

Package ‘KODAMA’

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Title Knowledge Discovery by Accuracy Maximization

Description KODAMA algorithm is an unsupervised and semi-supervised learning algorithm that performs feature extraction from noisy and high-dimensional data. It facilitates identification of patterns representing underlying groups on all samples in a data set. The algorithm was published by Cacciatore et al. 2014 <DOI:10.1073/pnas.1220873111>. Addition functions was introduced by Cacciatore et al. 2017 <DOI:10.1093/bioinformatics/btw705> to facilitate the identification of key features associated with the generated output and are easily interpretable for the user. Cross-validated techniques are also included in this package.

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VignetteBuilder knitr

SuggestsNote No suggestions

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categorical_table	<i>Categorical Information</i>
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Description

Summarization of the categorical information.

Usage

```
categorical_table (name,cat,label)
```

Arguments

name	the name of the feature.
cat	the information to summarize.
label	the classification of the cohort.

Value

The function returns a table with the summarized information. The p-value is computed using the Fisher's test.

Author(s)

Stefano Cacciatore

References

Cacciatore S, Luchinat C, Tenori L
Knowledge discovery by accuracy maximization.
Proc Natl Acad Sci U S A 2014;111(14):5117-22. doi: 10.1073/pnas.1220873111. [Link](#)

Cacciatore S, Tenori L, Luchinat C, Bennett PR, MacIntyre DA
KODAMA: an updated R package for knowledge discovery and data mining.
Bioinformatics 2017;33(4):621-623. doi: 10.1093/bioinformatics/btw705. [Link](#)

See Also

[continuous_table](#), [txtsummary](#)

Examples

```
data(clinical)

A=categorical_table("Gender",clinical[, "Gender"],clinical[, "Hospital"])
B=categorical_table("Gleason score",clinical[, "Gleason score"],clinical[, "Hospital"])
C=categorical_table("Ethnicity",clinical[, "Ethnicity"],clinical[, "Hospital"])

D=continuous_table("BMI",clinical[, "BMI"],clinical[, "Hospital"],digits=2)
E=continuous_table("Age",clinical[, "Age"],clinical[, "Hospital"],digits=1)

rbind(A,B,C,D,E)
```

clinical

Clinical Data of a Cohort of Prostate Cancer Patients

Description

The data belong to a cohort of 35 patients with prostate cancer from two different hospitals.

Usage

```
data(clinical)
```

Value

The data.frame "prcomp" with the following elements: "Hospital", "Gender", "Gleason score", "Ethnicity", "BMI", and "Age".

Examples

```
data(clinical)
```

```
head(clinical)
```

continuous_table	<i>Continuous Information</i>
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Description

Summarization of the continuous information.

Usage

```
continuous_table (name,num, label, digits=0,scientific=FALSE)
```

Arguments

name	the name of the feature.
num	the information to summarize.
label	the classification of the cohort.
digits	how many significant digits are to be used.
scientific	either a logical specifying whether result should be encoded in scientific format.

Value

The function returns a table with the summarized information. If the number of group is equal to two, the p-value is computed using the Wilcoxon rank-sum test, Kruskal-Wallis test otherwise.

Author(s)

Stefano Cacciatore

References

Cacciatore S, Luchinat C, Tenori L
 Knowledge discovery by accuracy maximization.
Proc Natl Acad Sci U S A 2014;111(14):5117-22. doi: 10.1073/pnas.1220873111. [Link](#)

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See Also

[categorical_table](#), [txtsummary](#)

Examples

```

data(clinical)

A=categorical_table("Gender",clinical[, "Gender"],clinical[, "Hospital"])
B=categorical_table("Gleason score",clinical[, "Gleason score"],clinical[, "Hospital"])
C=categorical_table("Ethnicity",clinical[, "Ethnicity"],clinical[, "Hospital"])

D=continuous_table("BMI",clinical[, "BMI"],clinical[, "Hospital"],digits=2)
E=continuous_table("Age",clinical[, "Age"],clinical[, "Hospital"],digits=1)

rbind(A,B,C,D,E)

```

core_cpp

*Maximization of Cross-Validated Accuracy Methods***Description**

This function performs the maximization of cross-validated accuracy by an iterative process

Usage

```

core_cpp(x,
         xTdata=NULL,
         clbest,
         Tcycle=20,
         FUN=c("KNN", "PLS-DA"),
         fpar=2,
         constrain=NULL,
         fix=NULL,
         shake=FALSE)

```

Arguments

x	a matrix.
xTdata	a matrix for projections. This matrix contains samples that are not used for the maximization of the cross-validated accuracy. Their classification is obtained by predicting samples on the basis of the final classification vector.
clbest	a vector to optimize.
Tcycle	number of iterative cycles that leads to the maximization of cross-validated accuracy.
FUN	classifier to be consider. Choices are "KNN" and "PLS-DA".
fpar	parameters of the classifier. If the classifier is KNN, fpar represents the number of neighbours. If the classifier is PLS-DA, fpar represents the number of components.

constrain	a vector of <code>nrow(data)</code> elements. Supervised constraints can be imposed by linking some samples in such a way that if one of them is changed, all other linked samples change in the same way (<i>i.e.</i> , they are forced to belong to the same class) during the maximization of the cross-validation accuracy procedure. Samples with the same identifying constrain will be forced to stay together.
fix	a vector of <code>nrow(data)</code> elements. The values of this vector must be TRUE or FALSE. By default all elements are FALSE. Samples with the TRUE fix value will not change the class label defined in <code>W</code> during the maximization of the cross-validation accuracy procedure. For more information refer to Cacciatore, <i>et al.</i> (2014).
shake	if <code>shake = FALSE</code> the cross-validated accuracy is computed with the class defined in <code>W</code> , before the maximization of the cross-validation accuracy procedure.

Value

The function returns a list with 3 items:

<code>clbest</code>	a classification vector with a maximized cross-validated accuracy.
<code>accbest</code>	the maximum cross-validated accuracy achieved.
<code>vect_acc</code>	a vector of all cross-validated accuracies obtained.
<code>vect_proj</code>	a prediction of samples in <code>xTdata</code> matrix using the vector <code>clbest</code> . This output is present only if <code>xTdata</code> is not NULL.

Author(s)

Stefano Cacciatore and Leonardo Tenori

References

Cacciatore S, Luchinat C, Tenori L
 Knowledge discovery by accuracy maximization.
Proc Natl Acad Sci U S A 2014;111(14):5117-22. doi: 10.1073/pnas.1220873111. [Link](#)

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See Also

[KODAMA](#)

Examples

```
# Here, the famous (Fisher's or Anderson's) iris data set was loaded
data(iris)
u=as.matrix(iris[,-5])
s=sample(1:150,150,TRUE)

# The maximization of the accuracy of the vector s is performed
```

```
results=core_cpp(u, clbest=s, fpar = 10)

print(as.numeric(results$clbest))
```

dinisurface

Ulisse Dini Data Set Generator

Description

This function creates a data set based upon data points distributed on a Ulisse Dini's surface.

Usage

```
dinisurface(N=1000)
```

Arguments

N Number of data points.

Value

The function returns a three dimensional data set.

Author(s)

Stefano Cacciatore and Leonardo Tenori

References

Cacciatore S, Luchinat C, Tenori L
Knowledge discovery by accuracy maximization.
Proc Natl Acad Sci U S A 2014;111(14):5117-22. doi: 10.1073/pnas.1220873111. [Link](#)

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See Also

[helicoid](#), [swissroll](#), [spirals](#)

Examples

```
require("rgl")
x=dinisurface()
open3d()
plot3d(x, col=rainbow(1000),box=FALSE,size=3)
rgl.postscript("dinisurface.pdf", fmt="pdf")
```

`floyd`*Find Shortest Paths Between All Nodes in a Graph*

Description

The `floyd` function finds all shortest paths in a graph using Floyd's algorithm.

Usage

```
floyd(data)
```

Arguments

`data` matrix or distance object

Value

`floyd` returns a matrix with the total lengths of the shortest path between each pair of points.

References

Floyd, Robert W
Algorithm 97: Shortest Path.
Communications of the ACM 1962; 5 (6): 345. doi:10.1145/367766.368168. [Link](#)

Examples

```
# build a graph with 5 nodes
x=matrix(c(0,NA,NA,NA,NA,30,0,NA,NA,NA,10,NA,0,NA,NA,NA,70,50,0,10,NA,40,20,60,0),ncol=5)
print(x)

# compute all path lengths
z=floyd(x)
print(z)
```

`frequency_matching`*Frequency Matching*

Description

A method to select unbalanced groupd in a cohort.

Usage

```
frequency_matching (data,label,times=5,seed=1234)
```


Arguments

data	a data.frame of data.
label	a classification of the groups.
times	The ratio between the two groups.
seed	a single number for random number generation.

Value

The function returns a list with 2 items or 4 items (if a test data set is present):

data	the data after the frequency matching.
label	the label after the frequency matching.
selection	the rows selected for the frequency matching.

Author(s)

Stefano Cacciatore

References

Cacciatore S, Luchinat C, Tenori L
 Knowledge discovery by accuracy maximization.
Proc Natl Acad Sci U S A 2014;111(14):5117-22. doi: 10.1073/pnas.1220873111. [Link](#)

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Bioinformatics 2017;33(4):621-623. doi: 10.1093/bioinformatics/btw705. [Link](#)

Examples

```
data(clinical)

A=categorical_table("Gender",clinical[, "Gender"],clinical[, "Hospital"])
B=categorical_table("Gleason score",clinical[, "Gleason score"],clinical[, "Hospital"])
C=categorical_table("Ethnicity",clinical[, "Ethnicity"],clinical[, "Hospital"])

D=continuous_table("BMI",clinical[, "BMI"],clinical[, "Hospital"],digits=2)
E=continuous_table("Age",clinical[, "Age"],clinical[, "Hospital"],digits=1)

# Analysis without matching
rbind(A,B,C,D,E)

# The order is important. Right is more important than left in the vector
# So, Ethnicity will be more important than Age
var=c("Age","BMI","Gleason score","Ethnicity")
t=frequency_matching(clinical[,var],clinical[, "Hospital"],times=1)
```

```
newdata=clinical[t$selection,]  
  
A=categorical_table("Gender",newdata[, "Gender"],newdata[, "Hospital"])  
B=categorical_table("Gleason score",newdata[, "Gleason score"],newdata[, "Hospital"])  
C=categorical_table("Ethnicity",newdata[, "Ethnicity"],newdata[, "Hospital"])  
  
D=continuous_table("BMI",newdata[, "BMI"],newdata[, "Hospital"],digits=2)  
E=continuous_table("Age",newdata[, "Age"],newdata[, "Hospital"],digits=1)  
  
# Analysis with matching  
rbind(A,B,C,D,E)
```

helicoid

Helicoid Data Set Generator

Description

This function creates a data set based upon data points distributed on a Helicoid surface.

Usage

```
helicoid(N=1000)
```

Arguments

N Number of data points.

Value

The function returns a three dimensional data set.

Author(s)

Stefano Cacciatore and Leonardo Tenori

References

Cacciatore S, Luchinat C, Tenori L
Knowledge discovery by accuracy maximization.
Proc Natl Acad Sci U S A 2014;111(14):5117-22. doi: 10.1073/pnas.1220873111. [Link](#)

Cacciatore S, Tenori L, Luchinat C, Bennett PR, MacIntyre DA
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Bioinformatics 2017;33(4):621-623. doi: 10.1093/bioinformatics/btw705. [Link](#)

See Also

[swissroll](#),[dini](#),[surface](#),[spirals](#)

Examples

```
require("rgl")
x=helicoid()
open3d()
plot3d(x, col=rainbow(1000),box=FALSE,size=3)
rgl.postscript("helicoid.pdf", fmt="pdf")
```

k.test

K-Test of Statistical Association

Description

This function performs a permutation test using PLS to assess association between the KODAMA output and any additional related parameters such as clinical metadata.

Usage

```
k.test(data, labels, n = 100)
```

Arguments

data	a matrix.
labels	a classification vector.
n	number of iterations of the permutation test.

Value

The p-value of the test.

Author(s)

Stefano Cacciatore

References

Cacciatore S, Luchinat C, Tenori L
Knowledge discovery by accuracy maximization.
Proc Natl Acad Sci U S A 2014;111(14):5117-22. doi: 10.1073/pnas.1220873111. [Link](#)

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See Also

[KODAMA](#)

Examples

```
# data(iris)
# data=iris[,-5]
# labels=iris[,5]
# kk=KODAMA(data,FUN="PLS-DA")
# kkplot=kk$pp
# k1=k.test(kkplot,labels)
# print(k1)
# k2=k.test(kkplot,sample(labels))
# print(k2)
```

knn.double.cv

Cross-Validation with k-Nearest Neighbors algorithm.

Description

This function performs a 10-fold cross validation on a given data set using k -Nearest Neighbors (k NN) model. To assess the prediction ability of the model, a 10-fold cross-validation is conducted by generating splits with a ratio 1:9 of the data set, that is by removing 10% of samples prior to any step of the statistical analysis, including PLS component selection and scaling. Best number of component for PLS was carried out by means of 10-fold cross-validation on the remaining 90% selecting the best Q^2 value. Permutation testing was undertaken to estimate the classification/regression performance of predictors.

Usage

```
knn.double.cv(Xdata,
              Ydata,
              constrain=1:nrow(Xdata),
              compmax=min(c(ncol(Xdata),nrow(Xdata))),
              perm.test=FALSE,
              optim=TRUE,
              scaling = c("centering","autoscaling"),
              times=100,
              runn=10)
```

Arguments

Xdata	a matrix.
Ydata	the responses. If Ydata is a numeric vector, a regression analysis will be performed. If Ydata is factor, a classification analysis will be performed.
constrain	a vector of nrow(data) elements. Sample with the same identifying constrain will be split in the training set or in the test set of cross-validation together.
compmax	the number of k to be used for classification.
perm.test	a classification vector.
optim	if perform the optimization of the number of k.

scaling	the scaling method to be used. Choices are "centering" or "autoscaling" (by default = "centering"). A partial string sufficient to uniquely identify the choice is permitted.
times	number of cross-validations with permuted samples
runn	number of cross-validations loops.

Value

A list with the following components:

Ypred	the vector containing the predicted values of the response variables obtained by cross-validation.
Yfit	the vector containing the fitted values of the response variables.
Q2Y	Q2y value.
R2Y	R2y value.
conf	The confusion matrix (only in classification mode).
acc	The cross-validated accuracy (only in classification mode).
txtQ2Y	a summary of the Q2y values.
txtR2Y	a summary of the R2y values.

Author(s)

Stefano Cacciatore

References

Cacciatore S, Luchinat C, Tenori L
 Knowledge discovery by accuracy maximization.
Proc Natl Acad Sci U S A 2014;111(14):5117-22. doi: 10.1073/pnas.1220873111. [Link](#)

Cacciatore S, Tenori L, Luchinat C, Bennett PR, MacIntyre DA
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Examples

```
data(iris)
data=iris[,-5]
labels=iris[,5]
pp=knn.double.cv(data,labels)
print(pp$Q2Y)
table(pp$Ypred,labels)

#
# data(MetRef)
# u=MetRef$data;
# u=u[,-which(colSums(u)==0)]
# u=normalization(u)$newXtrain
```

```
# u=scaling(u)$newXtrain
# pp=knn.double.cv(u,as.factor(MetRef$donor))
# print(pp$Q2Y)
# table(pp$Ypred, MetRef$donor)
#
```

knn.kodama

k-Nearest Neighbors Classifier.

Description

k-nearest neighbour classification for a test set from a training set.

Usage

```
knn.kodama(Xtrain,
           Ytrain,
           Xtest,
           Ytest=NULL,
           k,
           scaling = c("centering", "autoscaling"),
           perm.test=FALSE,
           times=1000)
```

Arguments

Xtrain	a matrix of training set cases.
Ytrain	a classification vector.
Xtest	a matrix of test set cases.
Ytest	a classification vector.
k	the number of nearest neighbors to consider.
scaling	the scaling method to be used. Choices are "centering" or "autoscaling" (by default = "centering"). A partial string sufficient to uniquely identify the choice is permitted.
perm.test	a classification vector.
times	a classification vector.

Details

The function utilizes the Approximate Nearest Neighbor (ANN) C++ library, which can give the exact nearest neighbours or (as the name suggests) approximate nearest neighbours to within a specified error bound. For more information on the ANN library please visit <http://www.cs.umd.edu/~mount/ANN/>.

Value

The function returns a vector of predicted labels.

Author(s)

Stefano Cacciatore and Leonardo Tenori

References

Bentley JL (1975)

Multidimensional binary search trees used for associative search.

Communication ACM 1975;18:309-517.

Arya S, Mount DM

Approximate nearest neighbor searching

Proc. 4th Ann. ACM-SIAM Symposium on Discrete Algorithms (SODA'93);271-280.

Arya S, Mount DM, Netanyahu NS, Silverman R, Wu AY

An optimal algorithm for approximate nearest neighbor searching

Journal of the ACM 1998;45:891-923.

Cacciatore S, Luchinat C, Tenori L

Knowledge discovery by accuracy maximization.

Proc Natl Acad Sci U S A 2014;111(14):5117-22. doi: 10.1073/pnas.1220873111. [Link](#)

Cacciatore S, Tenori L, Luchinat C, Bennett PR, MacIntyre DA

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See Also

[KODAMA](#)

Examples

```
data(iris)
data=iris[,-5]
labels=iris[,5]
ss=sample(150,15)

z=knn.kodama(data[-ss,], labels[-ss], data[ss,], k=5)
table(z$ypred[,5],labels[ss])
```

Description

KODAMA (KnOwledge Discovery by Accuracy MAximization) is an unsupervised and semi-supervised learning algorithm that performs feature extraction from noisy and high-dimensional data. Unlike other data mining methods, KODAMA is driven by an integrated procedure of cross validation of the results.

Usage

```
KODAMA(data,
        M = 100,
        Tcycle = 20,
        FUN_VAR = function(x) { ceiling(ncol(x)) },
        FUN_SAM = function(x) { ceiling(nrow(x) * 0.75)},
        bagging = FALSE,
        FUN = c("KNN", "PLS-DA"),
        f.par = 5,
        W = NULL,
        constrain = NULL,
        fix=NULL,
        epsilon = 0.05,
        dims=2,
        landmarks=5000)
```

Arguments

<code>data</code>	a matrix.
<code>M</code>	number of iterative processes (step I-III).
<code>Tcycle</code>	number of iterative cycles that leads to the maximization of cross-validated accuracy.
<code>FUN_VAR</code>	function to select the number of variables to select randomly. By default all variable are taken.
<code>FUN_SAM</code>	function to select the number of samples to select randomly. By default the 75 per cent of all samples are taken.
<code>bagging</code>	Should sampling be with replacement, <code>bagging = TRUE</code> . By default <code>bagging = FALSE</code> .
<code>FUN</code>	classifier to be considered. Choices are "KNN" and "PLS-DA".
<code>f.par</code>	parameters of the classifier.
<code>W</code>	a vector of <code>nrow(data)</code> elements. The KODAMA procedure can be started by different initializations of the vector <code>W</code> . Without any <i>a priori</i> information the vector <code>W</code> can be initialized with each element being different from the others (<i>i.e.</i> , each sample categorized in a one-element class). Alternatively, the vector <code>W</code> can be initialized by a clustering procedure, such as kmeans .

constrain	a vector of <code>nrow(data)</code> elements. Supervised constraints can be imposed by linking some samples in such a way that if one of them is changed the remaining linked samples must change in the same way (<i>i.e.</i> , they are forced to belong to the same class) during the maximization of the cross-validation accuracy procedure. Samples with the same identifying constrain will be forced to stay together.
fix	a vector of <code>nrow(data)</code> elements. The values of this vector must to be TRUE or FALSE. By default all elements are FALSE. Samples with the TRUE fix value will not change the class label defined in <code>W</code> during the maximization of the cross-validation accuracy procedure.
epsilon	cut-off value for low proximity. High proximity are typical of intracluster relationships, whereas low proximities are expected for intercluster relationships. Very low proximities between samples are ignored by (default) setting <code>epsilon = 0.05</code> .
dims	dimensions of the configurations of Sammon's non-linear mapping based on the KODAMA dissimilarity matrix.
landmarks	number of landmarks to use.

Details

KODAMA consists of five steps. These can be in turn divided into two parts: (i) the maximization of cross-validated accuracy by an iterative process (step I and II), resulting in the construction of a proximity matrix (step III), and (ii) the definition of a dissimilarity matrix (step IV and V). The first part entails the core idea of KODAMA, that is, the partitioning of data guided by the maximization of the cross-validated accuracy. At the beginning of this part, a fraction of the total samples (defined by `FUN_SAM`) are randomly selected from the original data. The whole iterative process (step I-III) is repeated `M` times to average the effects owing to the randomness of the iterative procedure. Each time that this part is repeated, a different fraction of samples is selected. The second part aims at collecting and processing these results by constructing a dissimilarity matrix to provide a holistic view of the data while maintaining their intrinsic structure (steps IV and V). Then, Sammon's non-linear mapping is used to visualise the results of KODAMA dissimilarity matrix. For additional information, visit <http://www.kodama-project.com/>.

Value

The function returns a list with 4 items:

dissimilarity	a dissimilarity matrix.
acc	a vector with the <code>M</code> cross-validated accuracies.
proximity	a proximity matrix.
v	a matrix containing the all classification obtained maximizing the cross-validation accuracy.
pp	a matrix containing the score of the Sammon's non-linear mapping.
res	a matrix containing all classification vectors obtained through maximizing the cross-validation accuracy.
f.par	parameters of the classifier.
entropy	Shannon's entropy of the KODAMA proximity matrix.
landpoints	indexes of the landmarks used.

Author(s)

Stefano Cacciatore and Leonardo Tenori

References

Cacciatore S, Luchinat C, Tenori L
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Proc Natl Acad Sci U S A 2014;111(14):5117-22. doi: 10.1073/pnas.1220873111. [Link](#)

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Examples

```
# data(iris)
# data=iris[,-5]
# labels=iris[,5]
# kk=KODAMA(data)
# plot(kk$pp,col=as.numeric(labels), xlab="First component", ylab="Second component",cex=2)
```

 loads

Variable Ranking

Description

This function can be used to extract the variable ranking when KODAMA is performed with the PLS-DA classifier.

Usage

```
loads(model,method=c("loadings","kruskal.test"))
```

Arguments

model	output of KODAMA.
method	method to be used. Choices are "loadings" and "kruskal.test".

Value

The function returns a vector of values indicating the "importance" of each variable. If "method="loadings" the average of the loading of the first component of PLS models based on the cross-validated accuracy maximized vector is computed. If "method="kruskal.test" the average of minus logarithm of p-value of Kruskal-Wallis Rank Sum test is computed.

Author(s)

Stefano Cacciatore

References

Cacciatore S, Luchinat C, Tenori L
Knowledge discovery by accuracy maximization.
Proc Natl Acad Sci U S A 2014;111(14):5117-22. doi: 10.1073/pnas.1220873111. [Link](#)

Cacciatore S, Tenori L, Luchinat C, Bennett PR, MacIntyre DA
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Bioinformatics 2017;33(4):621-623. doi: 10.1093/bioinformatics/btw705. [Link](#)

See Also[KODAMA](#)**Examples**

```
# data(iris)
# data=iris[,-5]
# labels=iris[,5]
# kk=KODAMA(data,FUN="PLS-DA")
# loads(kk)
```

lymphoma

Lymphoma Gene Expression Dataset

Description

This dataset consists of gene expression profiles of the three most prevalent adult lymphoid malignancies: diffuse large B-cell lymphoma (DLBCL), follicular lymphoma (FL), and B-cell chronic lymphocytic leukemia (B-CLL). The dataset consists of 4,682 mRNA genes for 62 samples (42 samples of DLBCL, 9 samples of FL, and 11 samples of B-CLL). Missing value are imputed and data are standardized as described in Dudoit, *et al.* (2002).

Usage

```
data(lymphoma)
```

Value

A list with the following elements:

data	Gene expression data. A matrix with 62 rows and 4,682 columns.
class	Class index. A vector with 62 elements.

References

- Cacciatore S, Luchinat C, Tenori L
Knowledge discovery by accuracy maximization.
Proc Natl Acad Sci U S A 2014;111(14):5117-22. doi: 10.1073/pnas.1220873111. [Link](#)
- Cacciatore S, Tenori L, Luchinat C, Bennett PR, MacIntyre DA
KODAMA: an updated R package for knowledge discovery and data mining.
Bioinformatics 2017;33(4):621-623. doi: 10.1093/bioinformatics/btw705. [Link](#)
- Alizadeh AA, Eisen MB, Davis RE, *et al.*
Distinct types of diffuse large B-cell lymphoma identified by gene expression profiling.
Nature 2000;403(6769):503-511.
- Dudoit S, Fridlyand J, Speed TP
Comparison of discrimination methods for the classification of tumors using gene expression data.
J Am Stat Assoc 2002;97(417):77-87.

Examples

```
data(lymphoma)
class=1+as.numeric(lymphoma$class)
cc=prcomp(lymphoma$data)$x
plot(cc,pch=21,bg=class,xlab="First Component",ylab="Second Component")

#
# kk=KODAMA(lymphoma$data)
# plot(kk$pp,pch=21,bg=class,xlab="First Component",ylab="Second Component")
#
```

mcplot

Evaluation of the Monte Carlo accuracy results

Description

This function can be used to plot the accuracy values obtained during KODAMA procedure.

Usage

```
mcplot(model)
```

Arguments

model output of KODAMA.

Author(s)

Stefano Cacciatore

References

Cacciatore S, Luchinat C, Tenori L
Knowledge discovery by accuracy maximization.
Proc Natl Acad Sci U S A 2014;111(14):5117-22. doi: 10.1073/pnas.1220873111. [Link](#)

Cacciatore S, Tenori L, Luchinat C, Bennett PR, MacIntyre DA
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See Also

[KODAMA](#)

Examples

```
# data=as.matrix(iris[,-5])  
# kk=KODAMA(data)  
# mcplot(kk)
```

MetRef

Nuclear Magnetic Resonance Spectra of Urine Samples

Description

The data belong to a cohort of 22 healthy donors (11 male and 11 female) where each provided about 40 urine samples over the time course of approximately 2 months, for a total of 873 samples. Each sample was analysed by Nuclear Magnetic Resonance Spectroscopy. Each spectrum was divided in 450 spectral bins.

Usage

```
data(MetRef)
```

Value

A list with the following elements:

data	Metabolomic data. A matrix with 873 rows and 450 columns.
gender	Gender index. A vector with 873 elements.
donor	Donor index. A vector with 873 elements.

References

- Assfalg M, Bertini I, Colangiuli D, *et al.*
 Evidence of different metabolic phenotypes in humans.
Proc Natl Acad Sci U S A 2008;105(5):1420-4. doi: 10.1073/pnas.0705685105. [Link](#)
- Cacciatore S, Luchinat C, Tenori L
 Knowledge discovery by accuracy maximization.
Proc Natl Acad Sci U S A 2014;111(14):5117-22. doi: 10.1073/pnas.1220873111. [Link](#)
- Cacciatore S, Tenori L, Luchinat C, Bennett PR, MacIntyre DA
 KODAMA: an updated R package for knowledge discovery and data mining.
Bioinformatics 2017;33(4):621-623. doi: 10.1093/bioinformatics/btw705. [Link](#)

Examples

```
data(MetRef)
u=MetRef$data;
u=u[,-which(colSums(u)==0)]
u=normalization(u)$newXtrain
u=scaling(u)$newXtrain
class=as.numeric(as.factor(MetRef$gender))
cc= prcomp(u)$x
plot(cc,pch=21,bg=class,xlab="First Component",ylab="Second Component")

class=as.numeric(as.factor(MetRef$donor))
plot(cc,pch=21,bg=rainbow(22)[class],xlab="First Component",ylab="Second Component")

#
# kk=KODAMA(u)
# plot(kk$pp,pch=21,bg=rainbow(22)[class],xlab="First Component",ylab="Second Component")
#
```

normalization

Normalization Methods

Description

Collection of Different Normalization Methods.

Usage

```
normalization(Xtrain,Xtest=NULL, method = "pqn",ref=NULL)
```

Arguments

Xtrain a matrix of data (training data set).
 Xtest a matrix of data (test data set).(by default = NULL).

method	the normalization method to be used. Choices are "none", "pqn", "sum", "median", "sqrt" (by default = "pqn"). A partial string sufficient to uniquely identify the choice is permitted.
ref	Reference sample for Probabilistic Quotient Normalization. (by default = NULL).

Details

A number of different normalization methods are provided:

- "none": no normalization method is applied.
- "pqn": the Probabilistic Quotient Normalization is computed as described in *Dieterle, et al.* (2006).
- "sum": samples are normalized to the sum of the absolute value of all variables for a given sample.
- "median": samples are normalized to the median value of all variables for a given sample.
- "sqrt": samples are normalized to the root of the sum of the squared value of all variables for a given sample.

Value

The function returns a list with 2 items or 4 items (if a test data set is present):

newXtrain	a normalized matrix (training data set).
coeXtrain	a vector of normalization coefficient of the training data set.
newXtest	a normalized matrix (test data set).
coeXtest	a vector of normalization coefficient of the test data set.

Author(s)

Stefano Cacciatore and Leonardo Tenori

References

Dieterle F, Ross A, Schlotterbeck G, Senn H.
Probabilistic Quotient Normalization as Robust Method to Account for Dilution of Complex Biological Mixtures. Application in ¹H NMR Metabolomics.
Anal Chem 2006;78:4281-90.

Cacciatore S, Luchinat C, Tenori L
Knowledge discovery by accuracy maximization.
Proc Natl Acad Sci U S A 2014;111(14):5117-22. doi: 10.1073/pnas.1220873111. [Link](#)

Cacciatore S, Tenori L, Luchinat C, Bennett PR, MacIntyre DA
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See Also[scaling](#)**Examples**

```

data(MetRef)
u=MetRef$data;
u=u[,-which(colSums(u)==0)]
u=normalization(u)$newXtrain
u=scaling(u)$newXtrain
class=as.numeric(as.factor(MetRef$gender))
cc=pca(u)
plot(cc$x,pch=21,bg=class,xlab=cc$txt[1],ylab=cc$txt[2])

```

pca

*Principal Components Analysis***Description**

Performs a principal components analysis on the given data matrix and returns the results as an object of class "prcomp".

Usage

```
pca(x, ...)
```

Arguments

x a matrix of data.
 ... arguments passed to [prcomp](#) function.

Value

The function returns a list with class `prcomp` containing the following components:

sdev	the standard deviations of the principal components (i.e., the square roots of the eigenvalues of the covariance/correlation matrix, though the calculation is actually done with the singular values of the data matrix).
rotation	the matrix of variable loadings (i.e., a matrix whose columns contain the eigenvectors). The function <code>princomp</code> returns this in the element <code>loadings</code> .
x	if <code>retx</code> is <code>TRUE</code> the value of the rotated data (the centred (and scaled if requested) data multiplied by the rotation matrix) is returned. Hence, <code>cov(x)</code> is the diagonal matrix <code>diag(sdev^2)</code> . For the formula method, <code>napredict()</code> is applied to handle the treatment of values omitted by the <code>na.action</code> .
center, scale	the centering and scaling used, or <code>FALSE</code> .
txt	the component of variance of each Principal Component.

Author(s)

Stefano Cacciatore

References

Pearson, K
On Lines and Planes of Closest Fit to Systems of Points in Space.
Philosophical Magazine 1901;2 (11): 559-572. doi:10.1080/14786440109462720. [Link](#)

See Also[prcomp](#)**Examples**

```
data(MetRef)
u=MetRef$data;
u=u[,-which(colSums(u)==0)]
u=normalization(u)$newXtrain
u=scaling(u)$newXtrain
class=as.numeric(as.factor(MetRef$gender))
cc=pca(u)
plot(cc$x,pch=21,bg=class,xlab=cc$txt[1],ylab=cc$txt[2])
```

pls.double.cv

Cross-Validation with PLS-DA.

Description

This function performs a 10-fold cross validation on a given data set using Partial Least Squares (PLS) model. To assess the prediction ability of the model, a 10-fold cross-validation is conducted by generating splits with a ratio 1:9 of the data set, that is by removing 10% of samples prior to any step of the statistical analysis, including PLS component selection and scaling. Best number of component for PLS was carried out by means of 10-fold cross-validation on the remaining 90% selecting the best Q^2_y value. Permutation testing was undertaken to estimate the classification/regression performance of predictors.

Usage

```
pls.double.cv(Xdata,
             Ydata,
             constrain=1:nrow(Xdata),
             compmax=min(c(ncol(Xdata),nrow(Xdata))),
             perm.test=FALSE,
             optim=TRUE,
             scaling = c("centering","autoscaling"),
             times=100,
             runn=10)
```

Arguments

Xdata	a matrix.
Ydata	the responses. If Ydata is a numeric vector, a regression analysis will be performed. If Ydata is factor, a classification analysis will be performed.
constrain	a vector of nrow(data) elements. Sample with the same identifying constrain will be split in the training set or in the test set of cross-validation together.
compmax	the number of latent components to be used for classification.
perm.test	a classification vector.
optim	if perform the optimization of the number of components.
scaling	the scaling method to be used. Choices are "centering" or "autoscaling" (by default = "centering"). A partial string sufficient to uniquely identify the choice is permitted.
times	number of cross-validations with permuted samples
runn	number of cross-validations loops.

Value

A list with the following components:

B	the (p x m x length(ncomp)) array containing the regression coefficients. Each row corresponds to a predictor variable and each column to a response variable. The third dimension of the matrix B corresponds to the number of PLS components used to compute the regression coefficients. If ncomp has length 1, B is just a (p x m) matrix.
Ypred	the vector containing the predicted values of the response variables obtained by cross-validation.
Yfit	the vector containing the fitted values of the response variables.
P	the (p x max(ncomp)) matrix containing the X-loadings.
Q	the (m x max(ncomp)) matrix containing the Y-loadings.
T	the (ntrain x max(ncomp)) matrix containing the X-scores (latent components)
R	the (p x max(ncomp)) matrix containing the weights used to construct the latent components.
Q2Y	Q2y value.
R2Y	R2y value.
R2X	vector containing the explained variance of X by each PLS component.
txtQ2Y	a summary of the Q2y values.
txtR2Y	a summary of the R2y values.

Author(s)

Stefano Cacciatore

References

Cacciatore S, Luchinat C, Tenori L
Knowledge discovery by accuracy maximization.
Proc Natl Acad Sci U S A 2014;111(14):5117-22. doi: 10.1073/pnas.1220873111. [Link](#)

Cacciatore S, Tenori L, Luchinat C, Bennett PR, MacIntyre DA
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Bioinformatics 2017;33(4):621-623. doi: 10.1093/bioinformatics/btw705. [Link](#)

Examples

```
data(iris)
data=iris[,-5]
labels=iris[,5]
pp=pls.double.cv(data,labels)
print(pp$Q2Y)
table(pp$Ypred,labels)

#
# data(MetRef)
# u=MetRef$data;
# u=u[,-which(colSums(u)==0)]
# u=normalization(u)$newXtrain
# u=scaling(u)$newXtrain
# pp=pls.double.cv(u,as.factor(MetRef$donor))
# print(pp$Q2Y)
# table(pp$Ypred, MetRef$donor)
#
```

pls.kodama

Partial Least Squares regression.

Description

Partial Least Squares (PLS) regression for test set from training set.

Usage

```
pls.kodama(Xtrain,
           Ytrain,
           Xtest,
           Ytest = NULL,
           ncomp,
           scaling = c("centering", "autoscaling"),
           perm.test=FALSE,
           times=1000)
```

Arguments

Xtrain	a matrix of training set cases.
Ytrain	a classification vector.
Xtest	a matrix of test set cases.
Ytest	a classification vector.
ncomp	the number of components to consider.
scaling	the scaling method to be used. Choices are "centering" or "autoscaling" (by default = "centering"). A partial string sufficient to uniquely identify the choice is permitted.
perm.test	a classification vector.
times	a classification vector.

Value

A list with the following components:

B	the ($p \times m \times \text{length}(\text{ncomp})$) matrix containing the regression coefficients. Each row corresponds to a predictor variable and each column to a response variable. The third dimension of the matrix B corresponds to the number of PLS components used to compute the regression coefficients. If ncomp has length 1, B is just a ($p \times m$) matrix.
Ypred	the ($n_{\text{test}} \times m \times \text{length}(\text{ncomp})$) containing the predicted values of the response variables for the observations from Xtest. The third dimension of the matrix Ypred corresponds to the number of PLS components used to compute the regression coefficients.
P	the ($p \times \max(\text{ncomp})$) matrix containing the X-loadings.
Q	the ($m \times \max(\text{ncomp})$) matrix containing the Y-loadings.
T	the ($n_{\text{train}} \times \max(\text{ncomp})$) matrix containing the X-scores (latent components)
R	the ($p \times \max(\text{ncomp})$) matrix containing the weights used to construct the latent components.

Author(s)

Stefano Cacciatore

References

- Cacciatore S, Luchinat C, Tenori L
 Knowledge discovery by accuracy maximization.
Proc Natl Acad Sci U S A 2014;111(14):5117-22. doi: 10.1073/pnas.1220873111. [Link](#)
- Cacciatore S, Tenori L, Luchinat C, Bennett PR, MacIntyre DA
 KODAMA: an updated R package for knowledge discovery and data mining.
Bioinformatics 2017;33(4):621-623. doi: 10.1093/bioinformatics/btw705. [Link](#)

See Also[KODAMA](#)**Examples**

```

data(iris)
data=iris[,-5]
labels=iris[,5]
ss=sample(150,15)
ncomponent=3

z=pls.kodama(data[-ss,], labels[-ss], data[ss,], ncomp=ncomponent)
table(z$Ypred[,ncomponent],labels[ss])

```

scaling

*Scaling Methods***Description**

Collection of Different Scaling Methods.

Usage

```
scaling(Xtrain,Xtest=NULL, method = "autoscaling")
```

Arguments

Xtrain	a matrix of data (training data set).
Xtest	a matrix of data (test data set).(by default = NULL).
method	the scaling method to be used. Choices are "none", "centering", "autoscaling", "rangescaling", "paretoscaling" (by default = "autoscaling"). A partial string sufficient to uniquely identify the choice is permitted.

Details

A number of different scaling methods are provided:

- "none": no scaling method is applied.
- "centering": centers the mean to zero.
- "autoscaling": centers the mean to zero and scales data by dividing each variable by the variance.
- "rangescaling": centers the mean to zero and scales data by dividing each variable by the difference between the minimum and the maximum value.
- "paretoscaling": centers the mean to zero and scales data by dividing each variable by the square root of the standard deviation. Unit scaling divides each variable by the standard deviation so that each variance equal to 1.

Value

The function returns a list with 1 item or 2 items (if a test data set is present):

`newXtrain` a scaled matrix (training data set).
`newXtest` a scale matrix (test data set).

Author(s)

Stefano Cacciatore and Leonardo Tenori

References

van den Berg RA, Hoefsloot HCJ, Westerhuis JA, *et al.*
Centering, scaling, and transformations: improving the biological information content of metabolomics data.
BMC Genomics 2006;7(1):142.

Cacciatore S, Luchinat C, Tenori L
Knowledge discovery by accuracy maximization.
Proc Natl Acad Sci U S A 2014;111(14):5117-22. doi: 10.1073/pnas.1220873111. [Link](#)

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Bioinformatics 2017;33(4):621-623. doi: 10.1093/bioinformatics/btw705. [Link](#)

See Also

[normalization](#)

Examples

```
data(MetRef)
u=MetRef$data;
u=u[,-which(colSums(u)==0)]
u=normalization(u)$newXtrain
u=scaling(u)$newXtrain
class=as.numeric(as.factor(MetRef$gender))
cc=pca(u)
plot(cc$x,pch=21,bg=class,xlab=cc$txt[1],ylab=cc$txt[2])
```

spirals

Spirals Data Set Generator

Description

Produces a data set of spiral clusters.

Usage

```
spirals(n=c(100,100,100),sd=c(0,0,0))
```

Arguments

n a vector of integer. The length of the vector is the number of clusters and each number corresponds to the number of data points in each cluster.

sd amount of noise for each spiral.

Value

The function returns a two dimensional data set.

Author(s)

Stefano Cacciatore and Leonardo Tenori

References

Cacciatore S, Luchinat C, Tenori L
Knowledge discovery by accuracy maximization.
Proc Natl Acad Sci U S A 2014;111(14):5117-22. doi: 10.1073/pnas.1220873111. [Link](#)

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Bioinformatics 2017;33(4):621-623. doi: 10.1093/bioinformatics/btw705. [Link](#)

See Also

[helicoid](#),[dinisurface](#),[swissroll](#)

Examples

```
pdf(file="spirals.pdf")
par(mfrow=c(2,2),mai=c(0,0,0,0))
v1=spirals(c(100,100,100),c(0.1,0.1,0.1))
plot(v1,col=rep(2:4,each=100))
v2=spirals(c(100,100,100),c(0.1,0.2,0.3))
plot(v2,col=rep(2:4,each=100))
v3=spirals(c(100,100,100,100,100),c(0,0,0.2,0,0))
plot(v3,col=rep(2:6,each=100))
v4=spirals(c(20,40,60,80,100),c(0.1,0.1,0.1,0.1,0.1))
plot(v4,col=rep(2:6,c(20,40,60,80,100)))
dev.off()
```

`swissroll`*Swiss Roll Data Set Generator*

Description

Computes the Swiss Roll data set of a given number of data points.

Usage

```
swissroll(N=1000)
```

Arguments

N Number of data points.

Value

The function returns a three dimensional matrix.

Author(s)

Stefano Cacciatore and Leonardo Tenori

References

Balasubramanian M, Schwartz EL
The isomap algorithm and topological stability.
Science 2002;295(5552):7.

Roweis ST, Saul LK
Nonlinear dimensionality reduction by locally linear embedding.
Science 2000;290(5500):2323-6.

Cacciatore S, Luchinat C, Tenori L
Knowledge discovery by accuracy maximization.
Proc Natl Acad Sci U S A 2014;111(14):5117-22. doi: 10.1073/pnas.1220873111. [Link](#)

Cacciatore S, Tenori L, Luchinat C, Bennett PR, MacIntyre DA
KODAMA: an updated R package for knowledge discovery and data mining.
Bioinformatics 2017;33(4):621-623. doi: 10.1093/bioinformatics/btw705. [Link](#)

See Also

[helicoid](#),[dini](#),[surface](#),[spirals](#)

Examples

```
require("rgl")
x=swissroll()
open3d()
plot3d(x, col=rainbow(1000),box=FALSE,size=3)
rgl.postscript("swissroll.pdf", fmt="pdf")
```

transformy

Conversion Classification Vector to Matrix

Description

This function converts a classification vector into a classification matrix.

Usage

```
transformy(y)
```

Arguments

y a vector or factor.

Details

This function converts a classification vector into a classification matrix.

Value

A matrix.

Author(s)

Stefano Cacciatore and Leonardo Tenori

References

Cacciatore S, Luchinat C, Tenori L
Knowledge discovery by accuracy maximization.
Proc Natl Acad Sci U S A 2014;111(14):5117-22. doi: 10.1073/pnas.1220873111. [Link](#)

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Bioinformatics 2017;33(4):621-623. doi: 10.1093/bioinformatics/btw705. [Link](#)

Examples

```
y=rep(1:10,3)
print(y)
z=transformy(y)
print(z)
```

txtsummary

Median and Coefficient Interval

Description

Summarization of a numeric vector.

Usage

```
txtsummary (x,digits=0,scientific=FALSE)
```

Arguments

x	a numeric vector.
digits	how many significant digits are to be used.
scientific	either a logical specifying whether result should be encoded in scientific format.

Value

The function returns the median and the 95% coefficient interval of numeric vector.

Author(s)

Stefano Cacciatore

References

Cacciatore S, Luchinat C, Tenori L
Knowledge discovery by accuracy maximization.
Proc Natl Acad Sci U S A 2014;111(14):5117-22. doi: 10.1073/pnas.1220873111. [Link](#)

Cacciatore S, Tenori L, Luchinat C, Bennett PR, MacIntyre DA
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Bioinformatics 2017;33(4):621-623. doi: 10.1093/bioinformatics/btw705. [Link](#)

See Also

[categorical_table](#),[continuous_table](#)

Examples

```
data(clinical)  
  
txtsummary(clinical[, "BMI"])
```

Description

This dataset consists of the spoken, not written, addresses from 1900 until the sixth address by Barack Obama in 2014. Punctuation characters, numbers, words shorter than three characters, and stop-words (e.g., "that", "and", and "which") were removed from the dataset. This resulted in a dataset of 86 speeches containing 834 different meaningful words each. Term frequency-inverse document frequency (TF-IDF) was used to obtain feature vectors. It is often used as a weighting factor in information retrieval and text mining. The TF-IDF value increases proportionally to the number of times a word appears in the document, but is offset by the frequency of the word in the corpus, which helps to control for the fact that some words are generally more common than others.

Usage

```
data(USA)
```

Value

A list with the following elements:

data	TF-IDF data. A matrix with 86 rows and 834 columns.
year	Year index. A vector with 86 elements.
president	President index. A vector with 86 elements.

Author(s)

Stefano Cacciatore and Leonardo Tenori

References

Cacciatore S, Luchinat C, Tenori L
Knowledge discovery by accuracy maximization.
Proc Natl Acad Sci U S A 2014;111(14):5117-22. doi: 10.1073/pnas.1220873111. [Link](#)

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Examples

```
# Here is reported the analysis on the State of the Union  
# of USA president as shown in Cacciatore, et al. (2014)  
#  
# data(USA)  
# kk=KODAMA(USA$data)  
# cc=cmdscale(kk$dissimilarity)
```

```
# par(cex=0.5,mar=c(15,6,2,2));  
# plot(USA$year,cc[,1],axes=F,pch=20,xlab="",ylab="First Component");  
# axis(1,at=USA$year,labels=rownames(USA$data),las=2);  
# axis(2,las=2);  
# box()  
#
```

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