Package 'loadings'

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Type Package

Title Loadings for Principal Component Analysis and Partial Least Squares

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Description

Computing statistical hypothesis testing for loading in principal component analysis (PCA) (Yamamoto, H. et al. (2014) <doi:10.1186/1471-2105-15-51>), orthogonal smoothed PCA (OSPCA) (Yamamoto, H. et al. (2021) <doi:10.3390/metabo11030149>), one-sided kernel PCA (Yamamoto, H. (2023) <doi:10.51094/jxiv.262>), partial least squares (PLS) and PLS discriminant analysis (PLS-DA) (Yamamoto, H. et al. (2009) <doi:10.1016/j.chemolab.2009.05.006>), PLS with rank order of groups (PLS-ROG) (Yamamoto, H. (2017) <doi:10.1002/cem.2883>), regularized canonical correlation analysis discriminant analysis (RCCA-DA) (Yamamoto, H. et al. (2008) <doi:10.1016/j.bej.2007.12.009>), multiset PLS and PLS-ROG (Yamamoto, H. (2022) <doi:10.1101/2022.08.30.505949>).

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`antibiotic` *Metagenome and metabolome data from antibiotic-treated mouse feces.*

Description

This is metagenome and metabolome data of antibiotic-treated mouse fecal samples [Y. Wakita, et al, BMC Microbiology, 18:188 (2018)]. This dataset includes six groups, comprising three types (Clea, CR, and Slc) of control mice and their antibiotic-treated counterparts.

Usage

```
data(antibiotic)
```

Format

The list object "antibiotic" contains the following elements:

data$X$microbiome$dist: Weighted UniFrac distance matrix for the metagenome.

data$X$microbiome$comp: Composition data for the metagenome.

data$X$metabolome : Metabolome data.

data$Y: A dummy matrix that includes group information with 0 or 1 in each column.

annotation$metabolome : Compound annotation for metabolome data.

Source

Y. Wakita, et al, Taxonomic classification for microbiome analysis, which correlates well with the metabolite milieu of the gut, BMC microbiology, 18:188 (2018)

`covid19` *Proteome and metabolome data of COVID-19 serum samples.*

Description

This is proteome and metabolome data of COVID-19 serum samples [B. Shen et al, Cell. 182 (2020) 59-72.e15.]. This dataset includes three groups of healthy control, mild and severe COVD-19.

Usage

```
data(covid19)
```

Format

The list object "covid19" contains the following elements:

X : List of data matrix that include samples in each rows and protein or metabolite in each columns for proteomics and metabolomics.

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

D : Example of differential matrix used in PLS-ROG or multiset PLS-ROG.

tau : Example of strength parameter matrix used in mutliset PLS or multiset PLS-ROG. All weights were set as the same value of 0.1.

K : List of kernel matrix by hyperbolic tangent kernel (scale=1, offset=1).

Source

B. Shen, et al, Proteomic and Metabolomic Characterization of COVID-19 Patient Sera, Cell. 182 (2020) 59-72.e15.

`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.

`multiplsrog_loading` *Multiset partial least squares rank order of groups loading*

Description

This function computes multiset partial least squares rank order of groups (PLS-ROG) loading from the result of the "multipls_rog" function.

Usage

```
multiplsrog_loading(multiplsrog)
```

Arguments

`multiplsrog`	The following variables (P,T,Q and U) are included in the multiplsrog object. P : A list of matrix with Multiset PLS-ROG coefficients for the explanatory variables in each column for each dataset T : A list of matrix with Multiset PLS-ROG scores for the explanatory variables in each column for each dataset Q : A matrix with Multiset PLS-ROG coefficients for the response variable in each column U : A matrix with Multiset PLS-ROG scores for the response variable in each column tau : Matrix for strength parameter of the connection between omics datasets or between omics dataset and group information.

Details

The multiset PLS-ROG loading and the p-value by statistical hypothesis testing is added to the multiplsrog object returned by the "multipls_rog" function in this package.

Value

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

Score : A list of matrix with Multiset PLS score for auxiliary variable in each column for each dataset

R : A list of matrix with Multiset PLS-ROG loadings in each column for each dataset

p.value : A list of matrix with p-value of multiset PLS-ROG loading in each column for each dataset

Author(s)

Hiroyuki Yamamoto

References

Yamamoto H. (2022) Multiset partial least squares with rank order of groups for integrating multi-omics data, bioRxiv.

Examples

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

multiplsrog <- multipls_rog(X,Y,tau,D)
# multiplsrog <- multipls_rog(X,Y,tau,D, kappa=0.999)

multiplsrog <- multiplsrog_loading(multiplsrog)
multiplsrog$loading$R
multiplsrog$loading$p.value
```

`multipls_geigen` *Multiset PLS : Multiset partial least squares*

Description

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

Usage

```
multipls_geigen(X,Y,tau)
```

Arguments

`X`	List of data matrix that include variables in each columns.
`Y`	Dummy matrix that include group information 0,1 in each columns.
`tau`	Matrix for strength parameter of the connection between omics datasets or between omics dataset and group information.

Details

Diagonal elements of matrix tau must be 0.

Value

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

P : A list of matrix with Multiset PLS coefficients for the explanatory variables in each column for each dataset

T : A list of matrix with Multiset PLS scores for the explanatory variables in each column for each dataset

Q : A matrix with Multiset PLS coefficients for the response variable in each column

U : A matrix with Multiset PLS scores for the response variable in each column

tau : Matrix for strength parameter of the connection between omics datasets or between omics dataset and group information (same as input value).

Author(s)

Hiroyuki Yamamoto

References

Yamamoto H. (2022) Multiset partial least squares with rank order of groups for integrating multi-omics data, bioRxiv.

Examples

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

multipls <- multipls_geigen(X,Y,tau)
```

---

multipls_loading *Multiset partial least squares loading*

Description

This function computes multiset partial least squares (PLS) loading from the result of the "multipls_geigen" function.

Usage

```
multipls_loading(multipls)
```

Arguments

multipls	The following variables (P,T,Q and U) are included in the multipls object.
	P : A list of matrix with Multiset PLS coefficients for the explanatory variables in each column for each dataset
	T : A list of matrix with Multiset PLS scores for the explanatory variables in each column for each dataset
	Q : A matrix with Multiset PLS coefficients for the response variable in each column
	U : A matrix with Multiset PLS scores for the response variable in each column
	tau : Matrix for strength parameter of the connection between omics datasets or between omics dataset and group information.

Details

The multiset PLS loading and the p-value by statistical hypothesis testing is added to the multipls object returned by the "multipls_geigen" function in this package.

Value

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

Score : A list of matrix with Multiset PLS score for auxiliary variable in each column for each dataset

R : A list of matrix with Multiset PLS loadings in each column for each dataset

p.value : A list of matrix with p-value of multiset PLS loading in each column for each dataset

Author(s)

Hiroyuki Yamamoto

References

Yamamoto H. (2022) Multiset partial least squares with rank order of groups for integrating multi-omics data, bioRxiv.

Examples

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

multipls <- multipls_geigen(X,Y,tau)

multipls <- multipls_loading(multipls)
multipls$loading$R
multipls$loading$p.value
```

`multipls_rog` *Multiset PLS-ROG : Multiset partial least squares with rank order of groups*

Description

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

Usage

```
multipls_rog(X,Y,tau,D,kappa)
```

Arguments

X	List of data matrix that include variables in each columns.
Y	Dummy matrix that include group information 0,1 in each columns.
tau	Matrix for strength parameter of the connection between omics datasets or between omics dataset and group information.
D	Differential matrix.
kappa	The smoothing parameter (default : 0.999).

Details

Diagonal elements of matrix tau must be 0.

Value

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

P : A list of matrix with Multiset PLS-ROG coefficients for the explanatory variables in each column for each dataset

T : A list of matrix with Multiset PLS-ROG scores for the explanatory variables in each column for each dataset

Q : A matrix with Multiset PLS-ROG coefficients for the response variable in each column

U : A matrix with Multiset PLS-ROG scores for the response variable in each column

tau : Matrix for strength parameter of the connection between omics datasets or between omics dataset and group information (same as input value).

Author(s)

Hiroyuki Yamamoto

References

Yamamoto H. (2022) Multiset partial least squares with rank order of groups for integrating multi-omics data, bioRxiv.

Examples

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

multiplsrog <- multipls_rog(X,Y,tau,D)
# multiplsrog <- multipls_rog(X,Y,tau,D, kappa=0.999)
```

onekpca_loading *One-sided kernel principal component loading*

Description

This function computes one-sided kernel principal component (one-sided KPC) loading from the result of the "one_kpca" function.

Usage

```
onekpca_loading(onekpca)
```

Arguments

onekpca	The following variables (P,T and U) are included in the onekpca object.
	P : A matrix with one-sided KPCA loading in each column
	T : A matrix with one-sided KPCA score for linear side in each column
	U : A matrix with one-sied KPCA score for nonlinear side in each column

Details

The one-sided KPC loading and the p-value by statistical hypothesis testing is added to the onekpca object returned by the "one_kpca" function.

Value

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

R : one-sided KPC loading (Correlation coefficient between one-sided KPC score of nonlinear variable (kernel matrix) and each variables in data matrix.)

p.value : p-value of one-sided KPC loading

Author(s)

Hiroyuki Yamamoto

References

Yamamoto H. (2023) One-sided Kernel Principal Component Analysis, Jxiv, <doi:10.51094/jxiv.262>.

Examples

```
# COVID-19 metabolome data
data(covid19)

X <- covid19$X$metabolomics
K <- covid19$K$metabolomics
```

```
onekpca <- one_kpca(X,K)

onekpca <- onekpca_loading(onekpca)

onekpca$loading$R
onekpca$loading$p.value
```

---

one_kpca *One-sided kernel principal component analysis*

Description

This function performs one-sided kernel principal component analysis (one-sided KPCA). In this function, data matrix is automatically scaled to zero mean and unit variance (i.e. autoscaling) for each variables.

Usage

```
one_kpca(X,K)
```

Arguments

X	Data matrix that include variables in each columns.
K	Kernel matrix computed from the data matrix X.

Details

The kernel matrix K, which is the argument of the one_kpca function, must be centered.

Value

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

P : A matrix with one-sided KPCA loading in each column

T : A matrix with one-sided KPCA score for linear side in each column

U : A matrix with one-sied KPCA score for nonlinear side in each column

Author(s)

Hiroyuki Yamamoto

References

Yamamoto H. (2023) One-sided Kernel Principal Component Analysis, Jxiv, <doi:10.51094/jxiv.262>.

Examples

```
# COVID-19 metabolome data
data(covid19)

X <- covid19$X$metabolomics
K <- covid19$K$metabolomics

onekpca <- one_kpca(X,K)
```

`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
```

plsda_loading *Partial least squares discriminant analysis (PLS-DA) loading*

Description

This function computes partial least squares discriminant analysis (PLS-DA) loading from the result of the 'pls_da' function.

Usage

```
plsda_loading(plsda)
```

Arguments

plsda	The following variables (P,T) are included in the plsda object.
	P: A matrix containing the PLS-DA loadings for each explanatory variable in the columns, before transformation.
	T : A matrix with PLS-DA score for explanatory variable in each column

Details

The PLS-DA loading and the p-value by statistical hypothesis testing is added to the pls object returned by the 'pls_da' function in this package.

Value

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

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

p.value : p-value of PLS-DA loading

Author(s)

Hiroyuki Yamamoto

References

Yamamoto, H. et al., Dimensionality reduction for metabolome data using PCA, PLS, OPLS, and RFDA with differential penalties to latent variables", Chemom. Intell. Lab. Syst., 98 (2009)

Examples

```
data(whhl)
X <- whhl$X$liver
Y <- whhl$Y
plsda <- pls_da(X,Y,2)
```

```
plsda <- plsda_loading(plsda)

plsda$loading$R
plsda$loading$p.value
```

---

plsrog_loading *Partial least squares rank order of groups loading*

Description

This function computes partial least squares rank rder of groups (PLS-ROG) loading from the result of the "pls_rog" function. PLS-ROG loading can also be computed from the result of the "pls_rog" function.

Usage

```
plsrog_loading(plsrog)
```

Arguments

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

Details

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

Value

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

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

p.value : p-value of PLS-ROG 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$X$liver
Y <- whhl$Y
D <- whhl$D

plsrog <- pls_rog(X,Y,D)

plsrog <- plsrog_loading(plsrog)
plsrog$loading$R
plsrog$loading$p.value
```

---

pls_da *Partial least squares discriminant analysis (PLS-DA)*

Description

This function performs partial least squares discriminant analysis (PLS-DA). 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_da(X,Y,k)
```

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.
k	Number of components.

Details

This function calculates PLS-DA. For PLS, use the 'pls_svd' function for PLS.

Value

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

P: A matrix containing the PLS-DA loadings for each explanatory variable in the columns, before transformation.

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

Author(s)

Hiroyuki Yamamoto

References

Yamamoto, H. et al., Dimensionality reduction for metabolome data using PCA, PLS, OPLS, and RFDA with differential penalties to latent variables", Chemom. Intell. Lab. Syst., 98 (2009)

Examples

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

plsda <- pls_da(X,Y,2)
```

---

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$X$liver
Y <- whhl$Y

pls <- pls_svd(X,Y)

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

`pls_rog` *PLS-ROG : Partial least squares with rank order of groups*

Description

This function performs partial least squares with 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$X$liver
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$X$liver
Y <- whhl$Y

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

---

rcca_da *Regularized canonical correlation analysis for discriminant analysis (RCCA-DA)*

Description

This function performs regularized canonical correlation analysis for discriminant analysis (RCCA-DA). In this function, data matrix for explanatory variable is automatically scaled to zero mean and unit variance (i.e. autoscaling) for each variables.

Usage

```
rcca_da(X,Y,lambda,k)
```

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.
lambda	The regularized parameter has a value in the range [0, 1), meaning it can be 0 but is less than 1."
k	Number of components.

Details

RCCA-DA is equivalent to Regularized Fisher discriminant analysis, theoretically.

Value

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

P: A matrix containing the RCCA-DA loadings for each explanatory variable in the columns, before transformation.

T : A matrix with RCCA-DA score for explanatory variable in each column

Author(s)

Hiroyuki Yamamoto

References

Yamamoto, H. et al., Canonical correlation analysis for multivariate regression and its application to metabolic fingerprinting", Biochem. Eng. Journal, 40 (2008) 199-204.

Yamamoto, H. et al., Dimensionality reduction for metabolome data using PCA, PLS, OPLS, and RFDA with differential penalties to latent variables", Chemom. Intell. Lab. Syst., 98 (2009)

Examples

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

rcca <- rcca_da(X,Y,0.5,2)
```

---

rcca_loading *Regularized canonical correlation analysis (RCCA-DA) loading*

Description

This function computes regularized canonical correlation analysis for discriminant analysis (RCCA-DA) loading from the result of the 'rcca_da' function.

Usage

```
rcca_loading(rcca)
```

Arguments

rcca	The following variables (Wx,P,T,Wy and S) are included in the rcca object. Wx : A matrix with RCCA-DA weight for explanatory variable in each column P: A matrix containing the RCCA-DA loadings for each explanatory variable in the columns, before transformation. T : A matrix with RCCA-DA score for explanatory variable in each column Wy : A matrix with RCCA-DA weight for explanatory variable in each column S : A matrix with RCCA-DA score for response variable in each column

Details

The RCCA-DA loading and the p-value by statistical hypothesis testing is added to the pls object returned by the 'rcca_da' function in this package.

Value

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

R : RCCA-DA loading (Correlation coefficient between PLS-DA score of explanatory variable and each variables in data matrix.)

p.value : p-value of RCCA-DA loading

Author(s)

Hiroyuki Yamamoto

References

Yamamoto, H. et al., Canonical correlation analysis for multivariate regression and its application to metabolic fingerprinting", Biochem. Eng. Journal, 40 (2008) 199-204.

Examples

```
data(whhl)
X <- whhl$X$liver
Y <- whhl$Y
rcca <- rcca_da(X,Y,0.5,2)

rcca <- rcca_loading(rcca)

rcca$loading$R
rcca$loading$p.value
```

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).

annotation : Compound annotation for metabolome data.

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)
```

unsvmultipls_loading *Unsupervised multiset partial least squares loading*

Description

This function computes unsupervised multiset partial least squares loading from the result of the "unsv_multipls" function.

Usage

```
unsvmultipls_loading(unsvmpls)
```

Arguments

unsvmpls	The following variables (P,T) are included in the unsvmpls object.
	P : A list of matrix with Multiset PLS coefficients in each column for each dataset
	T : A list of matrix with Multiset PLS scores in each column for each dataset

Details

The unsupervised multiset PLS loading and the p-value by statistical hypothesis testing is added to the unsvmpls object returned by the "unsv_multipls" function in this package.

Value

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

Score : A list of matrix with Multiset PLS score for auxiliary variable in each column for each dataset

R : A list of matrix with Unsupervised multiset PLS loadings in each column for each dataset

p.value : A list of matrix with p-value of Unsupervised multiset PLS loading in each column for each dataset

Author(s)

Hiroyuki Yamamoto

References

Yamamoto H. (2022) Multiset partial least squares with rank order of groups for integrating multi-omics data, bioRxiv.

Examples

```
data(whhl)
X <- whhl$X
tau <- rbind(c(0,1/4,1/4,1/4),c(1/4,0,1/4,1/4),c(1/4,1/4,0,1/4),c(1/4,1/4,1/4,0))

unsvmpls <- unsv_multipls(X,tau)

unsvmpls <- unsvmultipls_loading(unsvmpls)
unsvmpls$loading$R
unsvmpls$loading$p.value
```

unsv_multipls *Unsupervised multiset partial least squares*

Description

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

Usage

```
unsv_multipls(X,tau)
```

Arguments

X	List of data matrix that include variables in each columns.
tau	Matrix for strength parameter of the connection between omics datasets or between omics dataset and group information.

Details

Diagonal elements of matrix tau must be 0.

Value

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

P : A list of matrix with Multiset PLS coefficients in each column for each dataset

T : A list of matrix with Multiset PLS scores in each column for each dataset

Author(s)

Hiroyuki Yamamoto

References

Yamamoto H. (2022) Multiset partial least squares with rank order of groups for integrating multi-omics data, bioRxiv.

Examples

```
data(whhl)
X <- whhl$X
tau <- rbind(c(0,1/4,1/4,1/4),c(1/4,0,1/4,1/4),c(1/4,1/4,0,1/4),c(1/4,1/4,1/4,0))

unsvmpls <- unsv_multipls(X,tau)
```

whhl *Metabolome analysis of plasma, liver, heart and brain samples from rabbits with hyperlipidemia.*

Description

This is metabolome data from plasma, liver, heart and brain 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).

Usage

```
data(whhl)
```

Format

The list object "whhl" contains the following elements:

X : List of data matrix that include samples in each rows and metabolites in each columns for plasma, liver, heart and brain samples.

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

D : Example of differential matrix used in PLS-ROG or multiset PLS-ROG.

tau : Example of strength parameter matrix used in mutliset PLS or multiset PLS-ROG. All weights were set as the same value of 0.1.

Source

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.

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