca(X,D,0.999)

ospca <- ospca_loading(ospca)
ospca$loading$R
ospca$loading$p.value

# metabolome data

data(greentea)
X <- greentea$X
D <- greentea$D
M <- greentea$M

ospca <- os_pca(X,D,0.1,M)

ospca <- ospca_loading(ospca)
ospca$loading$R
ospca$loading$p.value
```

---

os_pca *Orthogonal smoothed principal component analysis*

Description

This function performs orthogonal smoothed principal component analysis (OS-PCA). In this function, data matrix is automatically scaled to zero mean and unit variance (i.e. autoscaling) for each variables.

Usage

```
os_pca(X,D,kappa,M)
```

Arguments

X	Data matrix that include variables in each columns.
D	Differential matrix.
kappa	The smoothing parameter (default : 0.999).
M	Averaging matrix for repeated data (default : Identity matrix).

Details

The kappa represents the degree of smoothing. The value of kappa increases, the strength of the smoothing increases.

Value

The return value is a list object that contains the following elements:

P : A matrix with OS-PC loading in each column

T : A matrix with OS-PC score in each column

MT : A matrix with averaging OS-PC score for repeated data in each column (If not for repeated data, the matrix MT equals to the matrix T)

Q : A matrix with OS-PC loading for auxiliary variable in each column

U : A matrix with OS-PC score for auxiliary variable in each column

Author(s)

Hiroyuki Yamamoto

References

Yamamoto H., Nakayama Y., Tsugawa H. (2021) OS-PCA: Orthogonal Smoothed Principal Component Analysis Applied to Metabolome Data, Metabolites, 11(3):149.

Examples

```
# metabolic turnover data
data(turnover)

X <- turnover$X
D <- turnover$D

ospca <- os_pca(X,D,0.999)

# metabolome data
data(greentea)

X <- greentea$X
D <- greentea$D
M <- greentea$M

ospca <- os_pca(X,D,0.1,M)
```

pca_loading *Principal component loading*

Description

This function computes principal component (PC) loading from the result of the "prcomp" function. (The "princomp" function is not supported. For "princomp" function, the "loadings" function in stats package should be used.) In this function, data matrix is should be scaled to zero mean and unit variance (i.e. autoscaling) for each variables.

Usage

```
pca_loading(pca)
```

Arguments

pca	The return object of the "prcomp" function.

Details

The PC loading and the p-value by statistical hypothesis testing is added to the pca object returned by the "prcomp" function.

Value

The return value is a list object that contains the following elements:

R : PC loading (Correlation coefficient between PC score and each variables in data matrix.)

p.value : p-value of PC loading

Author(s)

Hiroyuki Yamamoto

References

Yamamoto H., Fujimori T., Sato H., Ishikawa G., Kami K., Ohashi Y. (2014). "Statistical hypothesis testing of factor loading in principal component analysis and its application to metabolite set enrichment analysis". BMC Bioinformatics, (2014) 15(1):51.

Examples

```
data(fasting)
X <- fasting$X

pca <- prcomp(X, scale=TRUE)

pca <- pca_loading(pca)
pca$loading$R # PC loading
pca$loading$p.value # p-value
```

`pls_loading` *Partial least squares loading*

Description

This function computes partial least squares (PLS) loading from the result of the "pls_svd" function. PLS loading can also be computed from the result of the "pls_eigen" function in chemometrics package.

Usage

```
pls_loading(pls)
```

Arguments

`pls`	The following variables (P,T,Q and U) are included in the pls object.
	P : A matrix with PLS loading for explanatory variable in each column
	T : A matrix with PLS score for explanatory variable in each column
	Q : A matrix with PLS loading for response variable in each column
	U : A matrix with PLS score for response variable in each column

Details

The PLS loading and the p-value by statistical hypothesis testing is added to the pls object returned by the "pls_svd" function in this package or "pls_eigen" function in chemometrics package.

Value

The return value is a list object that contains the following elements:

R : PLS loading (Correlation coefficient between PLS score of response variable and each variables in data matrix.)

p.value : p-value of PLS loading

Author(s)

Hiroyuki Yamamoto

References

Yamamoto, H. (2017) PLS-ROG: Partial least squares with rank order of groups., Journal of Chemometrics, 31(3) (2017) e2883.

Examples

```
data(whhl)
X <- whhl$X
Y <- whhl$Y

pls <- pls_svd(X,Y)

pls <- pls_loading(pls)
pls$loading$R
pls$loading$p.value
```

---

pls_rog *Partial least squares rank order of groups*

Description

This function performs partial least squares rank order of groups (PLS-ROG). In this function, data matrix is automatically scaled to zero mean and unit variance (i.e. autoscaling) for each variables.

Usage

```
pls_rog(X,Y,D,kappa)
```

Arguments

X	Data matrix of explanatory variables that include variables in each columns.
Y	Dummy matrix that include group information 0,1 in each columns.
D	Differential matrix.
kappa	The smoothing parameter (default : kappa = 0.999).

Details

The kappa represents the degree of smoothing. The value of kappa increases, the strength of the smoothing increases.

Value

The return value is a list object that contains the following elements:

P : A matrix with PLS loading for explanatory variable in each column

T : A matrix with PLS score for explanatory variable in each column

Q : A matrix with PLS loading for response variable in each column

U : A matrix with PLS score for response variable in each column

Author(s)

Hiroyuki Yamamoto

References

Yamamoto, H. (2017) PLS-ROG: Partial least squares with rank order of groups., Journal of Chemometrics, 31(3) (2017) e2883.

Examples

```
data(whhl)
X <- whhl$X
Y <- whhl$Y
D <- whhl$D

plsrog <- pls_rog(X,Y,D)
```

`pls_svd` *Partial least squares*

Description

This function performs partial least squares. In this function, data matrix for explanatory variable is automatically scaled to zero mean and unit variance (i.e. autoscaling) for each variables.

Usage

```
pls_svd(X,Y)
```

Arguments

`X`	Data matrix of explanatory variables that include variables in each columns.
`Y`	Dummy matrix that include group information 0,1 in each columns.

Details

This function is wrapper function of "pls_rog" fucntion that the smoothing parameter kappa=0.

Value

The return value is a list object that contains the following elements:

P : A matrix with PLS loading for explanatory variable in each column

T : A matrix with PLS score for explanatory variable in each column

Q : A matrix with PLS loading for response variable in each column

U : A matrix with PLS score for response variable in each column

Author(s)

Hiroyuki Yamamoto

References

Barker, M. and Rayens, W. (2003) Partial Least Squares for Discrimination. Journal of Chemometrics, 17, 166-173.

Examples

```
data(whhl)
X <- whhl$X
Y <- whhl$Y

pls <- pls_svd(X,Y)
```

---

turnover *Metabolomic Turnover analysis of the yeast culture mediums*

Description

This includes differential isotopomer ratio from metabolomic turnover analysis of yeast cultures by gas chromatgraphy mass spectrometry. The data matrix contains 11 samping time for three groups of different yeast strains and culture condition (33 samples total) and 60 peaks.

Usage

```
data(turnover)
```

Format

The list object "turnover" contains the following elements:

X : Data matrix of explanatory variables that include variables in each columns.

Y : Dummy matrix that include group information 0,1 in each columns.

D : Differential matrix (Second order).

References

Nakayama Y., Tamada Y., Tsugawa H., Bamba T., Fukusaki E. Novel Strategy for Non-Targeted Isotope-Assisted Metabolomics by Means of Metabolic Turnover and Multivariate Analysis. Metabolites. 2014;4:722-739.

Examples

```
data(turnover)
```

whhl *Metabolome analysis of liver samples from rabbits with hyperlipidemia.*

Description

This is metabolome data from liver samples of normal, hyperlipidemic, and statin-treated rabbits measured by capillary electrophoresis time-of-flight mass spectrometry. The data matrix contains 9 samples (3 samples in each groups) and 168 metabolites.

Usage

```
data(whhl)
```

Arguments

The list object "whhl" contains the following elements:

X : Data matrix of explanatory variables that include variables in each columns.

Y : Dummy matrix that include group information 0,1 in each columns.

References

Ooga, T., Sato, H., Nagashima, A., Sasaki, K., Tomita, M., Soga T. and Ohashi, Y. (2011) Metabolomic Anatomy of Animal Model Revealing Homeostatic Imbalances in Dyslipidemia. Y. Mol. BioSyst.,7, 1217-23.

Examples

```
data(whhl)
```

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