Package: pdfCluster (via r-universe)

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Description Cluster analysis via nonparametric density estimation is performed. Operationally, the kernel method is used throughout to estimate the density. Diagnostics methods for evaluating the quality of the clustering are available. The package includes also a routine to estimate the probability density function obtained by the kernel method, given a set of data with arbitrary dimensions.
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Description

This package performs cluster analysis via kernel density estimation (Azzalini and Torelli, 2007; Menardi and Azzalini, 2014). Clusters are associated to the maximally connected components with estimated density above a threshold. As the threshold varies, these clusters may be represented according to a hierarchical structure in the form of a tree. Detection of the connected regions is conducted by means of the Delaunay tesselation when data dimensionality is low to moderate, following Azzalini and Torelli (2007). For higher dimensional data, detection of connected regions is performed according to the procedure described in Menardi and Azzalini (2013). In both cases, after that a number of high-density cluster-cores is identified, lower density data are allocated by following a supervised classification-like approach. The number of clusters, corresponding to the number of the modes of the estimated density, is automatically selected by the procedure. Diagnostics methods for evaluating the quality of clustering are also available (Menardi, 2011). Moreover, the package provides a routine to estimate the probability density function by kernel methods, given a set of data with arbitrary dimension. The main features of the package are described and illustrated in Azzalini and Menardi (2014).

Details

The pdfCluster-package makes use of classes and methods of the S4 system. It includes some foreign functions written in the C language: two of them compute the kernel density estimate of data and are interfaced by the R function kepdf. Other C routines included in the package allow for a quicker detection of the connected components of the subgraphs associated with the level sets of the data. Two of them are directly drawn from the homonymous ones in the spdep package.

Starting from version 1.0-0, new features have been introduced:

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 kernel density estimation may be performed by using either a a fixed or an adaptive bandwidth; moreover, the option of selecting a Student's t kernel has been included, for computational convenience;

- detection of connected components of the level sets is performed by means of the Delaunay triangulation when data dimensionality is up to 6, following Azzalini and Torelli (2007); for higher dimensional data a new procedure, which is less time-consuming, is now adopted (Menardi and Azzalini, 2014);
- the order of classification of lower density data depends now also on the standard error of the estimated density ratios; moreover, a cluster-specific bandwidth is the default option to classify low density data.

See examples below to understand how to set arguments of the main function of the package, in order to obtain the same results as the ones obtained with versions 0.1-x.

Author(s)

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References

Azzalini, A., Menardi, G. (2014). Clustering via Nonparametric Density Estimation: The R Package pdfCluster. *Journal of Statistical Software*, 57(11), 1-26, URL http://www.jstatsoft.org/v57/i11/.

Azzalini A., Torelli N. (2007). Clustering via nonparametric density estimation. *Statistics and Computing*, 17, 71-80.

Menardi G. (2011). Density based Silhouette diagnostics for clustering methods. *Statistics and Computing*, 21, 295-308.

Menardi G., Azzalini, A. (2014). An advancement in clustering via nonparametric density estimation. *Statistics and Computing*, DOI: 10.1007/s11222-013-9400-x, to appear.

Examples

```
# load data
data(wine)
gr <- wine[, 1]

# select a subset of variables
x <- wine[, c(2, 5, 8)]

#density estimation
pdf <- kepdf(x)
summary(pdf)
plot(pdf)

#clustering
cl <- pdfCluster(x)
summary(cl)
plot(cl)</pre>
```

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```
#comparison with original groups
table(groups(cl),gr)
#density based silhouette diagnostics
dsil <- dbs(cl)</pre>
plot(dsil)
##########
# higher dimensions
x <- wine[, -1]
#density estimation with adaptive bandwidth
pdf <- kepdf(x, bwtype="adaptive")</pre>
summary(pdf)
#density plot is not much clear for high- dimensional data
#select a few variables
plot(pdf, indcol = c(1,4,7))
#clustering
#when dimension is >= 6, default method to find connected components is "pairs"
#density is better estimated by using an adaptive bandwidth
cl <- pdfCluster(x, bwtype="adaptive")</pre>
summary(cl)
plot(cl)
########
# this example shows how to set the arguments in function pdfCluster
\# in order to obtain the same results as the ones of versions 0.1-x.
x \leftarrow wine[, c(2, 5, 8)]
# previous versions of the package
# do not run
# old code:
# cl <- pdfCluster(x)</pre>
# same result is obtained now obtained as follows:
cl <- pdfCluster(x, se=FALSE, hcores= TRUE, graphtype="delaunay", n.grid=50)</pre>
```

adj.rand.index

Adjusted Rand index

Description

Computes the adjusted Rand index to compare two alternative partitions of the same set.

Usage

```
adj.rand.index(cl1, cl2)
```

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Arguments

- cl1 the vector containing the class labels of the first partition.
- the vector containing the class labels of the second partition.

Details

The adjusted Rand index is a correction of the Rand index that measures the similarity between two classifications of the same objects by the proportions of agreements between the two partitions. The correction is obtained by subtracting from the Rand index its expected value.

Value

A numeric vector of length 1.

References

L. Hubert and P. Arabie (1985) Comparing partitions, Journal of Classification, 2, 193-218.

See Also

table

Examples

```
# load data
data(wine)
#actual groups
gr <- wine[, 1]

# select a subset of variables
x <- wine[, c(2, 5, 8)]

#clustering
cl <- pdfCluster(x)

#comparison with original groups
table(groups(cl), gr)
adj.rand.index(groups(cl), gr)</pre>
```

dbs

Density-based silhouette information methods

Description

Computes the density-based silhouette information of clustered data. Two methods are associated to this function. The first method applies to two arguments: the matrix of data and the vector of cluster labels; the second method applies to objects of pdfCluster-class.

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Usage

```
## S4 method for signature 'matrix'
dbs(x, clusters, h.funct="h.norm", hmult=1, prior, ...)
## S4 method for signature 'pdfCluster'
dbs(x, h.funct="h.norm", hmult = 1, prior =
    as.vector(table(x@cluster.cores)/sum(table(x@cluster.cores))),
    stage=NULL, ...)
```

Arguments

A matrix of data points partitioned by any density-based clustering method or an object of pdfCluster-class. clusters Cluster labels of grouped data. This argument has not to be set when x is a pdfCluster-class object. h.funct Function to estimate the smoothing parameters. Default is h.norm. hmult Shrink factor to be multiplied by the smoothing parameters. Default value is 1. prior Vector of prior probabilities of belonging to the groups. When x is of pdfCluster-class, default value is set proportional to the cluster cores cardinalities. Otherwise, equal prior probabilities are given to the clusters by default. When x is a pdfCluster-class object, this is the stage of classification of lowstage density data at which the dbs has to be computed. Default value is the number of stages of the procedure. Set it to 0 if the dbs has to be computed at cluster cores only.

Further arguments to be passed to methods (see dbs-methods) or arguments to kepdf. See details below.

Details

This function provides diagnostics for a clustering produced by any density-based clustering method. The dbs information is a suitable modification of the silhouette information aimed at evaluating the cluster quality in a density based framework. It is based on the estimation of data posterior probabilities of belonging to the clusters. It may be used to measure the quality of data allocation to the clusters. High values of the $d\hat{b}s$ are evidence of a good quality clustering.

Define

$$\hat{\tau}_m(x_i) = \frac{\pi_m \hat{f}(x_i | x \in m)}{\sum_{m=1}^{M} \pi_m \hat{f}(x_i | x_i \in m)} \quad m = 1, \dots, M,$$

where π_m is a prior probability of m and $\hat{f}(x_i|x_i \in m)$ is a density estimate at x_i evaluated with function kepdf by using the only data points in m. Density estimation is performed with fixed bandwidths h, as evaluated by function h. funct, possibly multiplied by the shrink factor hmult.

Density-based silhouette information of x_i , the i^{th} row of the data matrix x, is defined as follows:

$$d\hat{b}s_i = \frac{\log\left(\frac{\hat{\tau}_{m_0}(x_i)}{\hat{\tau}_{m_1}(x_i)}\right)}{\max_{x_i}\left|\log\left(\frac{\hat{\tau}_{m_0}(x_i)}{\hat{\tau}_{m_1}(x_i)}\right)\right|},$$

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where m_0 is the group where x_i has been allocated and m_1 is the group for which τ_m is maximum, $m \neq m_0$.

Note: when there exists x_j such that $\hat{\tau}_{m_1}(x_j)$ is zero, $d\hat{b}s_j$ is forced to 1 and $\max_{x_i} \left| \log \left(\frac{\hat{\tau}_{m_0}(x_i)}{\hat{\tau}_{m_1}(x_i)} \right) \right|$ is computed by excluding x_j from the data matrix x.

See Menardi (2011) for a detailed treatment.

Value

An object of class "dbs", with slots:

call The matched call.

x The matrix of clustered data points.

prior The vector of prior probabilities of belonging to the groups.

dbs A vector reporting the density-based silhouette information of the clustered data.

clusters Cluster labels of grouped data.

noc Number of clusters

stage If argument x of dbs is a pdfCluster-class object, this slot provides the stage

of the classification at which the dbs is computed.

See dbs-class for more details.

Methods

signature(x = "matrix", clusters = "numeric") Computes the density based silhouette information for objects partitioned according to any density-based clustering method.

signature(x = "pdfCluster", clusters = "missing") Computes the density based silhouette
information for objects of class "pdfCluster".

References

Menardi, G. (2011) Density-based Silhouette diagnostics for clustering methods. *Statistics and Computing*, 21, 295-308.

See Also

```
dbs-class, plot, dbs-method, silhouette.
```

Examples

```
#example 1: no groups in data
#random generation of group labels
set.seed(54321)
x <- rnorm(50)
groups <- sample(1:2, 50, replace = TRUE)
groups
dsil <- dbs(x = as.matrix(x), clusters=groups)
dsil
summary(dsil)</pre>
```

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```
plot(dsil, labels=TRUE, lwd=6)
#example 2: wines data
# load data
data(wine)

# select a subset of variables
x <- wine[, c(2,5,8)]

#clustering
cl <- pdfCluster(x)

dsil <- dbs(cl)
plot(dsil)</pre>
```

dbs-class

Class "dbs"

Description

This class pertains to results of the application of function dbs.

Objects from the Class

Objects can be created by calls of the form new("dbs", ...) or as a result from calling function dbs.

Slots

```
call: Object of class "call" reporting the matched call.
```

x: Object of class "matrix" representing the clustered data points.

prior: Object of class "numeric" being the prior probabilities of belonging to the groups.

dbs: Object of class "numeric" reporting the density-based silhouette information of the clustered data.

clusters: Object of class "numeric" reporting the group labels of grouped data.

noc: Object of class "numeric" indicating the number of clusters.

stage: Object of class "ANY" corresponding to the stage of the classification at which the density-based silhouette information is computed when dbs is applied to an object of pdfCluster-class.

Methods

```
plot signature(x = "dbs", y = "missing"):
```

S4 method for plotting objects of dbs-class. Data are partitioned into the clusters, sorted in a decreasing order with respect to their dbs value and displayed on a bar graph. See plot, dbs-method for further details.

groups 9

```
show signature(object = "dbs"):
```

S4 method for showing objects of dbs-class. The following elements are shown:

- the dbs index computed at the observed data;
- The cluster membership of each data point;

```
summary signature(object = "dbs"):
```

S4 method for summarizing objects of dbs-class. The following elements are shown:

- a summary (minimum, 1st quartile, median, mean, 3rd quartile, maximum) of the dbs values for each cluster;
- a summary (minimum, 1st quartile, median, mean, 3rd quartile, maximum) of the dbs values for all the observations.

See Also

```
dbs, silhouette, plot, dbs-method, plot-methods, show-methods, summary-methods.
```

Examples

```
showClass("dbs")

#wine example
#data loading
data(wine)

# select a subset of variables
x <- wine[, c(2,5,8)]

#clustering
cl <- pdfCluster(x)

dsil <- dbs(cl)
dsil
summary(dsil)</pre>
```

groups

Extracts groups

Description

Extracts the detected groups from objects of pdfCluster-class.

Usage

```
groups(obj, stage = length(obj@stages))
```

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Arguments

obj An object of pdfCluster-class

stage The stage of classification at which the clusters have to be extracted. Set this

value to 0 to extract the cluster cores. Default value is the total number of classification stages, that is, the final partition is given. When obj contains the

clusters cores only, these are given by default.

Details

This function is an user-friendly version of command obj@clusters, now obsolete, to ease extraction of groups from objects of pdfCluster-class.

Value

A numeric vector containing the group labels. NA values are associated to points not classified at the selected stage of the classification procedure.

See Also

pdfCluster

Examples

```
# load data
data(wine)

# select a subset of variables
x <- wine[, c(2, 5, 8)]

#clustering
cl <- pdfCluster(x)

groups(cl)

#equivalent to:
cl@clusters

#to extract the cluster cores
groups(cl, stage = 0)</pre>
```

h.norm

Normal optimal choice of smoothing parameter in density estimation

Description

This function computes the smoothing parameter to be used in kernel density estimation, as asymptotically optimal when the underlying distribution is Normal. Unidimensional as well as multidimensional data can be handled. When multidimensional data are supplied, a vector of smoothing parameters is computed having one element for each component.

h.norm

Usage

```
h.norm(x)
```

Arguments

x vector, matrix or data-frame of data.

Details

The smoothing parameter of component j of a $n \times d$ data matrix is estimated as follows:

$$\sigma_j \left(\frac{4}{(d+2)n} \right)^{\frac{1}{d+4}}$$

where σ_j is the estimated standard deviation of component j. See Section 2.4.2 of the reference below.

Value

Returns a numeric vector with the same length as the number of columns of x or with length one if x is a vector. When x is a matrix, a vector of smoothing parameters is provided having one element for each component.

References

Bowman, A.W. and Azzalini, A. (1997). *Applied smoothing techniques for data analysis: the kernel approach with S-Plus illustrations*. Oxford University Press, Oxford.

See Also

hnorm

Examples

```
set.seed(123)
x <- rnorm(30)
sm.par <- h.norm(x)
pdf <- kepdf(x, bwtype= "fixed", h = sm.par)
plot(pdf, eval.points=seq(-4,4,by=.2))</pre>
```

hprop2f

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Sample smoothing parameters in adaptive density estimation

Description

This function computes the sample smoothing parameters to be used in adaptive kernel density estimation, according to Silverman (1986).

Usage

```
hprop2f(x, h = h.norm(x), alpha = 1/2, kernel = "gaussian")
```

Arguments

X	Vector or matrix of data.
h	Vector of smoothing parameters to be used to get a pilot estimate of the density function. It has length equal to $NCOL(x)$.
alpha	Sensitivity parameter satysfying $0 \le \alpha \le 1$, giving the power to which raise the pilot density. Default value is 1/2. See details.
kernel	Kernel to be used to compute the pilot density estimate. It should be one of "gaussian" or "t7". See kepdf for further details.

Details

A vector of smoothing parameters h_i is chosen for each sample point x_i , as follows:

$$h_i = h \left(\frac{\hat{f}_h(x_i)}{g}\right)^{-\alpha}$$

where \hat{f}_h is a pilot kernel density estimate of the density function f, with vector of bandwidths h, and g is the geometric mean of $\hat{f}_h(x_i)$, i=1,...,n. See Section 5.3.1 of the reference below.

Value

Returns a matrix with the same dimensions of x where row i provides the vector of smoothing parameters for sample point x_i .

References

Silverman, B. (1986). *Density estimation for statistics and data analysis*. Chapman and Hall, London.

See Also

h.norm

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Examples

```
set.seed(123)
x <- rnorm(10)

sm.par <- hprop2f(x)
pdf <- kepdf(x, bwtype= "adaptive")

pdf@par$hx
sm.par

plot(pdf,eval.points=seq(-4,4,by=.2))</pre>
```

kepdf

Kernel estimate of a probability density function.

Description

Estimates density of uni- and multivariate data by the kernel method.

(1986) approach.

Usage

Arguments

х	A vector, a matrix or data-frame of data whose density should be estimated.
eval.points	A vector, a matrix or a data-frame of data points at which the density estimate should be evaluated.
kernel	Either 'gaussian' or 't7', it defines the kernel function to be used. See details below.
bwtype	Either 'fixed' or 'adaptive', corresponding to a kernel estimator with fixed or adaptive bandwidths respectively. See details below.
h	A vector of length set to $NCOL(x)$, defining the smoothing parameters to be used either to estimate the density in kernel estimation with fixed bandwidth or to estimate the pilot density in kernel estimation with adaptive bandwidths. Default value is the result of h . norm applied to x .
hx	A matrix with the same number of rows and columns as x , where each row defines the vector of smoothing parameters specific for each sample point. To be used when bwtype = "adaptive". Default value is the result of hprop2f applied to x . Set to NULL when bwtype= "fixed".
alpha	Sensitivity parameter to be given to hprop2f when bwtype= "adaptive" and the vectors of smoothing parameters are computed according to Silverman's

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Details

The current version of pdfCluster-package allows for computing estimates by a kernel product estimator of the form:

$$\hat{f}(y) = \sum_{i=1}^{n} \frac{1}{nh_{i,1} \cdots h_{i,d}} \prod_{j=1}^{d} K\left(\frac{y_j - x_{i,j}}{h_{i,j}}\right).$$

The kernel function K can either be a Gaussian density (if kernel = "gaussian") or a t_{ν} density, with $\nu=7$ degrees of freedom (when kernel = "t7"). Although uncommon, the option of selecting a t kernel is motivated by computational efficiency reasons. Hence, its use is suggested when either x or eval.points have a huge number of rows.

The vectors of bandwidths $h_i = (h_{i,1} \cdots h_{i,d})'$ are defined as follows:

Fixed bandwidth When bwtype='fixed', $h_i = h$ that is, a constant smoothing vector is used for all the observations x_i . Default values are set as asymptotically optimal for a multivariate Normal distribution (e.g., Bowman and Azzalini, 1997). See h. norm for further details.

Adaptive bandwidth When bwtype='adaptive', a vector of bandwidths h_i is specified for each observation x_i . Default values are selected according to Silverman (1986, Section 5.3.1). See hprop2f.

Value

An S4 object of kepdf-class with slots:

call The matched call.

x The data input, coerced to be a matrix.

eval.points The data points at which the density is evaluated.

estimate The values of the density estimate at the evaluation points.

kernel The selected kernel. bwtype The type of estimator.

par A list of parameters used to estimate the density, with elements:

- h the smoothing parameters used to estimate either the density or the pilot density;
- hx the matrix of sample smoothing parameters, when bwtype='adaptive';
- alpha sensitivity parameter used if bwtype='adaptive'.

References

Bowman, A.W. and Azzalini, A. (1997). *Applied smoothing techniques for data analysis: the kernel approach with S-Plus illustrations*. Oxford University Press, Oxford.

Silverman, B. (1986). Density estimation for statistics and data analysis. Chapman and Hall, London.

See Also

h.norm, hprop2f, kepdf-class.

kepdf-class 15

Examples

```
## A 1-dimensional example
data(wine)
x \leftarrow wine[,3]
pdf <- kepdf(x, eval.points=seq(0,7,by=.1))
plot(pdf, n.grid= 100, main="wine data")
## A 2-dimensional example
x <- wine[,c(2,8)]
pdf <- kepdf(x)
plot(pdf, main="wine data", props=c(5,50,90), ylim=c(0,4))
plot(pdf, main="wine data", method="perspective", phi=30, theta=60)
### A 3-dimensional example
x \leftarrow wine[,c(2,3,8)]
pdf <- kepdf(x)
plot(pdf, main="wine data", props=c(10,50,70), gap=0.2)
plot(pdf, main="wine data", method="perspective", gap=0.2, phi=30, theta=10)
### A 6-dimensional example
### adaptive kernel density estimate is preferable in high-dimensions
x \leftarrow wine[,c(2,3,5,7,8,10)]
pdf <- kepdf(x, bwtype="adaptive")</pre>
plot(pdf, main="wine data", props=c(10,50,70), gap=0.2)
plot(pdf, main="wine data", method="perspective", gap=0.2, phi=30, theta=10)
```

kepdf-class

Class "kepdf"

Description

This class encapsulates results of the application of function kepdf.

Objects from the Class

Objects can be created by calls of the form new("kepdf", ...) or as a result of a call to kepdf.

Slots

call: Object of class "call", corresponding to the matched call.

x: Object of class "matrix" representing the data points used to estimate the probability density function.

eval.points: Object of class "matrix" representing the data points at which the density is evaluated.

estimate The values of the density estimate at the evaluation points.

kernel: Object of class "character" giving the selected kernel.

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bwtype: Object of class "character" giving the selected type of estimator.

par: Object of class "list" providing the parameters used to estimate the density. Its elements are h, hx, and possibly alpha.

See kepdf for further details.

Methods

```
plot signature(x = "kepdf", y = "ANY")
```

Plots objects of kepdf-class. plot-methods are available for density estimates of:

- one-dimensional data;
- two-dimensional data: contour, image or perspective plots are available;
- multi-dimensional data: matrix of plots of all the pairs of two-dimensional marginal kernel density estimates.

See plot, kepdf-method for further details.

```
show signature(object = "kepdf")
```

Prints the following elements:

- the class of the object;
- the selected kernel;
- the selected type of estimator;
- either the fixed smoothing parameters or the smoothing parameters of each observation;
- the density estimates at the evaluation points.

```
summary signature(object = "kepdf")
```

Provides a summary of kepdf-class object by printing the highest density data point and the row or index position of a percentage top density data points, possibly given as optional argument prop.

See Also

 $\verb|h.norm|, \verb|kepdf|, \verb|plot|, \verb|kepdf-method|, \verb|plot-methods|, \verb|show-methods|, show-methods|, show-methods|,$

Examples

```
#
showClass("kepdf")

#
data(wine)
#select only "Barolo"-type wines
x <- wine[1:59,3]
pdf <- kepdf(x)
pdf
summary(pdf)
summary(pdf, props = 10*seq(1, 9, by = 1))</pre>
```

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oliveoil

Olive oil data

Description

This data set represents eight chemical measurements on different specimen of olive oil produced in various regions in Italy (northern Apulia, southern Apulia, Calabria, Sicily, inland Sardinia and coast Sardinia, eastern and western Liguria, Umbria) and further classifiable into three macro-areas: Centre-North, South, Sardinia. The data set is used to evaluate the pdfCluster ability of recunstructing the macro-area membership.

Usage

data(oliveoil)

Format

This data frame contains 572 rows, each corresponding to a different specimen of olive oil, and 10 columns. The first and the second column correspond to the macro-area and the region of origin of the olive oils respectively; here, the term "region" refers to a geographical area and only partially to administrative borders. Columns 3-10 represent the following eight chemical measurements on the acid components for the oil specimens: palmitic, palmitoleic, stearic, oleic, linoleic, linolenic, arachidic, eicosenoic.

Details

Since the raw data are of compositional nature, ideally totalling 10000, some preliminary transformations of data are advisable. In particular, Azzalini and Torelli (2007) adopt an additive log-ratio transformation (ALR). If x_j denotes the j^{th} chemical measurement $(j=1,\ldots,8)$, the ALR transformation is $y_j = \log x_j/x_k, j \neq k$, where k is an arbitrary but fixed variable. However, in this data set, the raw data do not always sum up exactly to 10000, because of measurement errors. Moreover, some 0's are present in the data, corresponding to measurements below the instrument sensitivity level. Therefore, it is suggested to add 1 to all raw data and normalize them by dividing each entry by the corresponding row sum $\sum_j (x_j + 1)$.

Source

Forina, M., Lanteri, S. Armanino, C., Casolino, C., Casale, M., Oliveri, P. (2008). V-PARVUS. *An Extendible Package of programs for explorative data analysis, classification and regression analysis*. Dip. Chimica e Tecnologie Farmaceutiche ed Alimentari, Università di Genova.

References

Azzalini A., Torelli N. (2007). Clustering via nonparametric density estimation. *Statistics and Computing*, 17, 71-80.

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Classification of low density data

Description

Allocates low density data points in a multi-stage procedure after that cluster cores have been detected by applying pdfCluster.

Usage

```
pdfClassification(obj, n.stage = 5, se = TRUE, hcores = FALSE)
```

Arguments

`		
	obj	An object of pdfCluster-class.
	n.stage	Allocation of low density data is performed by following a multi-stages procedure in $n.stage$ stages.
	se	Logical. Should the standard-error of the density estimates be taken into account to define the order of allocation? Default value is TRUE. See details below.
	hcores	Logical. Set this value to TRUE to build cluster density estimates by selecting the same bandwidths as the ones used to form the cluster cores. Otherwise, bandwidths specific for the clusters are selected. Default value is FALSE. See details below.

Details

The basic idea of the classification stage of the procedure is as follows: for an unallocated data point x_0 , compute the estimated density $\hat{f}_m(x_0)$ based on the data already assigned to group $m, m = 1, 2, \ldots, M$, and assign x_0 to the group with highest log ratio $\hat{f}_m(x_0)/\max_m \hat{f}_m(x_0)$.

In case $\hat{f}_m(x_0)=0$, for all $m=1,2,\ldots,M$, x_0 is considered as an outlier. The procedure gives a warning message and the outlier remains unclassified. The cluster label of x_0 will be set to zero.

The current implementation of this idea proceeds in n. stage stages, allocating a block of points at a time, updating the estimates $\hat{f}_m(\cdot)$ based on the new members of each group and then allocating a new block of points. When se = TRUE, classification is performed by further weighting the logratios inversely with their approximated standard error, so that points whose density estimate has highest precision are allocated first.

Each of the $f_m(\cdot)$ is built by selecting either the same bandwidths h_0 as the ones used to form the cluster cores (when hcores = TRUE) or cluster-specific bandwidths, obtained as follows:

$$h_m^* = \exp[(1 - a_m)\log(h_0) + a_m\log(h_m)],$$

where a_m is the proportion of data points in the m-th cluster core and h_m are asymptotically optimal for a normal distribution of the m-th cluster or computed according to the Silverman (1986) approach, if the kernel estimator has fixed or adaptive bandwidth, respectively.

Value

An object of pdfCluster-class with slot stages of class "list" having length equal to n. stage. See pdfCluster-class for further details.

Note

Function pdfClassification is called internally, from pdfCluster, when the argument n.stage is set to a value greater than zero. Alternatively, it may be called externally, by providing as argument an object of pdfCluster-class.

When pdfClassification is internally called from pdfCluster and one group only is detected, the slot stages is a list with n.stage elements, each of them being a vector with length equal to the number of data points and all elements equal to 1.

References

Azzalini A., Torelli N. (2007). Clustering via nonparametric density estimation. *Statistics and Computing*. 17, 71-80.

Silverman, B. (1986). Density estimation for statistics and data analysis. Chapman and Hall, London.

See Also

```
pdfCluster, pdfCluster-class
```

Examples

```
# load data
data(wine)

# select a subset of variables
x <- wine[, c(2,5,8)]

#whole procedure, included the classification phase
cl <- pdfCluster(x)
summary(cl)
table(groups(cl))

#use of bandwidths specific for the group
cl1 <- pdfClassification(cl, hcores= TRUE)
table(groups(cl1))</pre>
```

pdfCluster

Clustering via nonparametric density estimation

Description

Cluster analysis is performed by the density-based procedures described in Azzalini and Torelli (2007) and Menardi and Azzalini (2014), and summarized in Azzalini and Menardi (2014).

Usage

```
## S4 method for signature 'numeric'
pdfCluster(x, graphtype, hmult, Q = "QJ", lambda = 0.1,
    grid.pairs = 10, n.grid = min(round((5 + sqrt(NROW(x))) * 4), NROW(x)), ...)

## S4 method for signature 'matrix'
pdfCluster(x, graphtype, hmult, Q = "QJ", lambda = 0.1,
    grid.pairs = 10, n.grid = min(round((5 + sqrt(NROW(x))) * 4), NROW(x)), ...)

## S4 method for signature 'data.frame'
pdfCluster(x, graphtype, hmult, Q = "QJ", lambda = 0.1,
    grid.pairs = 10, n.grid = min(round((5 + sqrt(NROW(x))) * 4), NROW(x)), ...)

## S4 method for signature 'pdfCluster'
pdfCluster(x, graphtype, hmult, Q, lambda = 0.1,
    grid.pairs, n.grid = min(round((5 + sqrt(NROW(x))) * 4), NROW(x@x)), ...)
```

Arguments

A vector, a matrix or a data frame of numeric data to be partitioned. Since

density-based clustering is designed for continuous data only, if discrete data are provided, a warning message is displayed. Alternatively, x can be an object of pdfCluster-class itself, obtained when graphtype is set to "pairs". See

Section Details below.

graphtype Either "unidimensional", "delaunay" or "pairs", it defines the procedure used to build the graph associated with the data. If missing, a "delaunay" graph is built

for data having dimension less than 7, otherwise a "pairs" graph is built. See details below. This argument has not to be set when x is of pdfCluster-class.

hmult A shrink factor to be multiplied by the smoothing parameter h of function kepdf.

If missing, it is taken to be 1 when data have dimension greater than 6, 0.75

otherwise.

Q Optional arguments to be given when graphtype = "delaunay". See delaunayn

in package geometry for further details. This argument has not to be set when graphtype = "pairs", when graphtype = "unidimensional" or when x is of

pdfCluster-class.

lambda Tolerance threshold to be used when graphtype = "pairs". An edge is set between two observations if the density function, evaluated along the segment linking them, does not exhibit any valley having a measure exceeding lambda.

linking them, does not exhibit any valley having a measure exceeding lambda. Its range is [0,1) but a value larger than 0.3 is not recommended; default value is set to 0.10. This argument has not to be set when graphtype = "delaunay"

or graphtype = "unidimensional".

grid.pairs When graphtype = "pairs", this arguments defines the length of the grid of

points along the segment linking each pair of observations, on which the density is evaluated. Default is 10. This argument has not to be set when graphtype =

"delaunay", when graphtype = "unidimensional" or when x is of pdfCluster-class.

n.grid Defines the length of the grid on which evaluating the connected components of the density level sets. The default value is set to the minimum between the

number of data rows n and $\lfloor (5+\sqrt(n))4+0.5 \rfloor$, an empirical rule of thumb which indicates that the length of the grid grows with the square root of the number of rows data.

... Further arguments to be passed to kepdf or to pdfClassification.

Details

Clusters are associated to the connected components of the level sets of the density underlying the data. Density estimation is performed by kernel methods and the connected regions are approximated by the connected components of a graph built on data. Three alternative procedures to build the graph are adopted:

Unidimensional procedure When data are univariate an edge is set between two observations when all the data points included in the segment between the two candidate observations belong to the same level set.

Delaunay triangulation An edge is set between two observations when they are contiguous in the Voronoi diagram; see Azzalini and Torelli (2007).

Pairs evaluation An edge is set between two observations when the density function, evaluated along the segment joining them, does not exhibit any valley having a relative amplitude greater than a tolerance threshold $0 \le \lambda < 1$. Being a tolerance threshold, sensible values of λ are, in practice, included in [0, 0.3]; see Menardi and Azzalini (2013).

As the level set varies, the number of detected components gives rise to the tree of clusters, where each leave corresponds to a mode of the density function. Observations around these modes form a number of cluster cores, while the lower density observations are allocated according to a classification procedure; see also pdfClassification.

Value

An S4 object of pdfCluster-class with slots:

call The matched call.

x The matrix of data input. If a vector of data is provided as input, a one-column matrix is returned as output.

An object of class list providing information about the density estimate. It includes:

- kernel character vector defining the kernel function used to estimate the density;
- bwtype character vector defining if a fixed or an adaptive kernel estimator has been used;
- par list of components defining the parameters used in density estimation;
- estimate vector of density estimates evaluated at the data points.

See kepdf for further details.

An object of class list defining details about the identification of the connected regions. It includes:

• nc number of connected sets for each density level set.

pdf

nc

 p vector of level sets, giving the proportions of data with estimated density below a threshold.

- id group label of each point at different sections of the density estimate.
 Negative values of id mean that the estimated density is below the considered threshold.
- pq for each p gives the corresponding quantile q of the values of the density.

graph

An object of class list defining details about the graph built to find the connected sets of high density regions. Its length depends on the value of its first element:

- type either "unidimensional", "delaunay" or "pairs", defines the procedure used to set edges among the observations. In the last case only, the list includes also the following elements:
- comp.area a list containing the vector area and the matrix pairs.ord.
 The element i of vector area is the measure of the maximum valley in the density function linking the observations having row position as given in column i of pairs.ord.
- lambda tolerance threshold.

cluster.cores

A vector with the same length as NROW(x), defining the cluster cores membership. NA values correspond to low density, unlabeled data, to be classified in the second phase of the procedure by the intarnal call of pdfClassification.

tree

Cluster tree with leaves corresponding to the connected components associated to different sections of the density estimate. The object is of class dendrogram.

noc Number of clusters.

stages

List with elements corresponding to the data allocation to groups at the different stages of the classification procedure. NA values correspond to unlabeled data.

clusters

Set to NULL if n.stages = 0, that is, if data belonging to the cluster cores only have been allocated. Otherwise it reports the final label groups. This component is obsolete. Use function groups, instead.

Methods

signature(x="data.frame") This method applies the pdfCluster procedure to objects of class data.frame.

 ${\tt signature} ({\tt x="matrix"}) \ \ This \ method \ applies \ the \ pdf Cluster \ procedure \ to \ objects \ of \ class \ matrix.$

signature(x="numeric") This method applies the pdfCluster procedure to objects of class numeric.

signature(x="pdfCluster") This method applies to objects of pdfCluster-class when the graph has been built according to the "pairs" procedure. It allows to save time and computations if the user wants to compare results of cluster analysis for different values of the lambda parameter. See examples below.

Warning

It may happen that the variability of the estimated density is so high that not all jumps in the mode function can be detected by the selected grid scanning the density function. In that case, no

output is produced and a message is displayed. As this may be associated to the occurrence of some spurious connected components, which appear and disappear within the range between two subsequent values of the grid, a natural solution is to increase the value of n.grid. Alternatively either lambda or hmult may be increased to alleviate the chance of detecting spurious connected components.

Using graphtype='delaunay' when the dimensionality d of data is greater than 6 is highly time-consuming unless the number of rows n is fairly small, since the number of operations to run the Delaunay triangulation grows exponentially with d. Use graphtype= "pairs", instead, whose computational complexity grows quadratically with the number of observations.

References

Azzalini, A., Menardi, G. (2014). Clustering via nonparametric density estimation: the R package pdfCluster. *Journal of Statistical Software*, 57(11), 1-26, URL http://www.jstatsoft.org/v57/i11/.

Azzalini A., Torelli N. (2007). Clustering via nonparametric density estimation. *Statistics and Computing*. 17, 71-80.

Menardi, G., Azzalini, A. (2014). An advancement in clustering via nonparametric density estimation. *Statistics and Computing*. DOI: 10.1007/s11222-013-9400-x.

See Also

kepdf, pdfCluster-class, pdfClassification.

Examples

```
##########
#example 1
###########
# not run here for time reasons
#loading data
data(oliveoil)
#preparing data
olive1 <- 1 + oliveoil[, 3:10]
margin <- apply(data.matrix(olive1),1,sum)</pre>
olive1 <- olive1/margin
alr <- (-log( olive1[, -4]/olive1[, 4]))</pre>
#select the first 5 principal components
x <- princomp(alr, cor=TRUE)$scores[, 1:5]</pre>
#clustering
# not run here for time reasons
\#cl <- pdfCluster(x, h = h.norm(x), hmult=0.75)
#summary(cl)
#plot(cl)
#comparing groups with original macro-area membership
#groups <- groups(cl)</pre>
#table(oliveoil$macro.area, groups)
```

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```
#cluster cores
#table(groups(cl, stage = 0))
##########
#example 2
###########
# not run here for time reasons
# loading data
#data(wine)
#x <-wine[ ,-1]</pre>
#gr <- wine[ ,1]
# when data are high-dimensional, an adaptive kernel estimator is preferable
# building the Delaunay graph entails a too high computational effort
# use option "pairs" to build the graph
# it is the default option for dimension >6
# cl <- pdfCluster(x, graphtype="pairs", bwtype="adaptive")</pre>
# summary(cl)
# plot(cl)
#comparison with original groups
#table(groups(cl),gr)
# a better classification is obtained with larger value of lambda
# not necessary to run the whole procedure again
# a pdfCluster method applies on pdfCluster-class objects!
#cl1 <- pdfCluster(cl, lambda=0.25)</pre>
#table(gr, groups(cl1))
```

pdfCluster-class

Class "pdfCluster"

Description

This class pertains to results of the application of function pdfCluster.

Objects from the Class

Objects can be created by calls of the form new("pdfCluster", ...) or as a result to a call to pdfCluster.

Slots

```
call: Object of class "call" representing the matched call;x: Object of class "matrix" representing the clustered data points;pdf: Object of class "list" reporting details about the kernel density estimate at data points x.
```

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nc: Object of class "list" summarizing the result of the connected components search for different sections of the estimated density.

graph: An object of class "list" defining details about the graph built to find the connected sets of high density regions.

cluster.cores: Object of class "ANY" reporting the group labels of the data allocated to the cluster cores.

tree: Object of class "ANY", namely class dendrogram if the procedure detects more than one group, list otherwise. It reports the cluster tree structure associated to the different connected components for different density levels.

noc: Object of class "numeric" giving the number of clusters.

stages: Object of class "ANY", being NULL if the cluster cores only are detected, "list" when also the lower density data are allocated. The elements of the list correspond to the group labels at the different stages of the classification procedure. NA values correspond to unlabeled data.

clusters: Object of class "ANY" being NULL if the cluster cores only are detected, "numeric" when all the data are clustered. This slot is obsolete. Groups can be extracted by a call to function groups.

See pdfCluster for further details.

Methods

```
dbs signature(x = "pdfCluster", clusters = "missing")
```

Computes the density based Silhouette diagnostics of clustered data. See dbs for further details.

```
pdfCluster signature(x="pdfCluster")
```

Speeds up time for re-running the pdfCluster procedure with different values of tau when graphtype = "pairs"

```
plot signature(x = "pdfCluster", y = "missing")
```

Plots objects of pdfCluster-class. plot-methods are available for:

- the mode function: gives the number of connected components when the proportion of data points with density above a threshold varies. Set argument which to 1 to display this plot.
- the cluster tree: plot the hierarchical structure associated to the clusters detected by different sections of the density estimate. Set argument which to 2 to display this plot.
- the data points: scatterplot of data or of all the possible couples of coordinates reporting the label group. Set argument which to 3 to display this plot.
- the density-based Silhouette information: graphical diagnostics of the clustering. See plot, dbs-method. Set argument which to 4 to display this plot. Not available when noc=1.

See plot, pdfCluster-method for further details.

show signature(object = "pdfCluster").

Prints the following elements:

- the matched Call;
- the type of kernel estimator;

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- the type of graph built;
- the groups tree (if available);
- the cluster cores;
- the cluster labels at the different stages of the classification procedure;
- the final clustering.

```
summary signature(object = "pdfCluster").
```

Provides a summary of pdfCluster-class objects by printing the following elements:

- the matched call to pdfCluster function
- the frequency table of the cluster cores;
- the frequency table of the final grouping;
- the tree of clusters.

See Also

```
pdfCluster, plot, pdfCluster-method, show-methods, summary-methods
```

Examples

```
showClass("pdfCluster")

data(wine)
x <-wine[ ,-1]
gr <- wine[ ,1]

# clustering
cl <- pdfCluster(x, graphtype="pairs", bwtype="adaptive")
summary(cl)
cl
plot(cl)</pre>
```

plot,dbs-method

Plot objects of class dbs

Description

This function provides a graphical tool to display diagnostics of density-based cluster analysis by means of the density-based silhouette information.

Usage

```
## S4 method for signature 'dbs'
plot(x, y , xlab = "", ylab = "", col = NULL, lwd = 3, cex = 0.9,
    cex.axis = 0.5, main = NULL, labels = FALSE, ...)
```

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Arguments

X	An object of dbs-class;
У	Not used; for compatibility with generic plot;
xlab	A title for the x axis;
ylab	A title for the y axis;
col	A specification for the plotting color. Default are colors in palette corresponding to the group labels;
lwd	A specification for the width of the bars in the plot;
cex	A numerical value giving the amount by which plotting text and symbols should be magnified relative to the default;
cex.axis	The magnification to be used for axis annotation relative to the current setting of cex;
main	An overall title for the plot;
labels	Logical. Should row index of data be added to the plot?
	Further arguments to be passed to plot.

Details

After computing the density-based silhouette index by applying dbs-methods, data are partitioned into the clusters, sorted in a decreasing order with respect to their dbs value and displayed on a bar graph.

Methods

```
signature(x = "dbs", y = "missing") S4 method for plotting objects of dbs-class
```

See Also

```
dbs, dbs-class, silhouette.
```

Examples

```
#example 1: no groups in data
#random generation of group labels
set.seed(54321)
x <- rnorm(50)
groups <- sample(1:2, 50, replace=TRUE)
groups
dsil <- dbs(x=as.matrix(x), clusters=groups)
dsil
summary(dsil)
plot(dsil, labels=TRUE, lwd=6)

#example 2: wines data
# load data
data(wine)</pre>
```

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```
gr <- wine[,1]
# select a subset of variables
x <- wine[, c(2,5,8)]
#clustering
cl <- pdfCluster(x)
dsil <- dbs(cl)
plot(dsil)</pre>
```

plot,kepdf-method

Plot objects of class kepdf

Description

Functions and methods for plotting objects of kepdf-class.

Usage

```
## S4 method for signature 'kepdf'
plot(x, y, eval.points = NULL, n.grid = NULL,
  data = NULL, add = FALSE, main = NULL, xlab = NULL, ylab = NULL,
  zlab = NULL, col = NULL, col.data=2, type="1", props = c(75,50,25),
  method="contour", ticktype = "detailed", indcol = NULL,
  text.diag.panel = NULL, gap = 0.5, ...)
```

Arguments

X	An object of kepdf-class;
у	Not used; for compatibility with generic plot;
eval.points	A matrix of data points at which the density to be plotted has to be evaluated; the number of columns must correspond to the dimension of the sample data used to estimate the density. If not provided, density is evaluated on a grid defined on the range of sample data.
n.grid	A vector with length set to the number of column of sample data, defining the length of the grid on which the density to be plotted is evaluated; this argument is ignored when eval.points is not NULL.
data	Data to be optionally superimposed to the density plot.
add	Logical. If TRUE, add to a current plot.
main	An overall title for the plot.
xlab	A title for the x axis.
ylab	A title for the y axis.
zlab	A title for the z axis.
col	A specification for the plotting color.

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col.data	A specification for the color of data. Ignored if data is NULL.
type	What type of plot should be drawn. This argument applies when kernel density estimate is performed on unidimensional data only. Default value is "1".
props	A vector defining the fraction of the data to be included within each density level. This argument applies when kernel density estimate is performed on multidimensional data only.
method	One of c("contour", "image", "perspective"). To be used when two or higher dimensional data have been used to estimate the density.
ticktype	Character: "simple" draws just an arrow parallel to the axis to indicate direction of increase; "detailed" draws normal ticks; to be used if method="perspective" only.
indcol	Vector of the column positions to be plotted, when densities are estimated on higher than 2-dimensional data.
text.diag.pane	1
	Text to be displayed on the diagonal panels when plotting densities estimated on higher than 2-dimensional data.
gap	Distance between subplots, when plotting densities estimated of 2-dimensional data or higher-dimensional data.
• • •	Further arguments to be passed to plot, image, contour, persp.

Details

When density estimation is based on two or higher dimensional data, these functions make use of functions contour, image and persp. For densities estimated on higher than 2-d data, the pairwise marginal estimated densities are plotted for all possible pairs of coordinates or a chosen selection of them.

Value

A list containing the following elements:

eval.points data points at which the plotted density has been evaluated

estimate the estimated density at eval.points

Methods

```
signature(x = "kepdf", y = "missing") S4 method for plotting objects of kepdf-class.
```

See Also

```
kepdf-class, plot, contour, image, plot-methods, persp
```

Examples

```
#1-d example
set.seed(123)
x1 <- rnorm(50)
#normal optimal bandwidth
pdf1a \leftarrow kepdf(x1)
#shrink the smoothing parameter
pdf1b \leftarrow kepdf(x1, h=0.5*h.norm(x1))
plot(pdf1a, n.grid=50, data=x1, xlab="x1", ylim=c(0, max(c(pdf1a@estimate,
   pdf1b@estimate))))
plot(pdf1b, n.grid=50, lty=2, add=TRUE)
#2-d example
set.seed(123)
x2 <- cbind(rnorm(50),rnorm(50))</pre>
pdf2 \leftarrow kepdf(x2)
plot(pdf2, n.grid=c(50,50), data=x2)
plot(pdf2, n.grid=c(50,50), method="image")
plot(pdf2, n.grid=c(50,50), method="perspective", phi=30, theta=30)
#3-d example
set.seed(123)
x3 <- cbind(rnorm(50), rnorm(50), rnorm(50))
pdf3 <- kepdf(x3)
plot(pdf3, n.grid=c(50,50,50))
plot(pdf3, n.grid=c(50,50,50), method="image", col = terrain.colors(30))
plot(pdf3, n.grid=c(50,50,50), method="perspective", phi=30, theta=30)
```

plot,pdfCluster-method

Plot objects of class pdfCluster

Description

Functions and methods for plotting objects of pdfCluster-class.

Usage

```
## S4 method for signature 'pdfCluster'
plot(x, y, which = 1:4, stage = Inf, pch = NULL, col = NULL, ...)
```

Arguments

x An object of pdfCluster-class;

y Not used; for compatibility with generic plot;

which To be used to select the type of plot:

- when which = 1 plots the mode function, corresponding to the number of modes for different proportions of data points with density above a threshold.
- when which = 2 plots the cluster tree associated to different sections of the density estimate.
- when which = 3 displays the scatterplot of data or of all the possible pairs of coordinates reporting the label group.
- when which = 4 the plot.dbs is displayed.

Multiple choices are possible.

stage Plots the data points at the indicated stage of the classification procedure. Un-

allocated data are indicated by 0s. This argument applies if which=3 only.

Either an integer specifying a symbol or a single character to be used in plotting points. If a vector of the same length as the number of groups is given, different symbols or characters are used for different groups. The default value denotes points as their group label. This argument applies if which=3 only.

points as their group facer. This argument applies it writeries only.

Colors to be used in plotting points. If a vector of the same length as the number of groups is given, different colors or characters are used for different groups. The default value use colors in palette corresponding to the group labels of the data. This argument applies if which=3 only.

Further arguments to be passed to plot-methods.

Methods

pch

col

```
signature(x = "pdfCluster", y = "missing") S4 method for plotting objects of pdfCluster-class
```

References

Azzalini A., Torelli N. (2007). Clustering via nonparametric density estimation. *Statistics and Computing*. vol. 17, pp. 71-80.

See Also

```
pdfCluster-class, plot, plot-methods.
```

Examples

```
data(wine)
gr <- wine[,1]

# select a subset of variables
x <- wine[, c(2,5,8)]</pre>
```

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```
#clustering
cl <- pdfCluster(x)
plot(cl, which=3, stage=2)

table(cl@clusters, gr)
#set "B" for Barolo, "G" for Grignolino, "A" for Barbera
plot(cl, pch=c("B", "G", "A"), col=c(3,4,5))</pre>
```

plot-methods

Methods for function plot

Description

Methods for functions plot aimed at graphically displaying the S4 classes included in the pdfCluster-package.

Methods

```
signature(x = "kepdf", y = "ANY") S4 method for plotting objects of kepdf-class. See plot, kepdf-method
    for further details.
signature(x = "dbs", y = "missing") S4 method for plotting objects of kepdf-class. See plot, dbs-method
    for further details.
signature(x = "pdfCluster", y = "missing") S4 method for plotting objects of pdfCluster-class.
    See plot, pdfCluster-method for further details.
```

See Also

```
plot, dbs-method, plot, kepdf-method, plot, pdfCluster-method
```

show-methods

Methods for Function show

Description

Methods for function show aimed at showing the S4 classes included in the pdfCluster-package.

Methods

```
signature(object = "kepdf") S4 method for showing objects of kepdf-class.
signature(object = "dbs") S4 method for showing objects of dbs-class.
signature(object = "pdfCluster") S4 method for showing objects of pdfCluster-class.
```

See Also

```
dbs-class, kepdf-class, pdfCluster-class
```

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summary-methods Methods for Function summary
--

Description

Methods for function summary aimed at summarizing the S4 classes included in the pdfCluster-package.

Methods

```
signature(object = "dbs") S4 method for summarizing objects of dbs-class.
signature(object = "kepdf") S4 method for summarizing objects of kepdf-class.
signature(object = "pdfCluster") S4 method for summarizing objects of pdfCluster-class.
```

See Also

dbs-class, kepdf-class, pdfCluster-class.

wine	Wine data

Description

These data are the results of a chemical analysis of wines grown in the same region in Italy but derived from three different cultivars. The analysis determined the quantities of 13 constituents found in each of the three types of wine: Barolo, Grignolino, Barbera. The data set is used to evaluate the pdfCluster ability of understanding the type of wine, given the chemical measurement.

Usage

```
data(wine)
```

Format

This data frame contains 178 rows, each corresponding to a different cultivar of wine produced in Piedmont (Italy), and 14 columns. The first column is the type of wine, a factor variable with the following levels: Barolo, Grignolino, Barbera. The variables measured on the three types of wines are the following: Alcohol, Malic acid, Ash, Alcalinity, Magnesium, Phenols, Flavanoids, Nonflavanoids, Proanthocyanins, Color intensity, Hue, OD280.OD315Dilution, Proline. All variables but the label class are continuous.

Details

The original data set comprises 27 variables. Here a subset of 14 variables only has been included.

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Source

Forina, M., Lanteri, S. Armanino, C., Casolino, C., Casale, M., Oliveri, P. (2008). V-PARVUS. *An Extendible Pachage of programs for esplorative data analysis, classification and regression analysis*. Dip. Chimica e Tecnologie Farmaceutiche ed Alimentari, Università di Genova.

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