# The e1071 Package

October 7, 2003

**Version** 1.3-13

hanning.window

Date 2003-09-25
Title Misc Functions of the Department of Statistics (e1071), TU Wien
<b>Depends</b> R ( $>= 1.3.1$ ), mva, class, mlbench
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<b>Description</b> Functions for latent class analysis, short time Fourier transform, fuzzy clustering, support vector machines,
<b>License</b> GPL version 2. See COPYRIGHT.svm.cpp for the copyright of the svm C++ code.
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Discrete

Discrete Distribution

#### Description

These functions provide information about the discrete distribution where the probability of the elements of values is proportional to the values given in probs, which are normalized to sum up to 1. ddiscrete gives the density, pdiscrete gives the distribution function, qdiscrete gives the quantile function and rdiscrete generates random deviates.

## Usage

```
ddiscrete(x, probs, values = 1:length(probs))
pdiscrete(q, probs, values = 1:length(probs))
qdiscrete(p, probs, values = 1:length(probs))
rdiscrete(n, probs, values = 1:length(probs), ...)
```

#### Arguments

```
x,q
vector or array of quantiles.
p
vector or array of probabilites.
n
number of observations.
probs
probabilities of the distribution.
values
values of the distribution.
ignored (only there for backwards compatibility)
```

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#### **Details**

The random number generator is simply a wrapper for sample and provided for backwards compatibility only.

### Author(s)

Andreas Weingessel and Friedrich Leisch

#### Examples

```
## a vector of length 30 whose elements are 1 with probability 0.2
## and 2 with probability 0.8.
rdiscrete (30, c(0.2, 0.8))

## a vector of length 100 whose elements are A, B, C, D.
## The probabilities of the four values have the relation 1:2:3:3
rdiscrete (100, c(1,2,3,3), c("A","B","C","D"))
```

HouseVotes84

United States Congressional Voting Records 1984

## Description

This data set includes votes for each of the U.S. House of Representatives Congressmen on the 16 key votes identified by the CQA. The CQA lists nine different types of votes: voted for, paired for, and announced for (these three simplified to yea), voted against, paired against, and announced against (these three simplified to nay), voted present to avoid conflict of interest, and did not vote or otherwise make a position known (these three simplified to an unknown disposition).

#### Usage

data(HouseVotes84)

#### **Format**

A data frame with 435 observations on 17 variables:

- 1 Class Name: 2 (democrat, republican)
- 2 handicapped-infants: 2 (y,n)
- 3 water-project-cost-sharing: 2 (y,n)
- 4 adoption-of-the-budget-resolution: 2 (y,n)
- 5 physician-fee-freeze: 2 (y,n)
- 6 el-salvador-aid: 2 (y,n)
- 7 religious-groups-in-schools: 2 (y,n)
- 8 anti-satellite-test-ban: 2 (y,n)
- 9 aid-to-nicaraguan-contras: 2 (y,n)
- 10 mx-missile: 2 (y,n)
- 11 immigration: 2 (y,n)
- 12 synfuels-corporation-cutback: 2 (y,n)
- 13 education-spending: 2 (y,n)

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```
superfund-right-to-sue: 2 (y,n)
crime: 2 (y,n)
duty-free-exports: 2 (y,n)
export-administration-act-south-africa: 2 (y,n)
```

#### Source

- Source: Congressional Quarterly Almanac, 98th Congress, 2nd session 1984, Volume XL: Congressional Quarterly Inc., ington, D.C., 1985
- Donor: Jeff Schlimmer (Jeffrey.Schlimmer@a.gp.cs.cmu.edu)

These data have been taken from the UCI Repository Of Machine Learning Databases at

- ftp://ftp.ics.uci.edu/pub/machine-learning-databases
- http://www.ics.uci.edu/~mlearn/MLRepository.html

and were converted to R format by Friedrich.Leisch@ci.tuwien.ac.at.

bclust

Bagged Clustering

## Description

Cluster the data in x using the bagged clustering algorithm. A partitioning cluster algorithm such as kmeans is run repeatedly on bootstrap samples from the original data. The resulting cluster centers are then combined using the hierarchical cluster algorithm hclust.

#### Usage

### Arguments

x	Matrix of inputs (or object of class "bclust" for plot).
centers, k	Number of clusters.
iter.base	Number of runs of the base cluster algorithm.
minsize	Minimum number of points in a base cluster.
dist.method	Distance method used for the hierarchical clustering, see <code>dist</code> for available distances.

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hclust.method Linkage method used for the hierarchical clustering, see hclust for avail-

able methods.

base.method Partitioning cluster method used as base algorithm.

base.centers Number of centers used in each repetition of the base method.

verbose Output status messages.

final.kmeans If TRUE, a final kmeans step is performed using the output of the bagged

clustering as initialization.

docmdscale Logical, if TRUE a cmdscale result is included in the return value.

resample Logical, if TRUE the base method is run on bootstrap samples of x, else

directly on x.

weights Vector of length nrow(x), weights for the resampling. By default all

observations have equal weight.

maxcluster Maximum number of clusters memberships are to be computed for.

object Object of class "bclust".

main Main title of the plot.

... Optional arguments top be passed to the base method in bclust, ignored

in plot.

#### **Details**

First, iter.base bootstrap samples of the original data in x are created by drawing with replacement. The base cluster method is run on each of these samples with base.centers centers. The base.method must be the name of a partitioning cluster function returning a list with the same components as the return value of kmeans.

This results in a collection of iter.base \* base.centers centers, which are subsequently clustered using the hierarchical method hclust. Base centers with less than minsize points in there respective partitions are removed before the hierarchical clustering.

The resulting dendrogram is then cut to produce centers clusters. Hence, the name of the argument centers is a little bit misleading as the resulting clusters need not be convex, e.g., when single linkage is used. The name was chosen for compatibility with standard partitioning cluster methods such as kmeans.

A new hierarchical clustering (e.g., using another hclust.method) re-using previous base runs can be performed by running hclust.bclust on the return value of bclust.

#### Value

bclust and hclust.bclust return objects of class "bclust" including the components

hclust Return value of the hierarchical clustering of the collection of base centers

(Object of class "hclust").

cluster Vector with indices of the clusters the inputs are assigned to.

centers Matrix of centers of the final clusters. Only useful, if the hierarchical

clustering method produces convex clusters.

allcenters Matrix of all iter.base \* base.centers centers found in the base runs.

#### Author(s)

Friedrich Leisch

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#### References

Friedrich Leisch. Bagged clustering. Working Paper 51, SFB "Adaptive Information Systems and Modeling in Economics and Management Science", August 1999. http://www.ci.tuwien.ac.at/~leisch

## See Also

```
hclust, kmeans, boxplot.bclust
```

## Examples

```
data(iris)
bc1 <- bclust(iris[,1:4], 3, base.centers=5)
plot(bc1)

table(clusters.bclust(bc1, 3))
centers.bclust(bc1, 3)</pre>
```

bincombinations

Binary Combinations

## Description

Returns a matrix containing the  $2^p$  vectors of length p.

## Usage

```
bincombinations(p)
```

## Arguments

р

Length of binary vectors

## Author(s)

Friedrich Leisch

```
bincombinations(2)
bincombinations(3)
```

bootstrap.lca 7

bootstrap.lca $Boot$	strap Samples o	of LCA	Results
----------------------	-----------------	--------	---------

#### Description

This function draws bootstrap samples from a given LCA model and refits a new LCA model for each sample. The quality of fit of these models is compared to the original model.

## Usage

```
bootstrap.lca(1, nsamples=10, lcaiter=30, verbose=FALSE)
```

## Arguments

1 An LCA model as created by lca

nsamples Number of bootstrap samples

lcaiter Number of LCA iterations

verbose If TRUE some output is printed during the computations.

#### **Details**

From a given LCA model 1, nsamples bootstrap samples are drawn. For each sample a new LCA model is fitted. The goodness of fit for each model is computed via Likelihood Ratio and Pearson's Chisquare. The values for the fitted models are compared with the values of the original model 1. By this method it can be tested whether the data to which 1 was originally fitted come from an LCA model.

## Value

An object of class bootstrap.lca is returned, containing

 ${\tt loglsat} \quad {\tt The \ LogLikelihood \ of \ the \ models \ and \ of \ the \ corresponding \ saturated \ models}$ 

els

1ratio Likelihood quotient of the models and the coresponding saturated models

lratiomean, lratiosd

Mean and Standard deviation of lratio

1 Likelihood quotient of the original model and the corresponding satu-

rated model

zratio Z-Statistics of lratioorg

pvalzratio, pvalratio

P-Values for zratio, computed via normal distribution and empirical

distribution

chisq Pearson's Chisq of the models

chisqmean, chisqsd

Mean and Standard deviation of chisq

chisqorg Pearson's Chisq of the original model

zchisq Z-Statistics of chisqorg

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pvalzchisq, pvalchisq

P-Values for zchisq, computed via normal distribution and empirical

 $\operatorname{distribution}$ 

nsamples Number of bootstrap samples

lcaiter Number of LCA Iterations

## Author(s)

Andreas Weingessel

#### References

Anton K. Formann: "Die Latent-Class-Analysis", Beltz Verlag 1984

#### See Also

lca

### Examples

```
## Generate a 4-dim. sample with 2 latent classes of 500 data points each.
## The probabilities for the 2 classes are given by type1 and type2.
type1 <- c(0.8,0.8,0.2,0.2)
type2 <- c(0.2,0.2,0.8,0.8)
x <- matrix(runif(4000),nr=1000)
x[1:500,] <- t(t(x[1:500,])<type1)*1
x[501:1000,] <- t(t(x[501:1000,])<type2)*1

1 <- lca(x, 2, niter=5)
bl <- bootstrap.lca(1,nsamples=3,lcaiter=5)
bl</pre>
```

boxplot.bclust

Boxplot of cluster profiles

## Description

Makes boxplots of the results of a bagged clustering run.

### Usage

## Arguments

x Clustering result, object of class "bclust".

n Number of clusters to plot, by default the number of clusters used in the

call of bclust.

bycluster If TRUE (default), a boxplot for each cluster is plotted. If FALSE, a boxplot

for each variable is plotted.

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main Main title of the plot, by default the name of the cluster object.

oneplot If TRUE, all boxplots appear on one screen (using an appropriate rectan-

gular layout).

which Number of clusters which should be plotted, default is all clusters.

... Additional arguments for boxplot.

#### Author(s)

Friedrich Leisch

#### Examples

```
data(iris)
bc1 <- bclust(iris[,1:4], 3, base.centers=5)
boxplot(bc1)</pre>
```

classAgreement

Coefficients comparing classification agreement

### Description

classAgreement() computes several coefficients of agreement between the columns and rows of a 2-way contingency table.

### Usage

classAgreement(tab, match.names=FALSE)

#### Arguments

tab A 2-dimensional contingency table.

match.names Flag whether row and columns should be matched by name.

## Details

Suppose we want to compare two classifications summarized by the contingency table  $T = [t_{ij}]$  where  $i, j = 1, \ldots, K$  and  $t_{ij}$  denotes the number of data points which are in class i in the first partition and in class j in the second partition. If both classifications use the same labels, then obviously the two classification agree completely if only elements in the main diagonal of the table are non-zero. On the other hand, large off-diagonal elements correspond to smaller agreement between the two classifications. If match.names is TRUE, the class labels as given by the row and column names are matched, i.e. only columns and rows with the same dimnames are used for the computation.

If the two classification do not use the same set of labels, or if identical labels can have different meaning (e.g., two outcomes of cluster analysis on the same data set), then the situation is a little bit more complicated. Let A denote the number of all pairs of data points which are either put into the same cluster by both partitions or put into different clusters by both partitions. Conversely, let D denote the number of all pairs of data points that are put into one cluster in one partition, but into different clusters by the other partition. Hence, the partitions disagree for all pairs D and agree for all pairs A. We can measure the

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agreement by the Rand index A/(A+D) which is invariant with respect to permutations of the columns or rows of T.

Both indices have to be corrected for agreement by chance if the sizes of the classes are not uniform.

#### Value

A list with components

diag Percentage of data points in the main diagonal of tab.

kappa diag corrected for agreement by chance.

rand Rand index.

crand Rand index corrected for agreement by chance.

#### Author(s)

Friedrich Leisch

#### References

J. Cohen. A coefficient of agreement for nominal scales. Educational and Psychological Measurement, 20, 37–46, 1960.

Lawrence Hubert and Phipps Arabie. Comparing partitions. Journal of Classification, 2, 193-218, 1985.

#### See Also

matchClasses

```
## no class correlations: both kappa and crand almost zero
g1 <- sample(1:5, size=1000, replace=TRUE)
g2 <- sample(1:5, size=1000, replace=TRUE)
tab <- table(g1, g2)
classAgreement(tab)

## let pairs (g1=1,g2=1) and (g1=3,g2=3) agree better
k <- sample(1:1000, size=200)
g1[k] <- 1
g2[k] <- 1

k <- sample(1:1000, size=200)
g1[k] <- 3
g2[k] <- 3

tab <- table(g1, g2)

## both kappa and crand should be significantly larger than before classAgreement(tab)</pre>
```

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cmeans	Fuzzy C-Means Clustering	
--------	--------------------------	--

## Description

The fuzzy version of the known k means clustering algorithm as well as its online update (Unsupervised Fuzzy Competitive learning).

## Usage

#### Arguments

x	The data matrix where columns correspond to variables and rows to observations
centers	Number of clusters or initial values for cluster centers
iter.max	Maximum number of iterations
verbose	If TRUE, make some output during learning
dist	Must be one of the following: If "euclidean", the mean square error, if "manhattan", the mean absolute error is computed. Abbreviations are also accepted.
method	If "cmeans", then we have the cmeans fuzzy clustering method, if "ufcl" we have the On-line Update. Abbreviations in the method names are also accepted.
m	The degree of fuzzification. It is defined for values greater than 1
rate.par	The parameter of the learning rate

#### **Details**

The data given by  $\mathbf{x}$  is clustered by the fuzzy kmeans algorithm.

If centers is a matrix, its rows are taken as the initial cluster centers. If centers is an integer, centers rows of x are randomly chosen as initial values.

The algorithm stops when the maximum number of iterations (given by iter.max) is reached.

If verbose is TRUE, it displays for each iteration the number the value of the objective function.

If dist is "euclidean", the distance between the cluster center and the data points is the Euclidean distance (ordinary fuzzy k means algorithm). If "manhattan", the distance between the cluster center and the data points is the sum of the absolute values of the distances of the coordinates.

If method is "cmeans", then we have the kmeans fuzzy clustering method. If "ufcl" we have the On-line Update (Unsupervised Fuzzy Competitive learning) method, which works by performing an update directly after each input signal.

The parameters m defines the degree of fuzzification. It is defined for real values greater than 1 and the bigger it is the more fuzzy the membership values of the clustered data points are.

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The parameter rate.par of the learning rate for the "ufcl" algorithm which is by default set to rate.par=0.3 and is taking real values in (0, 1).

#### Value

cmeans returns an object of class "fclust".

centers The final cluster centers.

size The number of data points in each cluster.

cluster Vector containing the indices of the clusters where the data points are

assigned to. The maximum membership value of a point is considered for

partitioning it to a cluster.

iter The number of iterations performed,

membership a matrix with the membership values of the data points to the clusters.

withinerror Returns the sum of square distances within the clusters.

call Returns a call in which all of the arguments are specified by their names.

#### Author(s)

Evgenia Dimitriadou

#### References

Nikhil R. Pal, James C. Bezdek, and Richard J. Hathaway. Sequential Competitive Learning and the Fuzzy c-Means Clustering Algorithms. Neural Networks, Vol. 9, No. 5, pp. 787-796, 1996.

```
# a 2-dimensional example
x<-rbind(matrix(rnorm(100,sd=0.3),ncol=2),
         matrix(rnorm(100,mean=1,sd=0.3),ncol=2))
cl<-cmeans(x,2,20,verbose=TRUE,method="cmeans",m=2)</pre>
print(cl)
# a 3-dimensional example
x<-rbind(matrix(rnorm(150,sd=0.3),ncol=3),
         matrix(rnorm(150,mean=1,sd=0.3),ncol=3),
         matrix(rnorm(150,mean=2,sd=0.3),ncol=3))
cl<-cmeans(x,6,20,verbose=TRUE,method="cmeans")</pre>
print(cl)
# assign classes to some new data
y<-rbind(matrix(rnorm(33,sd=0.3),ncol=3),
         matrix(rnorm(33,mean=1,sd=0.3),ncol=3),
         matrix(rnorm(3,mean=2,sd=0.3),ncol=3))
          ycl<-predict(cl, y, type="both")</pre>
```

countpattern 13

count	pattern
Count	pattern

Count Binary Patterns

### Description

Every row of the binary matrix x is transformed into a binary pattern and these patterns are counted.

#### Usage

```
countpattern(x, matching=FALSE)
```

## Arguments

x A matrix of binary observations

matching If TRUE an additional vector is returned which stores which row belongs

to which pattern

#### Value

A vector of length 2^ncol(x) giving the number of times each pattern occurs in the rows of x. The names of this vector are the binary patterns. They are sorted according to their numeric value. If matching is TRUE, a list of the following two vectors is returned.

pat Numbers of patterns as described above.

matching Vector giving the position of the pattern of each row of x in pat.

## Author(s)

Andreas Weingessel

## Examples

```
xx \leftarrow rbind(c(1,0,0),c(1,0,0),c(1,0,1),c(0,1,1),c(0,1,1))

countpattern(xx)

countpattern(xx, matching=TRUE)
```

cshell

Fuzzy C-Shell Clustering

## Description

The c-shell clustering algorithm, the shell prototype-based version (ring prototypes) of the fuzzy kmeans clustering method.

## Usage

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#### Arguments

x The data matrix, were columns correspond to the variables and rows to

observations.

centers Number of clusters or initial values for cluster centers

iter.max Maximum number of iterations

verbose If TRUE, make some output during learning

dist Must be one of the following: If "euclidean", the mean square error, if

"manhattan", the mean absolute error is computed. Abbreviations are

also accepted.

method Currently, only the "cshell" method; the c-shell fuzzy clustering method

m The degree of fuzzification. It is defined for values greater than 1

radius The radius of resulting clusters

#### Details

The data given by x is clustered by the fuzzy c-shell algorithm.

If centers is a matrix, its rows are taken as the initial cluster centers. If centers is an integer, centers rows of x are randomly chosen as initial values.

The algorithm stops when the maximum number of iterations (given by iter.max) is reached.

If verbose is TRUE, it displays for each iteration the number the value of the objective function.

If dist is "euclidean", the distance between the cluster center and the data points is the Euclidean distance (ordinary kmeans algorithm). If "manhattan", the distance between the cluster center and the data points is the sum of the absolute values of the distances of the coordinates.

If method is "cshell", then we have the c-shell fuzzy clustering method.

The parameters m defines the degree of fuzzification. It is defined for real values greater than 1 and the bigger it is the more fuzzy the membership values of the clustered data points are.

The parameter radius is by default set to 0.2 for every cluster.

## Value

cshell returns an object of class "cshell".

centers The final cluster centers.

size The number of data points in each cluster.

cluster Vector containing the indices of the clusters where the data points are

assigned to. The maximum membership value of a point is considered for

partitioning it to a cluster.

iter The number of iterations performed.

membership a matrix with the membership values of the data points to the clusters.

withinerror Returns the sum of square distances within the clusters.

call Returns a call in which all of the arguments are specified by their names.

e1071-internal

## Author(s)

Evgenia Dimitriadou

#### References

Rajesh N. Dave. Fuzzy Shell-Clustering and Applications to Circle Detection in Digital Images. Int. J. of General Systems, Vol. 16, pp. 343-355, 1996.

## Examples

e1071-internal

Internal e1071 functions

## Description

Internal e1071 functions.

## Usage

```
prune.bclust(object, x, minsize=1, dohclust=FALSE, ...)
```

## **Details**

These are not to be called by the user.

element

Extract Elements of an Array

## Description

Returns the element of x specified by i.

## Usage

```
element(x, i)
```

## Arguments

Array of arbitrary dimensionality. х

i Vector of the same length as x has dimension

## Author(s)

Friedrich Leisch

#### See Also

Extract

## Examples

```
x \leftarrow array(1:20, dim=c(2,5,2))
element(x, c(1,4,2))
```

fclustIndex

Fuzzy Cluster Indexes (Validity/Performance Measures)

## Description

Calculates the values of several fuzzy validity measures. The values of the indexes can be independently used in order to evaluate and compare clustering partitions or even to determine the number of clusters existing in a data set.

#### Usage

```
fclustIndex(y, x, index = "all")
```

#### Arguments

An object of a fuzzy clustering result of class "fclust" у

x Data matrix

The validity measures used: "gath.geva", "xie.beni", "fukuyama.sugeno", index

"partition.coefficient", "partition.entropy", "proportion.exponent",

"separation.index" and "all" for all the indexes.

## Details

The validity measures and a short description of them follows, where N is the number of data points,  $u_{ij}$  the values of the membership matrix,  $v_i$  the centers of the clusters and k te number of clusters.

gath.geva: Gath and Geva introduced 2 main criteria for comparing and finding optimal partitions based on the heuristics that a better clustering assumes clear separation between the clusters, minimal volume of the clusters and maximal number of data points concentrated in the vicinity of the cluster centroids. These indexes are only

for the cmeans clustering algorithm valid. For the first, the "fuzzy hypervolume" we have: 
$$F_{HV} = \sum_{j=1}^{c} \left[ \det(F_j) \right]^{1/2}$$
, where  $F_j = \frac{\sum_{i=1}^{N} u_{ij} (x_i - v_j) (x_i - v_j)^T}{\sum_{i=1}^{N} u_{ij}}$ , for the case when

the defuzzification parameter is 2. For the second, the "average partition density":  $D_{PA} = \frac{1}{k} \sum_{j=1}^k \frac{S_j}{[\det(F_j)]^{1/2}}$ , where  $S_j = \sum_{i=1}^N u_{ij}$ . Moreover, the "partition density" which expresses the general partition density according to the physical definition of density is calculated by:  $P_D = \frac{S}{F_{HV}}$ , where  $S = \sum_{j=1}^k \sum_{i=1}^N u_{ij}$ .

- **xie.beni**: This index is a function of the data set and the centroids of the clusters. Xie and Beni explained this index by writing it as a ratio of the total variation of the partition and the centroids (U,V) and the separation of the centroids vectors. The minimum values of this index under comparison support the best partitions.  $u_{XB}(U,V;X) = \frac{\sum_{j=1}^{k} \sum_{i=1}^{N} u_{ij}^2 ||x_i v_j||^2}{N(\min_{j \neq l} \{||v_j v_l||^2\})}$
- **fukuyama.sugeno**: This index consists of the difference of two terms, the first combining the fuzziness in the membership matrix with the geometrical compactness of the representation of the data set via the prototypes, and the second the fuzziness in its row of the partition matrix with the distance from the *i*th prototype to the grand mean of the data. The minimum values of this index also propose a good partition.  $u_{FS}(U,V;X) = \sum_{i=1}^{N} \sum_{j=1}^{k} (u_{ij}^2)^q (||x_i v_j||^2 ||v_j \bar{v}||^2)$
- **partition.coefficient**: An index which measures the fuzziness of the partition but without considering the data set itself. It is a heuristic measure since it has no connection to any property of the data. The maximum values of it imply a good partition in the meaning of a least fuzzy clustering.  $F(U;k) = \frac{tr(UU^T)}{N} = \frac{\langle U,U \rangle}{N} = \frac{||U||^2}{N}$ 
  - F(U;k) shows the fuzziness or the overlap of the partition and depends on kN elements.
  - $1/k \le F(U;k) \le 1$ , where if F(U;k) = 1 then U is a hard partition and if F(U;k) = 1/k then U = [1/k] is the centroid of the fuzzy partion space  $P_{fk}$ . The converse is also valid.
- **partition.entropy**: It is a measure that provides information about the membership matrix without also considering the data itself. The minimum values imply a good partition in the meaning of a more crisp partition.  $H(U;k) = \sum_{i=1}^{N} h(u_i)/N$ , where  $h(u) = -\sum_{j=1}^{k} u_j \log_a(u_j)$  the Shannon's entropy.
  - H(U;k) shows the uncertainty of a fuzzy partition and depends also on kN elements. Specifically,  $h(u_i)$  is interpreted as the amount of fuzzy information about the membership of  $x_i$  in k classes that is retained by column  $u_j$ . Thus, at U = [1/k] the most information is withheld since the membership is the fuzziest possible.
  - $0 \le H(U;k) \le \log_a(k)$ , where for H(U;k) = 0 U is a hard partition and for  $H(U;k) = \log_a(k)$  U = [1/k].
- **proportion.exponent**: It is a measure P(U;k) of fuzziness adept to detect structural variations in the partition matrix as it becomes more fuzzier. A crisp cluster in the partition matrix can drive it to infinity when the partition coefficient and the partition entropy are more sensitive to small changes when approaching a hard partition. Its evaluation does not also involve the data or the algorithm used to partition them and its maximum implies the optimal partition but without knowing what maximum is a statistically significant maximum.
  - $0 \le P(U;k) < \infty$ , since the [0,1] values explode to  $[0,\infty)$  due to the natural logarithm. Specifically, P=0 when and only when U=[1/k], while  $P\to\infty$  when any column of U is crisp.
  - P(U;k) can easily explode and it is good for partitions with large column maximums and at detecting structural variations.
- separation.index (known as CS Index): This index identifies unique cluster structure with well-defined properties that depend on the data and a measure of distance. It

18 hamming.distance

answers the question if the clusters are compact and separated, but it rather seems computationally infeasible for big data sets since a distance matrix between all the data membership values has to be calculated. It also presupposes that a hard partition is derived from the fuzzy one.

 $D_1(U;k;X,d) = \min_{i+1 \le l \le k-1} \left\{ \min_{1 \le j \le k} \left\{ \frac{dis(u_j,u_l)}{\max_{1 \le m \le k} \{dia(u_m)\}} \right\} \right\}$ , where dia is the diameter of the subset, dis the distance of two subsets, and d a metric. U is a CS partition of  $X \Leftrightarrow D_1 > 1$ . When this holds then U is unique.

#### Value

Returns a vector with the validity measures values.

## Author(s)

Evgenia Dimitriadou

#### References

James C. Bezdek, *Pattern Recognition with Fuzzy Objective Function Algorithms*, Plenum Press, 1981, NY.

L. X. Xie and G. Beni, *Validity measure for fuzzy clustering*, IEEE Transactions on Pattern Analysis and Machine Intelligence, vol. 3, n. 8, p. 841-847, 1991.

I. Gath and A. B. Geva, *Unsupervised Optimal Fuzzy Clustering*, IEEE Transactions on Pattern Analysis and Machine Intelligence, vol. **11**, n. 7, p. 773-781, 1989.

Y. Fukuyama and M. Sugeno, A new method of choosing the number of clusters for the fuzzy c-means method, Proc. 5th Fuzzy Syst. Symp., p. 247-250, 1989 (in japanese).

#### See Also

cmeans

#### Examples

hamming.distance

Hamming Distances of Vectors

## Description

If both x and y are vectors, hamming.distance returns the Hamming distance (number of different bytes) between this two vectors. If x is a matrix, the Hamming distances between the rows of x are computed and y is ignored.

## Usage

```
hamming.distance(x, y)
```

hamming.window 19

## Arguments

x a vector or matrix.y an optional vector.

## Examples

```
x <- c(1, 0, 0)
y <- c(1, 0, 1)
hamming.distance(x, y)
z <- rbind(x,y)
rownames(z) <- c("Fred", "Tom")
hamming.distance(z)</pre>
```

hamming.window

Computes the Coefficients of a Hamming Window.

## Description

The filter coefficients  $w_i$  of a Hamming window of length  ${\tt n}$  are computed according to the formula

$$w_i = 0.54 - 0.46 \cos \frac{2\pi i}{n - 1}$$

## Usage

hamming.window(n)

## Arguments

n

The length of the window.

## Value

A vector containing the filter coefficients.

## Author(s)

Andreas Weingessel

## References

For a definition of the Hamming window, see for example Alan V. Oppenheim and Roland W. Schafer: "Discrete-Time Signal Processing", Prentice-Hall, 1989.

#### See Also

stft, hanning.window

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## Examples

```
hamming.window(10)

x<-rnorm(500)
y<-stft(x, wtype="hamming.window")
plot(y)</pre>
```

hanning.window

Computes the Coefficients of a Hanning Window.

## Description

The filter coefficients  $w_i$  of a Hanning window of length **n** are computed according to the formula

 $w_i = 0.5 - 0.5 \cos \frac{2\pi i}{n - 1}$ 

## Usage

hanning.window(n)

## Arguments

n

The length of the window.

## Value

A vector containing the filter coefficients.

## Author(s)

Andreas Weingessel

#### References

For a definition of the Hanning window, see for example Alan V. Oppenheim and Roland W. Schafer: "Discrete-Time Signal Processing", Prentice-Hall, 1989.

## See Also

stft, hamming.window

```
hanning.window(10)

x<-rnorm(500)
y<-stft(x, wtype="hanning.window")
plot(y)</pre>
```

ica 21

ica Independent Component Analysis

#### Description

This is an R-implementation of the Matlab-Function of Petteri.Pajunen@hut.fi.

For a data matrix X independent components are extracted by applying a nonlinear PCA algorithm. The parameter fun determines which nonlinearity is used. fun can either be a function or one of the following strings "negative kurtosis", "positive kurtosis", "4th moment" which can be abbreviated to uniqueness. If fun equals "negative (positive) kurtosis" the function fun tanh fun is used which provides ICA for sources with negative (positive) kurtosis. For fun == "4th moments" the signed square function is used.

#### Usage

```
ica(X, lrate, epochs=100, ncomp=dim(X)[2], fun="negative")
```

#### **Arguments**

X The matrix for which the ICA is to be computed

lrate learning rate

epochs number of iterations

ncomp number of independent components

fun function used for the nonlinear computation part

## Value

An object of class "ica" which is a list with components

weights ICA weight matrix
projection Projected data
epochs Number of iterations

fun Name of the used function

## Note

Currently, there is no reconstruction from the ICA subspace to the original input space.

#### Author(s)

Andreas Weingessel

#### References

Oja et al., "Learning in Nonlinear Constrained Hebbian Networks", in Proc. ICANN-91, pp. 385–390.

Karhunen and Joutsensalo, "Generalizations of Principal Component Analysis, Optimization Problems, and Neural Networks", Neural Networks, v. 8, no. 4, pp. 549–562, 1995.

22 interpolate

impute

Replace Missing Values

## Description

Replaces missing values of a matrix or dataframe with the medians (what="median") or means (what="mean") of the respective columns.

#### Usage

```
impute(x, what="median")
```

## Arguments

x A matrix or dataframe.

what What to impute.

## Value

A matrix or dataframe.

## Author(s)

Friedrich Leisch

## Examples

```
x<- matrix(1:10, ncol=2)
x[c(1,3,7)] <- NA
print(x)
print(impute(x))</pre>
```

interpolate

Interpolate Values of Array

## Description

For each row in matrix x, the hypercube of a containing this point is searched. The corners of the hypercube are linearly interpolated. By default, dimnames(a) is taken to contain the coordinate values for each point in a. This can be overridden using adims. If method=="constant", the value of the "lower left" corner of the hypercube is returned.

## Usage

kurtosis 23

#### Arguments

x Matrix of values at which interpolation shall take place.

a Array of arbitrary dimension.

adims List of the same structure as dimnames (a).

method Interpolation method, one of "linear" or "constant".

## Author(s)

Friedrich Leisch

#### See Also

```
approx, spline
```

## Examples

```
x <- seq(0,3,0.2)
z <- outer(x,x, function(x,y) sin(x*y))
dimnames(z) <- list(x,x)
sin(1.1*2.1)
interpolate(c(1.1, 2.1),z)</pre>
```

kurtosis

Kurtosis

#### Description

Computes the kurtosis.

## Usage

kurtosis(x, na.rm=FALSE)

## Arguments

x a numeric vector containing the values whose kurtosis is to be computed.na.rm a logical value indicating whether NA values should be stripped before the computation proceeds.

### **Details**

If N = length(x), then the kurtosis of x is defined as

$$N^{-1}\operatorname{sd}(x)^{-4}\sum_{i}(x_{i}-\operatorname{mean}(x))^{4}-3.$$

#### Value

The kurtosis of x.

```
x <- rnorm(100)
kurtosis(x)</pre>
```

24 lca

 ${\it Latent Class Analysis (LCA)}$ 

## Description

A latent class analysis with k classes is performed on the data given by x.

#### Usage

lca(x, k, niter=100, matchdata=FALSE, verbose=FALSE)

## Arguments

x Either a data matrix of binary observations or a list of patterns as created

by countpattern

k Number of classes used for LCA

niter Number of Iterations

matchdata If TRUE and x is a data matrix, the class membership of every data point

is returned, otherwise the class membership of every pattern is returned.

verbose If TRUE some output is printed during the computations.

#### Value

An object of class "lca" is returned, containing

w Probabilities to belong to each class

p Probabilities of a '1' for each variable in each class

matching Depending on matchdata either the class membership of each pattern or

of each data point

logl, loglsat The LogLikelihood of the model and of the saturated model

bic, bicsat The BIC of the model and of the saturated model

chisq Pearson's Chisq

1hquot Likelihood quotient of the model and the saturated model

n Number of data points.np Number of free parameters.

## Author(s)

Andreas Weingessel

### References

Anton K. Formann: "Die Latent-Class-Analysis", Beltz Verlag 1984

## See Also

countpattern, bootstrap.lca

matchClasses 25

#### Examples

```
## Generate a 4-dim. sample with 2 latent classes of 500 data points each.
## The probabilities for the 2 classes are given by type1 and type2.
type1 <- c(0.8,0.8,0.2,0.2)
type2 <- c(0.2,0.2,0.8,0.8)
x <- matrix(runif(4000),nr=1000)
x[1:500,] <- t(t(x[1:500,])<type1)*1
x[501:1000,] <- t(t(x[501:1000,])<type2)*1

1 <- lca(x, 2, niter=5)
print(1)
summary(1)
p <- predict(1, x)
table(p, c(rep(1,500),rep(2,500)))</pre>
```

matchClasses

Find similar classes in two-way contingency tables

### Description

Try to find a mapping between the two groupings, such that as many cases as possible are in one of the matched pairs.

#### Usage

#### Arguments

tab	Two-way contingency table of class memberships
method	One of "rowmax", "greedy" or "exact".
iter	Number of iterations used in greedy search.
verbose	If TRUE, display some status messages during computation.
maxexact	Maximum number of variables for which all possible permutations are computed.
x, y	Vectors or matrices with class memberships.

## Details

If method="rowmax", then each class defining a row in the contingency table is mapped to the column of the correspoding row maximum. Hence, some columns may be mapped to more than one row (while each row is mapped to a single column).

If method="greedy" or method="exact", then the contingency table must be a square matrix and a unique mapping is computed. This corresponds to a permutation of columns and rows, such that sum of the main diagonal, i.e., the trace of the matrix, gets as large as possible. For both methods, first all pairs where row and columns maxima correspond and are bigger than the sum of all other elements in the corresponding columns and rows together are located and fixed (this is a necessary condition for maximal trace).

26 moment

If method="exact", then for the remaining rows and columns, all possible permutations are computed and the optimum is returned. This can get computationally infeasible very fast. If more than maxexact rows and columns remain after applying the necessary condition, then method is reset to "greedy". If method="greedy", then a greedy heuristic is tried iter times. Repeatedly a row is picked at random and matched to the free column with the maximum value.

compareMatchedClasses() computes the contingency table for each combination of columns from x and y and applies matchClasses to that table. The columns of the table are permuted accordingly and then the table is passed to classAgreement. The resulting agreement coefficients (diag, kappa, ...) are returned. The return value of compareMatchedClasses() is a list containing a matrix for each coefficient; with element (k,l) corresponding to the k-th column of x and l-th column of y. If y is missing, then the columns of x are compared with each other.

#### Author(s)

Friedrich Leisch

#### See Also

classAgreement

#### Examples

```
## a stupid example with no class correlations:
g1 <- sample(1:5, size=1000, replace=TRUE)
g2 <- sample(1:5, size=1000, replace=TRUE)</pre>
tab <- table(g1, g2)
matchClasses(tab, "exact")
## let pairs (g1=1,g2=4) and (g1=3,g2=1) agree better
k <- sample(1:1000, size=200)
g1[k] <- 1
g2[k] < -4
k <- sample(1:1000, size=200)
g1[k] <- 3
g2[k] <- 1
tab <- table(g1, g2)
matchClasses(tab, "exact")
## get agreement coefficients:
compareMatchedClasses(g1, g2, method="exact")
```

moment

Statistical Moment

#### Description

Computes the (optionally centered and/or absolute) sample moment of a certain order.

naiveBayes 27

#### Usage

```
moment(x, order=1, center=FALSE, absolute=FALSE, na.rm=FALSE)
```

#### Arguments

a numeric vector containing the values whose moment is to be computed.

order of the moment to be computed, the default is to compute the first moment, i.e., the mean.

center a logical value indicating whether centered moments are to be computed.

absolute a logical value indicating whether absolute moments are to be computed.

a logical value indicating whether NA values should be stripped before the computation proceeds.

#### **Details**

When center and absolute are both FALSE, the moment is simply  $sum(x ^ order) / length(x)$ .

## Author(s)

Kurt Hornik and Friedrich Leisch

#### See Also

```
mean, var
```

## Examples

```
x <- rnorm(100)
## Compute the mean
moment(x)
## Compute the 2nd centered moment (!= var)
moment(x, order=2, center=TRUE)
## Compute the 3rd absolute centered moment
moment(x, order=3, center=TRUE, absolute=TRUE)</pre>
```

naiveBayes

Naive Bayes Classifier

## Description

Computes the conditional a-posterior probabilities of a categorical class variable given independent categorical predictor variables using the Bayes rule.

## Usage

```
naiveBayes(formula, data, ..., subset, na.action = na.pass)
```

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### Arguments

formula A formula of the form class ~ x1 + x2 + .... Interactions are not

allowed.

data Either a data frame of factors or a contingency table.

... Currently not used.

subset For data given in a data frame, an index vector specifying the cases to

be used in the training sample. (NOTE: If given, this argument must be

named.)

na.action A function to specify the action to be taken if NAs are found. The default

action is not to count them for the computation of the probability factors. An alternative is na.omit, which leads to rejection of cases with missing values on any required variable. (NOTE: If given, this argument must be

named.)

#### Value

An object of class "naiveBayes" including components:

apriori Class distribution for the dependent variable.

tables A list of probability tables, one for each predictor variable, giving, for each

attribute level, the conditional probabilities given the predictor classes.

## Author(s)

David Meyer \( \)david.meyer@ci.tuwien.ac.at \( \)

#### See Also

```
predict.naiveBayes
```

```
data(HouseVotes84)
model <- naiveBayes(Class ~ ., data = HouseVotes84)
predict(model, HouseVotes84[1:10,-1])
predict(model, HouseVotes84[1:10,-1], type = "raw")

pred <- predict(model, HouseVotes84[,-1])
table(pred, HouseVotes84$Class)

data(Titanic)
m <- naiveBayes(Survived ~ ., data = Titanic)
m
predict(m, as.data.frame(Titanic)[,1:3])</pre>
```

permutations 29

permutations

All permutations of integers 1:n

#### Description

Returns a matrix containing all permutations of the integers 1:n (one permutation per row).

#### Usage

```
permutations(n)
```

#### Arguments

n

Number of element to permute.

## Author(s)

Friedrich Leisch

## Examples

permutations(3)

plot.stft

Plot Short Time Fourier Transforms

## Description

An object of class "stft" is plotted as a gray scale image. The x-axis corresponds to time, the y-axis to frequency. If the default colormap is used, dark regions in the plot correspond to high values at the particular time/frequency location.

#### Usage

```
plot(x, col = gray(63:0/63), ...)
```

## Arguments

x An object of class "stft" as obtained by the function stft.

col An optional colormap. By default 64 gray values are used, where white

corresponds to the minimum value and black to the maximum.

... further arguments to be passed to or from methods.

## Value

No return value. This function is only for plotting.

## Author(s)

Andreas Weingessel

30 plot.svm

## See Also

stft

## Examples

```
x<-rnorm(500)
y<-stft(x)
plot(y)</pre>
```

plot.svm

 $Plot\ svm\ objects$ 

## Description

Generates a scatter plot of the input data of a svm fit for classification models by highlighting the classes and support vectorts. Optionally, draws filled contour plot of the class regions.

## Usage

```
plot.svm(x, data, formula, fill = TRUE, grid = 50, slice = list(), ...)
```

## Arguments

x	An object of class svm
data	data to visualize. Should be the same used for fitting.
formula	formula selecting the visualized two dimensions. Only needed if more than two input variables are used. $$
fill	switch indicating whether a contour plot for the class regions should be added.
grid	granularity for the contour plot.
slice	a list of named numeric values for the dimensions held constant (only needed if more than two variables are used). Dimensions not specified are fixed at $0$ .
	additional graphics parameters passed to filled.contour and plot.

## Author(s)

```
\begin{array}{l} {\rm David\ Meyer} \\ \langle {\rm david.meyer@ci.tuwien.ac.at} \rangle \end{array}
```

## See Also

svm

plot.tune 31

#### Examples

plot.tune

Plot tuning object

#### Description

Visualizes the results of parameter tuning.

## Usage

#### **Arguments**

an object of class tune Х choose whether a contour plot or a perspective plot is used if two patype rameters are to be visualized. Ignored if only one parameter has been tuned. angle of azimuthal direction. theta col the color(s) of the surface facets. Transparent colours are ignored. main title main titles for the axes. N.B. These must be character strings; expressions are xlab, ylab not accepted. Numbers will be coerced to character strings. swapxy if TRUE, the parameter axes are swaped (only used in case of two parameters). transform.x, transform.y, transform.z functions to transform the parameters (x and y) and the error measures (z). Ignored if NULL. color.palette color palette used in contour plot. nlevels number of levels used in contour plot. Further graphics parameters. . . .

32 predict.naiveBayes

#### Author(s)

```
David Meyer (based on C/C++-code by Chih-Chung Chang and Chih-Jen Lin) \langle david.meyer@ci.tuwien.ac.at \rangle
```

#### See Also

tune

#### Examples

predict.naiveBayes

Naive Bayes Classifier

### Description

Computes the conditional a-posterior probabilities of a categorical class variable given independent categorical predictor variables using the Bayes rule.

### Usage

```
predict.naiveBayes(object, newdata, type = c("class", "raw"), threshold = 0.001, ...)
```

## Arguments

object An object of class "naiveBayes".

newdata A dataframe with new predictors.

type see value.

threshold Value replacing cells with 0 probabilities.

... Currently not used.

#### Details

For attributes with missing values, the corresponding conditional probabilities are omitted for prediction.

#### Value

If type = "raw", the conditional a-posterior probabilities for each class are returned, and the class with maximal probability else.

## Author(s)

David Meyer (david.meyer@ci.tuwien.ac.at)

predict.svm 33

#### See Also

```
naiveBayes
```

#### Examples

```
data(HouseVotes84)
model <- naiveBayes(Class ~ ., data = HouseVotes84)
predict(model, HouseVotes84[1:10,-1])
predict(model, HouseVotes84[1:10,-1], type = "raw")

pred <- predict(model, HouseVotes84[,-1])
table(pred, HouseVotes84$Class)

data(Titanic)
m <- naiveBayes(Survived ~ ., data = Titanic)
m
predict(m, as.data.frame(Titanic)[,1:3])</pre>
```

predict.svm

Predict method for Support Vector Machines

#### Description

This function predicts values based upon a model trained by svm.

### Usage

```
predict(object, newdata, ..., na.action = na.omit)
```

#### **Arguments**

object Object of class "svm", created by svm.

newdata A matrix containing the new input data. A vector will be transformed to

a n x 1 matrix.

na.action A function to specify the action to be taken if 'NA's are found. The

default action is na.omit, which leads to rejection of cases with missing values on any required variable. An alternative is na.fail, which causes an error if NA cases are found. (NOTE: If given, this argument must be

named.)

... Currently not used.

## Value

The predicted value (for classification: the label, for density estimation: TRUE or FALSE).

## Note

If the training set was scaled by svm (done by default), the new data is scaled accordingly using scale and center of the training data.

34 predict.svm

#### Author(s)

```
David Meyer (based on C++-code by Chih-Chung Chang and Chih-Jen Lin) \langle david.meyer@ci.tuwien.ac.at \rangle
```

#### References

• Chang, Chih-Chung and Lin, Chih-Jen:

LIBSVM 2.0: Solving Different Support Vector Formulations.

http://www.csie.ntu.edu.tw/~cjlin/papers/libsvm2.ps.gz

• Chang, Chih-Chung and Lin, Chih-Jen:

Libsvm: Introduction and Benchmarks

http://www.csie.ntu.edu.tw/~cjlin/papers/q2.ps.gz

#### See Also

svm

```
data(iris)
attach(iris)
## classification mode
# default with factor response:
model <- svm (Species~., data=iris)</pre>
# alternatively the traditional interface:
x \leftarrow subset (iris, select = -Species)
y <- Species
model \leftarrow svm (x, y)
print (model)
summary (model)
# test with train data
pred <- predict (model, x)</pre>
# (same as:)
pred <- predict (model)</pre>
# Check accuracy:
table (pred,y)
## try regression mode on two dimensions
# create data
x \leftarrow seq (0.1,5,by=0.05)
y \leftarrow log(x) + rnorm(x, sd=0.2)
# estimate model and predict input values
m <- svm (x,y)
new <- predict (m,x)</pre>
# visualize
plot (x,y)
points (x, log(x), col=2)
points (x, new, col=4)
```

rbridge 35

```
## density-estimation

# create 2-dim. normal with rho=0:
X <- data.frame (a=rnorm (1000), b=rnorm (1000))
attach (X)

# traditional way:
m <- svm (X, gamma=0.1)

# formula interface:
m <- svm (~., data=X, gamma=0.1)
# or:
m <- svm (~a+b, gamma=0.1)

# test:
newdata <- data.frame(a=c(0,4), b=c(0,4))
predict (m, newdata)</pre>
```

rbridge

Simulation of Brownian Bridge

#### Description

rwiener returns a time series containing a simulated realization of the Brownian bridge on the interval [0,end]. If W(t) is a Wiener process, then the Brownian bridge is defined as W(t) - t W(1).

## Usage

```
rbridge(end = 1, frequency = 1000)
```

## Arguments

end the time of the last observation.

frequency the number of observations per unit of time.

## See Also

rwiener

```
# simulate a Brownian bridge on [0,1] and plot it
x <- rbridge()
plot(x,type="l")</pre>
```

36 read.matrix.csr

read.matrix.csr

read/write sparse data

## Description

reads and writes a file in sparse data format.

### Usage

```
read.matrix.csr(file, fac = TRUE, ncol = NULL)
write.matrix.csr(x, file = "out.dat", y = NULL)
```

## Arguments

х	An object of class matrix.csr
У	A vector (either numeric or a factor)
file	The filename.
fac	If TRUE and y-values are stored in the file, the values are interpreted as factor levels.
ncol	Number of columns, detected automatically. Can be used to add empty

columns (these are not stored in the sparse format).

#### Value

If the data file includes no y variable, read.matrix.csr returns an object of class matrix.csr, else a list with components:

```
x object of class matrix.csry vector of numeric values or factor levels, depending on fac.
```

## Author(s)

```
David Meyer (based on C/C++-code by Chih-Chung Chang and Chih-Jen Lin) \langle david.meyer@ci.tuwien.ac.at \rangle
```

## See Also

```
matrix.csr
```

```
library(methods)
if (require(SparseM)) {
  data(iris)
  x <- as.matrix(iris[,1:4])
  y <- iris[,5]
  xs <- as.matrix.csr(x)
  write.matrix.csr(xs, y = y, file="iris.dat")
  xs2 <- read.matrix.csr("iris.dat")$x
  if (!all(as.matrix(xs) == as.matrix(xs2)))
    stop("Error: objects are not equal!")</pre>
```

read.octave 37

}

read.octave

Read Octave Data File

## Description

Read a vector or matrix from an Octave ASCII data file created using the command save -ascii in Octave.

## Usage

```
read.octave(file, quiet=FALSE)
```

#### Arguments

file the name of a Octave data file to read.

quiet do not print information on type and size of the object read in.

#### **Details**

read.octave reads only the first object found in the file and ignores the rest.

#### Value

read.octave returns an object of type vector or matrix.

#### See Also

```
scan, read.table
```

rectangle.window

Computes the Coefficients of a Rectangle Window.

## Description

Returns the filter coefficents of a rectangle window. That is a vector of n 1.

The purpose of this function is just to have a name for the R command rep (1, n).

## Usage

```
rectangle.window(n)
```

## Arguments

n The length of the window.

## Value

A vector of length n filled with 1.

38 allShortestPaths

## Author(s)

Andreas Weingessel

#### See Also

stft

#### Examples

```
x<-rnorm(500)
y<-stft(x, wtype="rectangle.window")
plot(y)</pre>
```

rwiener

Simulation of Wiener Process

## Description

rwiener returns a time series containing a simulated realization of the Wiener process on the interval [0,end]

## Usage

```
rwiener(end = 1, frequency = 1000)
```

## Arguments

end the time of the last observation.

frequency the number of observations per unit of time.

## Examples

```
# simulate a Wiener process on [0,1] and plot it
x <- rwiener()
plot(x,type="l")</pre>
```

allShortestPaths

Find Shortest Paths Between All Nodes in a Directed Graph

#### Description

allShortestPaths finds all shortest paths in a directed (or undirected) graph using Floyd's algorithm. extractPath can be used to actually extract the path between a given pair of nodes.

## Usage

```
allShortestPaths(x)
extractPath(obj, start, end)
```

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#### Arguments

x	matrix or distance object
obj	${\rm return} \ {\rm value} \ {\rm of} \ {\tt allShortestPaths}$
start	integer, starting point of path
end	integer, end point of path

#### **Details**

If x is a matrix, then x[i,j] has to be the length of the direct path from point i to point j. If no direct connection from point i to point j exist, then x[i,j] should be either NA or Inf. Note that the graph can be directed, hence x[i,j] need not be the same as x[j,i]. The main diagonal of x is ignored. Alternatively, x can be a distance object as returned by dist (corresponding to an undirected graph).

#### Value

allShortestPaths returns a list with components

length A matrix with the total lengths of the shortest path between each pair of

points.

middlePoints A matrix giving a point in the middle of each shortest path (or 0 if the

direct connection is the shortest path), this is mainly used as input for

extractPath.

extractPath returns a vector of node numbers giving with the shortest path between two points.

## Author(s)

Friedrich Leisch

## References

Kumar, V., Grama, A., Gupta, A. and Karypis, G. Introduction to Parallel Programming - Design and Analysis of Algorithms, Benjamin Cummings Publishing, 1994, ISBN 0-8053-3170-0

## Examples

```
## build a graph with 5 nodes
x <- matrix(NA, 5, 5)
diag(x) <- 0
x[1,2] <- 30; x[1,3] <- 10
x[2,4] <- 70; x[2,5] <- 40
x[3,4] <- 50; x[3,5] <- 20
x[4,5] <- 60
x[5,4] <- 10
print(x)

## compute all path lengths
z <- allShortestPaths(x)
print(z)

## the following should give 1 -> 3 -> 5 -> 4
extractPath(z, 1, 4)
```

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sigmoid

The logistic function and derivatives

#### Description

```
Sigmoid 1/(1 + \exp(-x)), first and second derivative.
```

## Usage

```
sigmoid(x)
dsigmoid(x)
d2sigmoid(x)
```

#### Arguments

Х

a numeric vector

## Author(s)

Friedrich Leisch

#### Examples

```
plot(sigmoid, -5, 5, ylim = c(-.2, 1))
plot(dsigmoid, -5, 5, add = TRUE, col = 2)
plot(d2sigmoid, -5, 5, add = TRUE, col = 3)
```

skewness

Skewness

## Description

Computes the skewness.

#### Usage

```
skewness(x, na.rm=FALSE)
```

## Arguments

x na.rm a numeric vector containing the values whose skewness is to be computed.

a logical value indicating whether  $\mathtt{NA}$  values should be stripped before the computation proceeds.

## Details

If N = length(x), then the skewness of x is defined as

$$N^{-1} \operatorname{sd}(x)^{-3} \sum_{i} (x_i - \operatorname{mean}(x))^3.$$

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#### Value

The skewness of x.

#### Examples

```
x <- rnorm(100)
skewness(x)</pre>
```

stft

Computes the Short Time Fourier Transform of a Vector

#### Description

This function computes the Short Time Fourier Transform of a given vector X.

First, time-slices of length win are extracted from the vector. The shift of one time-slice to the next one is given by inc. The values of these time-slices are smoothed by mulitplying them with a window function specified in wtype. For the thus obtained windows, the Fast Fourier Transform is computed.

## Usage

```
stft(X, win=min(80,floor(length(X)/10)), inc=min(24, floor(length(X)/30)), coef=64, wtype="hanning")
```

## Arguments

X	The vector from which the stft is computed.	
win	Length of the window. For long vectors the default window size is 80, for short vectors the window size is chosen so that 10 windows fit in the vector.	
inc	Increment by which the window is shifted. For long vectors the default increment is 24, for short vectors the increment is chosen so that 30 in-	

crements fit in the vector.

Number of Fourier coefficients

wtype Type of window used

## Value

coef

Object of type stft. Contains the values of the stft and information about the parameters.

values A matrix containing the results of the stft. Each row of the matrix con-

tains the coef Fourier coefficients of one window.

windowsize The value of the parameter win increment The value of the parameter inc windowtype The value of the parameter wtype

## Author(s)

Andreas Weingessel

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#### See Also

plot.stft

## Examples

```
x<-rnorm(500)
y<-stft(x)
plot(y)</pre>
```

svm

Support Vector Machines

## Description

svm is used to train a support vector machine. It can be used to carry out general regression and classification (of nu and epsilon-type), as well as density-estimation. A formula interface is provided.

## Usage

```
svm(formula, data = list(), ..., subset, na.action =
na.omit, scale = TRUE)
svm(x, y = NULL, scale = TRUE, type = NULL, kernel =
"radial", degree = 3, gamma = 1 / dim(x)[2], coef0 = 0, cost = 1, nu = 0.5,
class.weights = NULL, cachesize = 40, tolerance = 0.001, epsilon = 0.5,
shrinking = TRUE, cross = 0, fitted = TRUE, ..., subset, na.action = na.omit)
```

## Arguments

formula	a symbolic description of the model to be fit. Note, that an intercept is always included, whether given in the formula or not.
data	an optional data frame containing the variables in the model. By default the variables are taken from the environment which 'svm' is called from.
x	a data matrix, a vector, or a sparse matrix (object of class matrix.csr as provided by the package SparseM).
У	a response vector with one label for each row/component of $\mathbf{x}$ . Can be either a factor (for classification tasks) or a numeric vector (for regression).
scale	A logical vector indicating the variables to be scaled. If $\mathtt{scale}$ is of length 1, the value is recycled as many times as needed. Per default, data are scaled internally (both $\mathtt{x}$ and $\mathtt{y}$ variables) to zero mean and unit variance. The center and scale values are returned and used for later predictions.
type	svm can be used as a classification machine, as a regresson machine, or for novelty detection. Depending of whether y is a factor or not, the default setting for type is C-classification or eps-regression, respectively, but may be overwritten by setting an explicit value. Valid options are:

- C-classification
- nu-classification
- one-classification (for novelty detection)

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• eps-regression

• nu-regression

the kernel used in training and predicting. You might consider changing

some of the following parameters, depending on the kernel type.

linear: u'v

polynomial:  $(\gamma u'v + coef0)^{degree}$ radial basis:  $e^{(-\gamma|u-v|^2)}$ sigmoid:  $tanh(\gamma u'v + coef0)$ 

degree parameter needed for kernel of type polynomial (default: 3)

gamma parameter needed for all kernels except linear (default: 1/(data dimen-

 $\operatorname{sion}))$ 

coef0 parameter needed for kernels of type polynomial and sigmoid (default:

0)

cost cost of constraints violation (default: 1)—it is the 'C'-constant of the

regularization term in the Lagrange formulation.

nu parameter needed for nu-classification and one-classification

class.weights a named vector of weights for the different classes, used for asymetric class

sizes. Not all factor levels have to be supplied (default weight: 1). All

components have to be named.

cachesize cache memory in MB (default 40)

tolerance tolerance of termination criterion (default: 0.001)
epsilon epsilon in the insensitive-loss function (default: 0.5)

shrinking option whether to use the shrinking-heuristics (default: TRUE)

cross if a integer value k>0 is specified, a k-fold cross validation on the training

data is performed to assess the quality of the model: the accuracy rate

for classification and the Mean Sqared Error for regression

fitted indicates whether the fitted values should be computed and included in

the model or not (default: TRUE)

... additional parameters for the low level fitting function svm.default

subset An index vector specifying the cases to be used in the training sample.

(NOTE: If given, this argument must be named.)

na.action A function to specify the action to be taken if NAs are found. The default

action is na.omit, which leads to rejection of cases with missing values on any required variable. An alternative is na.fail, which causes an error if NA cases are found. (NOTE: If given, this argument must be named.)

#### Details

For multiclass-classification with k levels, k>2, libsvm uses the 'one-against-one'-approach, in which k(k-1)/2 binary classifiers are trained; the appropriate class is found by a voting scheme.

libsvm internally uses a sparse data representation, which is also high-level supported by the package SparseM.

If the predictor variables include factors, the formula interface must be used to get a correct model matrix. plot.svm allows a simple graphical visualization of classification models.

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#### Value

An object of class "svm" containing the fitted model, including:

SV The resulting support vectors (possibly scaled).

index The index of the resulting support vectors in the data matrix. Note that

this index refers to the preprocessed data (after the possible effect of

na.omit and subset)

coefs The corresponding coefficients times the training labels.

rho The negative intercept.

#### Note

Data are scaled internally, usually yielding better results.

#### Author(s)

David Meyer (based on C/C++-code by Chih-Chung Chang and Chih-Jen Lin) \( \david.meyer@ci.tuwien.ac.at \)

#### References

 Chang, Chih-Chung and Lin, Chih-Jen: LIBSVM: a library for Support Vector Machines http://www.csie.ntu.edu.tw/~cjlin/libsvm

• Exact formulations of models, algorithms, etc. can be found in the document:

Chang, Chih-Chung and Lin, Chih-Jen:

LIBSVM: a library for Support Vector Machines

http://www.csie.ntu.edu.tw/~cjlin/papers/libsvm.ps.gz

• Chang, Chih-Chung and Lin, Chih-Jen:

Libsvm: Introduction and Benchmarks

http://www.csie.ntu.edu.tw/~cjlin/papers/q2.ps.gz

## See Also

```
predict.svm plot.svm matrix.csr (in package 'SparseM')
```

#### Examples

```
data(iris)
attach(iris)

## classification mode
# default with factor response:
model <- svm(Species~., data=iris)

# alternatively the traditional interface:
x <- subset(iris, select = -Species)
y <- Species
model <- svm(x, y)

print(model)
summary(model)

# test with train data</pre>
```

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```
pred <- predict(model, x)</pre>
# Check accuracy:
table(pred, y)
## try regression mode on two dimensions
# create data
x \leftarrow seq(0.1, 5, by = 0.05)
y \leftarrow log(x) + rnorm(x, sd = 0.2)
# estimate model and predict input values
m < - svm(x, y)
new <- predict(m, x)</pre>
# visualize
plot(x, y)
points(x, log(x), col = 2)
points(x, new, col = 4)
## density-estimation
# create 2-dim. normal with rho=0:
X <- data.frame(a = rnorm(1000), b = rnorm(1000))</pre>
attach(X)
# traditional way:
m \leftarrow svm(X, gamma = 0.1)
# formula interface:
m <- svm(~., data = X, gamma = 0.1)</pre>
m \leftarrow svm(^a a + b, gamma = 0.1)
# test:
newdata <- data.frame(a = c(0,4), b = c(0,4))
newdata
predict(m, newdata)
# visualization:
plot(as.matrix(X))
points(as.matrix(X)[m$index,], col = 2)
```

tune

Parameter tuning of fuctions using grid search

## Description

This generic function tunes hyperparameters of statistical methods using a grid search over supplied parameter ranges.

## Usage

```
tune(method, train.x, train.y = NULL, data = list(), validation.x =
    NULL, validation.y = NULL, ranges = NULL, predict.func = predict,
    control = tune.control(), ...)
```

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### Arguments

function to be tuned. method either a formula or a matrix of predictors. train.x the response variable if train.x is a predictor matrix. Ignored if train.x train.y data data, if a formula interface is used. Ignored, if predictor matrix and response are supplied directly. an optional validation set. Depending on whether a formula interface is validation.x used or not, the response can be included in validation.x or separately speciefied using validation.y. if no formula interface is used, the response of the (optional) validation validation.y a named list of parameter vectors spanning the sampling space. The ranges vectors will usually be created by seq. predict.func optional predict function, if the standard predict behaviour is inadequate. object of class "tune.control", as created by the function tune.control(). control

#### **Details**

As performance measure, the classification error is used for classification, and the mean squared error for regression. It is possible to specify only one parameter combination (i.e., vectors of length 1) to obtain an error estimation of the specified type (bootstrap, cross-classification, etc.) on the given data set. For conveneince, there are several tune.foo() wrappers defined, e.g., for nnet(), randomForest(), rpart(), svm(), and knn().

Further parameters passed to the training functions.

#### Value

An object of class tune, including the components:

best.parameters

a 1 x k data frame, k number of parameters.

best.performance

best achieved performance.

performances if requested, a data frame of all parameter combinations along with the

corresponding performance results.

if requested, the model trained on the complete training data using the best parameter comb

#### Author(s)

 $\begin{array}{l} {\bf David\ Meyer} \\ \langle {\bf david.meyer@ci.tuwien.ac.at} \rangle \end{array}$ 

#### See Also

```
tune.control, plot.tune, tune.svm, tune.wrapper
```

tune.control 47

#### Examples

```
data(iris)
## tune 'svm' for classification with RBF-kernel (default in svm),
## using one split for training/validation set
obj <- tune(svm, Species~., data = iris,</pre>
            ranges = list(gamma = 2^{(-1:1)}, cost = 2^{(2:4)}),
            control = tune.control(sampling = "fix")
## alternatively:
## obj <- tune.svm(Species~., data = iris, gamma = 2^(-1:1), cost = 2^(2:4))
summary(obj)
plot(obj)
## tune 'knn' using a convenience function; this time with the
## conventional interface and bootstrap sampling:
x <- iris[,-5]
y <- iris[,5]</pre>
obj2 <- tune.knn(x, y, k = 1:5, control = tune.control(sampling = "boot"))
summary(obj2)
plot(obj2)
## tune 'rpart' for regression, using 10-fold cross validation (default)
obj3 <- tune.rpart(mpg~., data = mtcars, minsplit = c(5,10,15))
summary(obj3)
plot(obj3)
## simple error estimation for lm using 10-fold cross validation
tune(lm, mpg~., data = mtcars)
```

tune.control

control parameters for the tune function

## Description

Creates an object of class tune.control to be used with the tune function, containing various control parameters.

#### Usage

```
tune.control(random = FALSE, nrepeat = 1, repeat.aggregate = min,
sampling = c("cross", "fix", "bootstrap"), sampling.aggregate = mean,
cross = 10, fix = 2/3, nboot = 10, boot.size = 9/10, best.model = TRUE,
performances = TRUE)
```

## Arguments

random if an integer value is specified, random parameter vectors are drawn from

the parameter space.

nrepeat specifies how often training shall be repeated.

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#### repeat.aggregate

function for aggregating the repeated training results.

sampling

sampling scheme. If sampling = "cross", a cross-times cross validation is performed. If sampling = "boot", nboot training sets of size boot.size (part) are sampled from the supplied data. If sampling = "fix", a single split into training/validation set is used, the training set containing a fix part of the supplied data. Note that a separate validation set can be supplied via validation.x and validation.y. It is only used for sampling = "boot" and sampling = "fix"; in the latter case, fix is set to 1.

sampling.aggregate

function for aggregating the training results on the generated training

samples.

cross number of partitions for cross-validation.

fix part of the data used for training in fixed sampling.

nboot number of bootstrap replications.

boot.size size of the bootstrap samples.

best.model if TRUE, the best model is trained and returned (the best parameter set

is used for training on the complete training set).

performances if TRUE, the performance results for all parameter combinations are re-

turned.

#### Value

An object of class "tune.control" containing all the above parameters (either the defaults or the user specified values).

## Author(s)

David Meyer (david.meyer@ci.tuwien.ac.at)

## See Also

tune

tune.wrapper

Convenience tuning wrapper functions

## Description

Convenience tuning wrapper functions, using tune.

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#### Usage

```
tune.svm(x, y = NULL, data = NULL, degree = NULL, gamma = NULL, coef0 = NULL, cost = NULL,
         nu = NULL, ...)
best.svm(x, ...)
tune.nnet(x, y = NULL, data = NULL, size = NULL, decay = NULL, trace = FALSE, nrepeat = 5,
best.nnet(x, ...)
tune.rpart(formula, data, na.action = na.omit, minsplit = NULL,
           minbucket = NULL, cp = NULL, maxcompete = NULL, maxsurrogate = NULL,
           usesurrogate = NULL, xval = NULL, surrogatestyle = NULL, maxdepth =
           NULL, predict.func = NULL, ...)
best.rpart(formula, ...)
rpart.wrapper(formula, minsplit=20, minbucket=round(minsplit/3), cp=0.01,
              maxcompete=4, maxsurrogate=5, usesurrogate=2, xval=10,
              surrogatestyle=0, maxdepth=30, ...)
tune.randomForest(x, y = NULL, data = NULL, nodesize = NULL, mtry = NULL, ntree = NULL, ...
best.randomForest(x, ...)
tune.knn(x, y, k = NULL, l = NULL, ...)
knn.wrapper(x, y, k = 1, 1 = 0, ...)
```

## Arguments

```
formula, x, y, data
                                                                                          formula and data arguments of function to be tuned.
                                                                                         predicting function.
predict.func
na.action
                                                                                          function handling missingness.
minsplit, minbucket, cp, maxcompete, maxsurrogate, usesurrogate, xval, surrogatestyle, maxdomete, m
                                                                                          rpart parameters.
degree, gamma, coef0, cost, nu
                                                                                          svm parameters.
k, 1
                                                                                         knn parameters.
mtry, nodesize, ntree
                                                                                          randomForest parameters.
size, decay, nrepeat, trace
                                                                                          nnet parameters.
```

Further parameters passed to tune.

## Details

For examples, see the help page of tune().

#### Value

tune.foo() returns a tuning object including the best parameter set obtained by optimizing over the specified parameter vectors. best.foo() directly returns the best model, i.e. the fit of a new model using the optimal parameters found by tune.foo.

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## Author(s)

 $\begin{array}{l} {\rm David\ Meyer} \\ \langle {\rm david.meyer@ci.tuwien.ac.at} \rangle \end{array}$ 

## See Also

tune

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