

Package ‘cluster’

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| | |
|------------------------|----|
| agnes | 3 |
| agnes.object | 5 |
| agriculture | 7 |
| animals | 8 |
| bannerplot | 9 |
| chorSub | 10 |

| | |
|-----------------------------------|----|
| clara | 11 |
| clara.object | 14 |
| clusplot | 15 |
| clusplot.default | 16 |
| coef.hclust | 20 |
| daisy | 21 |
| diana | 24 |
| dissimilarity.object | 27 |
| ellipsoidhull | 28 |
| fanny | 30 |
| fanny.object | 32 |
| flower | 34 |
| lower.to.upper.tri.inds | 35 |
| mona | 36 |
| mona.object | 37 |
| pam | 38 |
| pam.object | 40 |
| partition.object | 42 |
| plantTraits | 43 |
| plot.agnes | 45 |
| plot.diana | 47 |
| plot.mona | 49 |
| plot.partition | 50 |
| pltree | 52 |
| pltree.twins | 52 |
| pluton | 54 |
| predict.ellipsoid | 55 |
| print.agnes | 56 |
| print.clara | 57 |
| print.diana | 57 |
| print.dissimilarity | 58 |
| print.fanny | 59 |
| print.mona | 59 |
| print.pam | 60 |
| ruspini | 60 |
| silhouette | 61 |
| sizeDiss | 64 |
| summary.agnes | 65 |
| summary.clara | 66 |
| summary.diana | 67 |
| summary.mona | 67 |
| summary.pam | 68 |
| twins.object | 68 |
| volume.ellipsoid | 69 |
| votes.repub | 70 |
| xclara | 70 |

 agnes

Agglomerative Nesting (Hierarchical Clustering)

Description

Computes agglomerative hierarchical clustering of the dataset.

Usage

```
agnes(x, diss = inherits(x, "dist"), metric = "euclidean",
      stand = FALSE, method = "average", par.method,
      keep.diss = n < 100, keep.data = !diss)
```

Arguments

| | |
|------------|---|
| x | <p>data matrix or data frame, or dissimilarity matrix, depending on the value of the <code>diss</code> argument.</p> <p>In case of a matrix or data frame, each row corresponds to an observation, and each column corresponds to a variable. All variables must be numeric. Missing values (NAs) are allowed.</p> <p>In case of a dissimilarity matrix, <code>x</code> is typically the output of <code>daisy</code> or <code>dist</code>. Also a vector with length $n*(n-1)/2$ is allowed (where n is the number of observations), and will be interpreted in the same way as the output of the above-mentioned functions. Missing values (NAs) are not allowed.</p> |
| diss | <p>logical flag: if TRUE (default for <code>dist</code> or dissimilarity objects), then <code>x</code> is assumed to be a dissimilarity matrix. If FALSE, then <code>x</code> is treated as a matrix of observations by variables.</p> |
| metric | <p>character string specifying the metric to be used for calculating dissimilarities between observations. The currently available options are "euclidean" and "manhattan". Euclidean distances are root sum-of-squares of differences, and manhattan distances are the sum of absolute differences. If <code>x</code> is already a dissimilarity matrix, then this argument will be ignored.</p> |
| stand | <p>logical flag: if TRUE, then the measurements in <code>x</code> are standardized before calculating the dissimilarities. Measurements are standardized for each variable (column), by subtracting the variable's mean value and dividing by the variable's mean absolute deviation. If <code>x</code> is already a dissimilarity matrix, then this argument will be ignored.</p> |
| method | <p>character string defining the clustering method. The six methods implemented are "average" ([unweighted pair-]group average method, UPGMA), "single" (single linkage), "complete" (complete linkage), "ward" (Ward's method), "weighted" (weighted average linkage) and its generalization "flexible" which uses (a constant version of) the Lance-Williams formula and the <code>par.method</code> argument. Default is "average".</p> |
| par.method | <p>if <code>method == "flexible"</code>, numeric vector of length 1, 3, or 4, see in the details section.</p> |

`keep.diss, keep.data`

logicals indicating if the dissimilarities and/or input data `x` should be kept in the result. Setting these to `FALSE` can give much smaller results and hence even save memory allocation *time*.

Details

`agnes` is fully described in chapter 5 of Kaufman and Rousseeuw (1990). Compared to other agglomerative clustering methods such as `hclust`, `agnes` has the following features: (a) it yields the agglomerative coefficient (see [agnes.object](#)) which measures the amount of clustering structure found; and (b) apart from the usual tree it also provides the banner, a novel graphical display (see [plot.agnes](#)).

The `agnes`-algorithm constructs a hierarchy of clusterings.

At first, each observation is a small cluster by itself. Clusters are merged until only one large cluster remains which contains all the observations. At each stage the two *nearest* clusters are combined to form one larger cluster.

For `method="average"`, the distance between two clusters is the average of the dissimilarities between the points in one cluster and the points in the other cluster.

In `method="single"`, we use the smallest dissimilarity between a point in the first cluster and a point in the second cluster (nearest neighbor method).

When `method="complete"`, we use the largest dissimilarity between a point in the first cluster and a point in the second cluster (furthest neighbor method).

The `method = "flexible"` allows (and requires) more details: The Lance-Williams formula specifies how dissimilarities are computed when clusters are agglomerated (equation (32) in K.&R., p.237). If clusters C_1 and C_2 are agglomerated into a new cluster, the dissimilarity between their union and another cluster Q is given by

$$D(C_1 \cup C_2, Q) = \alpha_1 * D(C_1, Q) + \alpha_2 * D(C_2, Q) + \beta * D(C_1, C_2) + \gamma * |D(C_1, Q) - D(C_2, Q)|,$$

where the four coefficients $(\alpha_1, \alpha_2, \beta, \gamma)$ are specified by the vector `par.method`:

If `par.method` is of length 1, say $= \alpha$, `par.method` is extended to give the "Flexible Strategy" (K. & R., p.236 f) with Lance-Williams coefficients $(\alpha_1 = \alpha_2 = \alpha, \beta = 1 - 2\alpha, \gamma = 0)$.

If of length 3, $\gamma = 0$ is used.

Care and expertise is probably needed when using `method = "flexible"` particularly for the case when `par.method` is specified of longer length than one. The *weighted average* (`method="weighted"`) is the same as `method="flexible"`, `par.method = 0.5`.

Value

an object of class "`agnes`" representing the clustering. See [agnes.object](#) for details.

BACKGROUND

Cluster analysis divides a dataset into groups (clusters) of observations that are similar to each other.

Hierarchical methods like `agnes`, [diana](#), and [mona](#) construct a hierarchy of clusterings, with the number of clusters ranging from one to the number of observations.

Partitioning methods like [pam](#), [clara](#), and [fanny](#) require that the number of clusters be given by the user.

References

- Kaufman, L. and Rousseeuw, P.J. (1990). *Finding Groups in Data: An Introduction to Cluster Analysis*. Wiley, New York.
- Anja Struyf, Mia Hubert & Peter J. Rousseeuw (1996): Clustering in an Object-Oriented Environment. *Journal of Statistical Software*, **1**. <http://www.stat.ucla.edu/journals/jss/>
- Struyf, A., Hubert, M. and Rousseeuw, P.J. (1997). Integrating Robust Clustering Techniques in S-PLUS, *Computational Statistics and Data Analysis*, **26**, 17–37.
- Lance, G.N., and W.T. Williams (1966). A General Theory of Classifactory Sorting Strategies, I. Hierarchical Systems. *Computer J.* **9**, 373–380.

See Also

[agnes.object](#), [daisy](#), [diana](#), [dist](#), [hclust](#), [plot.agnes](#), [twins.object](#).

Examples

```
data(votes.repub)
agn1 <- agnes(votes.repub, metric = "manhattan", stand = TRUE)
agn1
plot(agn1)

op <- par(mfrow=c(2,2))
agn2 <- agnes(daisy(votes.repub), diss = TRUE, method = "complete")
plot(agn2)
agnS <- agnes(votes.repub, method = "flexible", par.meth = 0.6)
plot(agnS)
par(op)

data(agriculture)
## Plot similar to Figure 7 in ref
## Not run: plot(agnes(agriculture), ask = TRUE)
```

agnes.object

Agglomerative Nesting (AGNES) Object

Description

The objects of class "agnes" represent an agglomerative hierarchical clustering of a dataset.

Value

A legitimate agnes object is a list with the following components:

| | |
|-------|---|
| order | a vector giving a permutation of the original observations to allow for plotting, in the sense that the branches of a clustering tree will not cross. |
|-------|---|

| | |
|-----------|--|
| order.lab | a vector similar to order, but containing observation labels instead of observation numbers. This component is only available if the original observations were labelled. |
| height | a vector with the distances between merging clusters at the successive stages. |
| ac | the agglomerative coefficient, measuring the clustering structure of the dataset. For each observation i , denote by $m(i)$ its dissimilarity to the first cluster it is merged with, divided by the dissimilarity of the merger in the final step of the algorithm. The ac is the average of all $1 - m(i)$. It can also be seen as the average width (or the percentage filled) of the banner plot. Because ac grows with the number of observations, this measure should not be used to compare datasets of very different sizes. |
| merge | an $(n-1)$ by 2 matrix, where n is the number of observations. Row i of merge describes the merging of clusters at step i of the clustering. If a number j in the row is negative, then the single observation $ j $ is merged at this stage. If j is positive, then the merger is with the cluster formed at stage j of the algorithm. |
| diss | an object of class "dissimilarity" (see dissimilarity.object), representing the total dissimilarity matrix of the dataset. |
| data | a matrix containing the original or standardized measurements, depending on the stand option of the function agnes. If a dissimilarity matrix was given as input structure, then this component is not available. |

GENERATION

This class of objects is returned from [agnes](#).

METHODS

The "agnes" class has methods for the following generic functions: print, summary, plot.

INHERITANCE

The class "agnes" inherits from "twins". Therefore, the generic functions [pltree](#) and [as.hclust](#) are available for agnes objects. After applying [as.hclust\(\)](#), all *its* methods are available, of course.

See Also

[agnes](#), [diana](#), [as.hclust](#), [hclust](#), [plot.agnes](#), [twins.object](#).

agriculture*European Union Agricultural Workforces*

Description

Gross National Product (GNP) per capita and percentage of the population working in agriculture for each country belonging to the European Union in 1993.

Usage

```
data(agriculture)
```

Format

A data frame with 12 observations on 2 variables:

| | | | |
|--------|---|---------|---------------------------|
| [, 1] | x | numeric | per capita GNP |
| [, 2] | y | numeric | percentage in agriculture |

The row names of the data frame indicate the countries.

Details

The data seem to show two clusters, the “more agricultural” one consisting of Greece, Portugal, Spain, and Ireland.

Source

Eurostat (European Statistical Agency, 1994): *Cijfers en feiten: Een statistisch portret van de Europese Unie*.

References

Anja Struyf, Mia Hubert & Peter J. Rousseeuw (1996): Clustering in an Object-Oriented Environment. *Journal of Statistical Software*, **1**. <http://www.stat.ucla.edu/journals/jss/>

See Also

[agnes](#), [daisy](#), [diana](#).

Examples

```
data(agriculture)

## Compute the dissimilarities using Euclidean metric and without
## standardization
daisy(agriculture, metric = "euclidean", stand = FALSE)
```

```
## 2nd plot is similar to Figure 3 in Struyf et al (1996)
plot(pam(agriculture, 2))

## Plot similar to Figure 7 in Struyf et al (1996)
## Not run: plot(agnes(agriculture), ask = TRUE)

## Plot similar to Figure 8 in Struyf et al (1996)
## Not run: plot(diana(agriculture), ask = TRUE)
```

animals

Attributes of Animals

Description

This data set considers 6 binary attributes for 20 animals.

Usage

```
data(animals)
```

Format

A data frame with 20 observations on 6 variables:

| | | |
|--------|-----|----------------|
| [, 1] | war | warm-blooded |
| [, 2] | fly | can fly |
| [, 3] | ver | vertebrate |
| [, 4] | end | endangered |
| [, 5] | gro | live in groups |
| [, 6] | hai | have hair |

All variables are encoded as 1 = 'no', 2 = 'yes'.

Details

This dataset is useful for illustrating monothetic (only a single variable is used for each split) hierarchical clustering.

Source

Leonard Kaufman and Peter J. Rousseeuw (1990): *Finding Groups in Data* (pp 297ff). New York: Wiley.

References

Anja Struyf, Mia Hubert & Peter J. Rousseeuw (1996): Clustering in an Object-Oriented Environment. *Journal of Statistical Software*, **1**. <http://www.stat.ucla.edu/journals/jss/>

Examples

```
data(animals)
apply(animals,2, table) # simple overview

ma <- mona(animals)
ma
## Plot similar to Figure 10 in Struyf et al (1996)
plot(ma)
```

| | |
|------------|---|
| bannerplot | <i>Plot Banner (of Hierarchical Clustering)</i> |
|------------|---|

Description

Draws a “banner”, i.e. basically a horizontal [barplot](#) visualizing the (agglomerative or divisive) hierarchical clustering or an other binary dendrogram structure.

Usage

```
bannerplot(x, w = rev(x$height), fromLeft = TRUE,
           main=NULL, sub=NULL, xlab = "Height", adj = 0,
           col = c(2, 0), border = 0, axes = TRUE, frame.plot = axes,
           rev.xax = !fromLeft, xax.pretty = TRUE,
           labels = NULL, nmax.lab = 35, max.strlen = 5,
           yax.do = axes && length(x$order) <= nmax.lab,
           yaxRight = fromLeft, y.mar = 2.4 + max.strlen/2.5, ...)
```

Arguments

| | |
|-----------|--|
| x | a list with components order, order.lab and height when w, the next argument is not specified. |
| w | non-negative numeric vector of bar widths. |
| fromLeft | logical, indicating if the banner is from the left or not. |
| main, sub | main and sub titles, see title . |
| xlab | x axis label (with ‘correct’ default e.g. for <code>plot.agnes</code>). |
| adj | passed to title (main, sub) for string adjustment. |
| col | vector of length 2, for two horizontal segments. |
| border | color for bar border; now defaults to background (no border). |
| axes | logical indicating if axes (and labels) should be drawn at all. |

| | |
|-------------------------|---|
| <code>frame.plot</code> | logical indicating the banner should be framed; mainly used when <code>border = 0</code> (as per default). |
| <code>rev.xax</code> | logical indicating if the x axis should be reversed (as in <code>plot.diana</code>). |
| <code>xax.pretty</code> | logical or integer indicating if <code>pretty()</code> should be used for the x axis. <code>xax.pretty = FALSE</code> is mainly for back compatibility. |
| <code>labels</code> | labels to use on y-axis; the default is constructed from x. |
| <code>nmax.lab</code> | integer indicating the number of labels which is considered too large for single-name labelling the banner plot. |
| <code>max.strlen</code> | positive integer giving the length to which strings are truncated in banner plot labeling. |
| <code>yax.do</code> | logical indicating if a y axis and banner labels should be drawn. |
| <code>yaxRight</code> | logical indicating if the y axis is on the right or left. |
| <code>y.mar</code> | positive number specifying the margin width to use when banners are labeled (along a y-axis). The default adapts to the string width and optimally would also depend on the font. |
| <code>...</code> | graphical parameters (see <code>par</code>) may also be supplied as arguments to this function. |

Note

This is mainly a utility called from `plot.agnes`, `plot.diana` and `plot.mona`.

Author(s)

Martin Maechler (from original code of Kaufman and Rousseeuw).

Examples

```
data(agriculture)
bannerplot(agnes(agriculture), main = "Bannerplot")
```

chorSub

Subset of C-horizon of Kola Data

Description

This is a small rounded subset of the C-horizon data `chorizon` from package `mvoutlier`.

Usage

```
data(chorSub)
```

Format

A data frame with 61 observations on 10 variables. The variables contain scaled concentrations of chemical elements.

Details

This data set was produced from chorizon via these statements:

```
data(chorizon, package = "mvoutlier")
chorSub <- round(100*scale(chorizon[,101:110]))[190:250,]
storage.mode(chorSub) <- "integer"
colnames(chorSub) <- gsub("_.*", "", colnames(chorSub))
```

Source

Kola Project (1993-1998)

See Also

[chorizon](#) in package **mvoutlier** and other Kola data in the same package.

Examples

```
data(chorSub)
summary(chorSub)
pairs(chorSub, gap= .1)# some outliers
```

clara

Clustering Large Applications

Description

Computes a "clara" object, a list representing a clustering of the data into k clusters.

Usage

```
clara(x, k, metric = "euclidean", stand = FALSE, samples = 5,
      sampsize = min(n, 40 + 2 * k), trace = 0, medoids.x = TRUE,
      keep.data = medoids.x, rngR = FALSE, pamLike = FALSE)
```

Arguments

- | | |
|--------|---|
| x | data matrix or data frame, each row corresponds to an observation, and each column corresponds to a variable. All variables must be numeric. Missing values (NAs) are allowed. |
| k | integer, the number of clusters. It is required that $0 < k < n$ where n is the number of observations (i.e., $n = \text{nrow}(x)$). |
| metric | character string specifying the metric to be used for calculating dissimilarities between observations. The currently available options are "euclidean" and "manhattan". Euclidean distances are root sum-of-squares of differences, and manhattan distances are the sum of absolute differences. |

| | |
|-----------|--|
| stand | logical, indicating if the measurements in <code>x</code> are standardized before calculating the dissimilarities. Measurements are standardized for each variable (column), by subtracting the variable's mean value and dividing by the variable's mean absolute deviation. |
| samples | integer, number of samples to be drawn from the dataset. The default, 5, is rather small for historical (and now back compatibility) reasons and we recommend to set samples an order of magnitude larger. |
| sampsize | integer, number of observations in each sample. <code>sampsize</code> should be higher than the number of clusters (<code>k</code>) and at most the number of observations (<code>n = nrow(x)</code>). |
| trace | integer indicating a <i>trace level</i> for diagnostic output during the algorithm. |
| medoids.x | logical indicating if the medoids should be returned, identically to some rows of the input data <code>x</code> . If FALSE, <code>keep.data</code> must be false as well, and the medoid indices, i.e., row numbers of the medoids will still be returned (<code>i.med</code> component), and the algorithm saves space by needing one copy less of <code>x</code> . |
| keep.data | logical indicating if the (<i>scaled</i> if <code>stand</code> is true) data should be kept in the result. Setting this to FALSE saves memory (and hence time), but disables <code>clusplot()</code> ing of the result. Use <code>medoids.x = FALSE</code> to save even more memory. |
| rngR | logical indicating if R's random number generator should be used instead of the primitive <code>clara()</code> -builtin one. If true, this also means that each call to <code>clara()</code> returns a different result – though only slightly different in good situations. |
| pamLike | logical indicating if the “swap” phase (see <code>pam</code> , in C code) should use the same algorithm as <code>pam()</code> . Note that from Kaufman and Rousseeuw's description this <i>should</i> have been true always, but as the original Fortran code and the subsequent port to C has always contained a small one-letter change (a typo according to Martin Maechler) with respect to PAM, the default, <code>pamLike = FALSE</code> has been chosen to remain back compatible rather than “PAM compatible”. |

Details

`clara` is fully described in chapter 3 of Kaufman and Rousseeuw (1990). Compared to other partitioning methods such as `pam`, it can deal with much larger datasets. Internally, this is achieved by considering sub-datasets of fixed size (`sampsize`) such that the time and storage requirements become linear in n rather than quadratic.

Each sub-dataset is partitioned into k clusters using the same algorithm as in `pam`.

Once k representative objects have been selected from the sub-dataset, each observation of the entire dataset is assigned to the nearest medoid.

The mean (equivalent to the sum) of the dissimilarities of the observations to their closest medoid is used as a measure of the quality of the clustering. The sub-dataset for which the mean (or sum) is minimal, is retained. A further analysis is carried out on the final partition.

Each sub-dataset is forced to contain the medoids obtained from the best sub-dataset until then. Randomly drawn observations are added to this set until `sampsize` has been reached.

Value

an object of class “`clara`” representing the clustering. See `clara.object` for details.

Note

By default, the random sampling is implemented with a *very* simple scheme (with period $2^{16} = 65536$) inside the Fortran code, independently of R's random number generation, and as a matter of fact, deterministically. Alternatively, we recommend setting `rngR = TRUE` which uses R's random number generators. Then, `clara()` results are made reproducible typically by using `set.seed()` before calling `clara`.

The storage requirement of `clara` computation (for small k) is about $O(n \times p) + O(j^2)$ where $j = \text{samplesize}$, and $(n, p) = \text{dim}(x)$. The CPU computing time (again assuming small k) is about $O(n \times p \times j^2 \times N)$, where $N = \text{samples}$.

For “small” datasets, the function `pam` can be used directly. What can be considered *small*, is really a function of available computing power, both memory (RAM) and speed. Originally (1990), “small” meant less than 100 observations; in 1997, the authors said “*small (say with fewer than 200 observations)*”; as of 2006, you can use `pam` with several thousand observations.

Author(s)

Kaufman and Rousseeuw (see `agnes`), originally. All arguments from `trace` on, and most R documentation and all tests by Martin Maechler.

See Also

`agnes` for background and references; `clara.object`, `pam`, `partition.object`, `plot.partition`.

Examples

```
## generate 500 objects, divided into 2 clusters.
x <- rbind(cbind(rnorm(200,0,8), rnorm(200,0,8)),
           cbind(rnorm(300,50,8), rnorm(300,50,8)))
clarax <- clara(x, 2, samples=50)
clarax
clarax$clusinfo
## using pamLike=TRUE gives the same (apart from the 'call'):
all.equal(clarax[-8],
          clara(x, 2, samples=50, pamLike = TRUE)[-8])
plot(clarax)

## 'xclara' is an artificial data set with 3 clusters of 1000 bivariate
## objects each.
data(xclara)
(clx3 <- clara(xclara, 3))
## "better" number of samples
cl.3 <- clara(xclara, 3, samples=100)
## but that did not change the result here:
stopifnot(cl.3$clustering == clx3$clustering)
## Plot similar to Figure 5 in Struyf et al (1996)
## Not run: plot(clx3, ask = TRUE)

## Try 100 times *different* random samples -- for reliability:
nSim <- 100
```

```

nCl <- 3 # = no.classes
set.seed(421)# (reproducibility)
cl <- matrix(NA,nrow(xclara), nSim)
for(i in 1:nSim)
  cl[,i] <- clara(xclara, nCl, medoids.x = FALSE, rngR = TRUE)$cluster
tcl <- apply(cl,1, tabulate, nbins = nCl)
## those that are not always in same cluster (5 out of 3000 for this seed):
(iDoubt <- which(apply(tcl,2, function(n) all(n < nSim))))
if(length(iDoubt)) { # (not for all seeds)
  tabD <- tcl[,iDoubt, drop=FALSE]
  dimnames(tabD) <- list(cluster = paste(1:nCl), obs = format(iDoubt))
  t(tabD) # how many times in which clusters
}

```

clara.object

Clustering Large Applications (CLARA) Object

Description

The objects of class "clara" represent a partitioning of a large dataset into clusters and are typically returned from [clara](#).

Value

A legitimate clara object is a list with the following components:

| | |
|------------|---|
| sample | labels or case numbers of the observations in the best sample, that is, the sample used by the clara algorithm for the final partition. |
| medoids | the medoids or representative objects of the clusters. It is a matrix with in each row the coordinates of one medoid. Possibly NULL, namely when the object resulted from clara(*, medoids.x=FALSE). Use the following i.med in that case. |
| i.med | the <i>indices</i> of the medoids above: medoids <- x[i.med,] where x is the original data matrix in clara(x,*). |
| clustering | the clustering vector, see partition.object . |
| objective | the objective function for the final clustering of the entire dataset. |
| clusinfo | matrix, each row gives numerical information for one cluster. These are the cardinality of the cluster (number of observations), the maximal and average dissimilarity between the observations in the cluster and the cluster's medoid. The last column is the maximal dissimilarity between the observations in the cluster and the cluster's medoid, divided by the minimal dissimilarity between the cluster's medoid and the medoid of any other cluster. If this ratio is small, the cluster is well-separated from the other clusters. |
| diss | dissimilarity (maybe NULL), see partition.object . |
| silinfo | list with silhouette width information for the best sample, see partition.object . |
| call | generating call, see partition.object . |
| data | matrix, possibly standardized, or NULL, see partition.object . |

Methods, Inheritance

The "clara" class has methods for the following generic functions: print, summary.

The class "clara" inherits from "partition". Therefore, the generic functions plot and clusplot can be used on a clara object.

See Also

[clara](#), [dissimilarity.object](#), [partition.object](#), [plot.partition](#).

| | |
|----------|--|
| clusplot | <i>Bivariate Cluster Plot (of a Partitioning Object)</i> |
|----------|--|

Description

Draws a 2-dimensional "clusplot" (clustering plot) on the current graphics device. The generic function has a default and a partition method.

Usage

```
clusplot(x, ...)

## S3 method for class 'partition'
clusplot(x, main = NULL, dist = NULL, ...)
```

Arguments

| | |
|------|---|
| x | an R object, here, specifically an object of class "partition", e.g. created by one of the functions pam , clara , or fanny . |
| main | title for the plot; when NULL (by default), a title is constructed, using x\$call. |
| dist | when x does not have a diss nor a data component, e.g., for pam (dist(*), keep.diss=FALSE), dist must specify the dissimilarity for the clusplot. |
| ... | optional arguments passed to methods, notably the clusplot.default method (except for the diss one) may also be supplied to this function. Many graphical parameters (see par) may also be supplied as arguments here. |

Details

The `clusplot.partition()` method relies on [clusplot.default](#).

If the clustering algorithms [pam](#), [fanny](#) and [clara](#) are applied to a data matrix of observations-by-variables then a clusplot of the resulting clustering can always be drawn. When the data matrix contains missing values and the clustering is performed with [pam](#) or [fanny](#), the dissimilarity matrix will be given as input to clusplot. When the clustering algorithm [clara](#) was applied to a data matrix with NAs then clusplot will replace the missing values as described in [clusplot.default](#), because a dissimilarity matrix is not available.

Value

For the partition (and default) method: An invisible list with components Distances and Shading, as for [clusplot.default](#), see there.

Side Effects

a 2-dimensional clusplot is created on the current graphics device.

See Also

[clusplot.default](#) for references; [partition.object](#), [pam](#), [pam.object](#), [clara](#), [clara.object](#), [fanny](#), [fanny.object](#), [par](#).

Examples

```
## For more, see ?clusplot.default

## generate 25 objects, divided into 2 clusters.
x <- rbind(cbind(rnorm(10,0,0.5), rnorm(10,0,0.5)),
           cbind(rnorm(15,5,0.5), rnorm(15,5,0.5)))
clusplot(pam(x, 2))
## add noise, and try again :
x4 <- cbind(x, rnorm(25), rnorm(25))
clusplot(pam(x4, 2))
```

clusplot.default

*Bivariate Cluster Plot (clusplot) Default Method***Description**

Creates a bivariate plot visualizing a partition (clustering) of the data. All observation are represented by points in the plot, using principal components or multidimensional scaling. Around each cluster an ellipse is drawn.

Usage

```
## Default S3 method:
clusplot(x, clus, diss = FALSE, cor = TRUE, stand = FALSE,
         lines = 2, shade = FALSE, color = FALSE,
         labels = 0, plotchar = TRUE,
         col.p = "dark green", col.txt = col.p,
         col.clus = if(color) c(2, 4, 6, 3) else 5, cex = 1, cex.txt = cex,
         span = TRUE,
         add = FALSE,
         xlim = NULL, ylim = NULL,
         main = paste("CLUSPLOT(", deparse(substitute(x)), ")"),
         sub = paste("These two components explain",
                     round(100 * var.dec, digits = 2), "% of the point variability."),
```



```
verbose = getOption("verbose"),
...)
```

Arguments

| | |
|---------------|---|
| x | <p>matrix or data frame, or dissimilarity matrix, depending on the value of the diss argument.</p> <p>In case of a matrix (alike), each row corresponds to an observation, and each column corresponds to a variable. All variables must be numeric. Missing values (NAs) are allowed. They are replaced by the median of the corresponding variable. When some variables or some observations contain only missing values, the function stops with a warning message.</p> <p>In case of a dissimilarity matrix, x is the output of daisy or dist or a symmetric matrix. Also, a vector of length $n * (n - 1) / 2$ is allowed (where n is the number of observations), and will be interpreted in the same way as the output of the above-mentioned functions. Missing values (NAs) are not allowed.</p> |
| clus | <p>a vector of length n representing a clustering of x. For each observation the vector lists the number or name of the cluster to which it has been assigned. clus is often the clustering component of the output of pam, fanny or clara.</p> |
| diss | <p>logical indicating if x will be considered as a dissimilarity matrix or a matrix of observations by variables (see x argument above).</p> |
| cor | <p>logical flag, only used when working with a data matrix (diss = FALSE). If TRUE, then the variables are scaled to unit variance.</p> |
| stand | <p>logical flag: if true, then the representations of the n observations in the 2-dimensional plot are standardized.</p> |
| lines | <p>integer out of 0, 1, 2, used to obtain an idea of the distances between ellipses. The distance between two ellipses E1 and E2 is measured along the line connecting the centers $m1$ and $m2$ of the two ellipses.</p> <p>In case E1 and E2 overlap on the line through $m1$ and $m2$, no line is drawn. Otherwise, the result depends on the value of lines: If</p> <p>lines = 0, no distance lines will appear on the plot;</p> <p>lines = 1, the line segment between $m1$ and $m2$ is drawn;</p> <p>lines = 2, a line segment between the boundaries of E1 and E2 is drawn (along the line connecting $m1$ and $m2$).</p> |
| shade | <p>logical flag: if TRUE, then the ellipses are shaded in relation to their density. The density is the number of points in the cluster divided by the area of the ellipse.</p> |
| color | <p>logical flag: if TRUE, then the ellipses are colored with respect to their density. With increasing density, the colors are light blue, light green, red and purple. To see these colors on the graphics device, an appropriate color scheme should be selected (we recommend a white background).</p> |
| labels | <p>integer code, currently one of 0,1,2,3,4 and 5. If</p> <p>labels= 0, no labels are placed in the plot;</p> <p>labels= 1, points and ellipses can be identified in the plot (see identify);</p> <p>labels= 2, all points and ellipses are labelled in the plot;</p> |

| | |
|---------------------------|---|
| | labels= 3 , only the points are labelled in the plot; |
| | labels= 4 , only the ellipses are labelled in the plot. |
| | labels= 5 , the ellipses are labelled in the plot, and points can be identified. |
| | The levels of the vector <code>clus</code> are taken as labels for the clusters. The labels of the points are the rownames of <code>x</code> if <code>x</code> is matrix like. Otherwise (<code>diss = TRUE</code>), <code>x</code> is a vector, point labels can be attached to <code>x</code> as a "Labels" attribute (<code>attr(x, "Labels")</code>), as is done for the output of <code>daisy</code> . |
| | A possible <code>names</code> attribute of <code>clus</code> will not be taken into account. |
| <code>plotchar</code> | logical flag: if <code>TRUE</code> , then the plotting symbols differ for points belonging to different clusters. |
| <code>span</code> | logical flag: if <code>TRUE</code> , then each cluster is represented by the ellipse with smallest area containing all its points. (This is a special case of the minimum volume ellipsoid.) If <code>FALSE</code> , the ellipse is based on the mean and covariance matrix of the same points. While this is faster to compute, it often yields a much larger ellipse. There are also some special cases: When a cluster consists of only one point, a tiny circle is drawn around it. When the points of a cluster fall on a straight line, <code>span=FALSE</code> draws a narrow ellipse around it and <code>span=TRUE</code> gives the exact line segment. |
| <code>add</code> | logical indicating if ellipses (and labels if <code>labels</code> is true) should be <i>added</i> to an already existing plot. If false, neither a <code>title</code> or sub title, see <code>sub</code> , is written. |
| <code>col.p</code> | color code(s) used for the observation points. |
| <code>col.txt</code> | color code(s) used for the labels (if <code>labels >= 2</code>). |
| <code>col.clus</code> | color code for the ellipses (and their labels); only one if <code>color</code> is false (as per default). |
| <code>cex, cex.txt</code> | character expansion (size), for the point symbols and point labels, respectively. |
| <code>xlim, ylim</code> | numeric vectors of length 2, giving the x- and y- ranges as in <code>plot.default</code> . |
| <code>main</code> | main title for the plot; by default, one is constructed. |
| <code>sub</code> | sub title for the plot; by default, one is constructed. |
| <code>verbose</code> | a logical indicating, if there should be extra diagnostic output; mainly for 'debugging'. |
| <code>...</code> | Further graphical parameters may also be supplied, see <code>par</code> . |

Details

`clusplot` uses the functions `princomp` and `cmdscale`. These functions are data reduction techniques. They will represent the data in a bivariate plot. Ellipses are then drawn to indicate the clusters. The further layout of the plot is determined by the optional arguments.

Value

An invisible list with components:

| | |
|-----------|--|
| Distances | When <code>lines</code> is 1 or 2 we obtain a <code>k</code> by <code>k</code> matrix (<code>k</code> is the number of clusters). The element in <code>[i, j]</code> is the distance between ellipse <code>i</code> and ellipse <code>j</code> . If <code>lines = 0</code> , then the value of this component is <code>NA</code> . |
|-----------|--|

Shading A vector of length k (where k is the number of clusters), containing the amount of shading per cluster. Let y be a vector where element i is the ratio between the number of points in cluster i and the area of ellipse i . When the cluster i is a line segment, $y[i]$ and the density of the cluster are set to NA. Let z be the sum of all the elements of y without the NAs. Then we put $\text{shading} = y/z * 37 + 3$.

Side Effects

a visual display of the clustering is plotted on the current graphics device.

Note

When we have 4 or fewer clusters, then the `color=TRUE` gives every cluster a different color. When there are more than 4 clusters, `clusplot` uses the function `pam` to cluster the densities into 4 groups such that ellipses with nearly the same density get the same color. `col.clus` specifies the colors used.

The `col.p` and `col.txt` arguments, added for R, are recycled to have length the number of observations. If `col.p` has more than one value, using `color = TRUE` can be confusing because of a mix of point and ellipse colors.

References

- Pison, G., Struyf, A. and Rousseeuw, P.J. (1999) Displaying a Clustering with CLUSPLOT, *Computational Statistics and Data Analysis*, **30**, 381–392.
 A version of this is available as technical report from <http://www.agoras.ua.ac.be/abstract/Disclu99.htm>
- Kaufman, L. and Rousseeuw, P.J. (1990). *Finding Groups in Data: An Introduction to Cluster Analysis*. Wiley, New York.
- Struyf, A., Hubert, M. and Rousseeuw, P.J. (1997). Integrating Robust Clustering Techniques in S-PLUS, *Computational Statistics and Data Analysis*, **26**, 17-37.

See Also

`princomp`, `cmdscale`, `pam`, `clara`, `daisy`, `par`, `identify`, `cov.mve`, `clusplot.partition`.

Examples

```
## plotting votes.diss(dissimilarity) in a bivariate plot and
## partitioning into 2 clusters
data(votes.repub)
votes.diss <- daisy(votes.repub)
pamv <- pam(votes.diss, 2, diss = TRUE)
clusplot(pamv, shade = TRUE)
## is the same as
votes.clus <- pamv$clustering
clusplot(votes.diss, votes.clus, diss = TRUE, shade = TRUE)

clusplot(pamv, col.p = votes.clus, labels = 4) # color points and label ellipses
# "simple" cheap ellipses: larger than minimum volume:
# here they are *added* to the previous plot:
```

```

clusplot(pamv, span = FALSE, add = TRUE, col.clus = "midnightblue")

## a work-around for setting a small label size:
clusplot(votes.diss, votes.clus, diss = TRUE)
op <- par(new=TRUE, cex = 0.6)
clusplot(votes.diss, votes.clus, diss = TRUE,
          axes=FALSE,ann=FALSE, sub="", col.p=NA, col.txt="dark green", labels=3)
par(op)
## MM: This should now be as simple as
clusplot(votes.diss, votes.clus, diss = TRUE, labels = 3, cex.txt = 0.6)

if(interactive()) { # uses identify() *interactively* :
  clusplot(votes.diss, votes.clus, diss = TRUE, shade = TRUE, labels = 1)
  clusplot(votes.diss, votes.clus, diss = TRUE, labels = 5)# ident. only points
}

## plotting iris (data frame) in a 2-dimensional plot and partitioning
## into 3 clusters.
data(iris)
iris.x <- iris[, 1:4]
cl3 <- pam(iris.x, 3)$clustering
op <- par(mfrow= c(2,2))
clusplot(iris.x, cl3, color = TRUE)
U <- par("usr")
## zoom in :
rect(0,-1, 2,1, border = "orange", lwd=2)
clusplot(iris.x, cl3, color = TRUE, xlim = c(0,2), ylim = c(-1,1))
box(col="orange",lwd=2); mtext("sub region", font = 4, cex = 2)
## or zoom out :
clusplot(iris.x, cl3, color = TRUE, xlim = c(-4,4), ylim = c(-4,4))
mtext("'super' region", font = 4, cex = 2)
rect(U[1],U[3], U[2],U[4], lwd=2, lty = 3)

# reset graphics
par(op)

```

coef.hclust

Agglomerative Coefficient for 'hclust' Objects

Description

Computes the “agglomerative coefficient”, measuring the clustering structure of the dataset.

For each observation i , denote by $m(i)$ its dissimilarity to the first cluster it is merged with, divided by the dissimilarity of the merger in the final step of the algorithm. The agglomerative coefficient is the average of all $1 - m(i)$. It can also be seen as the average width (or the percentage filled) of the banner plot.

Because it grows with the number of observations, this measure should not be used to compare datasets of very different sizes.

Usage

```
coef.hclust(object, ...)
## S3 method for class 'hclust'
coef(object, ...)
## S3 method for class 'twins'
coef(object, ...)
```

Arguments

| | |
|--------|--|
| object | an object of class "hclust" or "twins", i.e., typically the result of <code>hclust(.)</code> , <code>agnes(.)</code> , or <code>diana(.)</code> . Since <code>coef.hclust</code> only uses <code>object\$heights</code> , and <code>object\$merge</code> , <code>object</code> can be any list-like object with appropriate merge and heights components. |
| ... | currently unused potential further arguments |

Value

a number specifying the *agglomerative* (or *divisive* for diana objects) coefficient as defined by Kaufman and Rousseeuw, see `agnes.object $ ac` or `diana.object $ dc`.

Examples

```
data(agriculture)
aa <- agnes(agriculture)
coef(aa) # really just extracts aa$ac
coef(as.hclust(aa))# recomputes
```

daisy

Dissimilarity Matrix Calculation

Description

Compute all the pairwise dissimilarities (distances) between observations in the data set. The original variables may be of mixed types. In that case, or whenever `metric = "gower"` is set, a generalization of Gower's formula is used, see 'Details' below.

Usage

```
daisy(x, metric = c("euclidean", "manhattan", "gower"),
      stand = FALSE, type = list(), weights = rep.int(1, p))
```

Arguments

| | |
|----------------------|--|
| <code>x</code> | numeric matrix or data frame, of dimension $n \times p$, say. Dissimilarities will be computed between the rows of <code>x</code> . Columns of mode numeric (i.e. all columns when <code>x</code> is a matrix) will be recognized as interval scaled variables, columns of class factor will be recognized as nominal variables, and columns of class ordered will be recognized as ordinal variables. Other variable types should be specified with the <code>type</code> argument. Missing values (NAs) are allowed. |
| <code>metric</code> | character string specifying the metric to be used. The currently available options are "euclidean" (the default), "manhattan" and "gower". Euclidean distances are root sum-of-squares of differences, and manhattan distances are the sum of absolute differences. "Gower's distance" is chosen by metric "gower" or automatically if some columns of <code>x</code> are not numeric. Also known as Gower's coefficient (1971), expressed as a dissimilarity, this implies that a particular standardisation will be applied to each variable, and the "distance" between two units is the sum of all the variable-specific distances, see the details section. |
| <code>stand</code> | logical flag: if TRUE, then the measurements in <code>x</code> are standardized before calculating the dissimilarities. Measurements are standardized for each variable (column), by subtracting the variable's mean value and dividing by the variable's mean absolute deviation. If not all columns of <code>x</code> are numeric, <code>stand</code> will be ignored and Gower's standardization (based on the range) will be applied in any case, see argument <code>metric</code> , above, and the details section. |
| <code>type</code> | list for specifying some (or all) of the types of the variables (columns) in <code>x</code> . The list may contain the following components: "ordratio" (ratio scaled variables to be treated as ordinal variables), "logratio" (ratio scaled variables that must be logarithmically transformed), "asymm" (asymmetric binary) and "symm" (symmetric binary variables). Each component's value is a vector, containing the names or the numbers of the corresponding columns of <code>x</code> . Variables not mentioned in the <code>type</code> list are interpreted as usual (see argument <code>x</code>). |
| <code>weights</code> | an optional numeric vector of length $p(=ncol(x))$; to be used in "case 2" (mixed variables, or <code>metric = "gower"</code>), specifying a weight for each variable (<code>x[,k]</code>) instead of 1 in Gower's original formula. |

Details

The original version of `daisy` is fully described in chapter 1 of Kaufman and Rousseeuw (1990). Compared to [dist](#) whose input must be numeric variables, the main feature of `daisy` is its ability to handle other variable types as well (e.g. nominal, ordinal, (a)symmetric binary) even when different types occur in the same data set.

The handling of nominal, ordinal, and (a)symmetric binary data is achieved by using the general dissimilarity coefficient of Gower (1971). If `x` contains any columns of these data-types, both arguments `metric` and `stand` will be ignored and Gower's coefficient will be used as the metric. This can also be activated for purely numeric data by `metric = "gower"`. With that, each variable (column) is first standardized by dividing each entry by the range of the corresponding variable, after subtracting the minimum value; consequently the rescaled variable has range $[0, 1]$, exactly.

Note that setting the type to `symm` (symmetric binary) gives the same dissimilarities as using `nominal` (which is chosen for non-ordered factors) only when no missing values are present, and more efficiently.

Note that `daisy` now gives a warning when 2-valued numerical variables do not have an explicit type specified, because the reference authors recommend to consider using `"asymm"`.

In the `daisy` algorithm, missing values in a row of `x` are not included in the dissimilarities involving that row. There are two main cases,

1. If all variables are interval scaled (and `metric` is *not* "gower"), the metric is "euclidean", and n_g is the number of columns in which neither row i and j have NAs, then the dissimilarity $d(i,j)$ returned is $\sqrt{p/n_g}$ ($p = \text{ncol}(x)$) times the Euclidean distance between the two vectors of length n_g shortened to exclude NAs. The rule is similar for the "manhattan" metric, except that the coefficient is p/n_g . If $n_g = 0$, the dissimilarity is NA.
2. When some variables have a type other than interval scaled, or if `metric = "gower"` is specified, the dissimilarity between two rows is the weighted mean of the contributions of each variable. Specifically,

$$d_{ij} = d(i, j) = \frac{\sum_{k=1}^p w_k \delta_{ij}^{(k)} d_{ij}^{(k)}}{\sum_{k=1}^p w_k \delta_{ij}^{(k)}}.$$

In other words, d_{ij} is a weighted mean of $d_{ij}^{(k)}$ with weights $w_k \delta_{ij}^{(k)}$, where $w_k = \text{weights}[k]$, $\delta_{ij}^{(k)}$ is 0 or 1, and $d_{ij}^{(k)}$, the k -th variable contribution to the total distance, is a distance between $x[i, k]$ and $x[j, k]$, see below.

The 0-1 weight $\delta_{ij}^{(k)}$ becomes zero when the variable $x[, k]$ is missing in either or both rows (i and j), or when the variable is asymmetric binary and both values are zero. In all other situations it is 1.

The contribution $d_{ij}^{(k)}$ of a nominal or binary variable to the total dissimilarity is 0 if both values are equal, 1 otherwise. The contribution of other variables is the absolute difference of both values, divided by the total range of that variable. Note that "standard scoring" is applied to ordinal variables, i.e., they are replaced by their integer codes 1:K. Note that this is not the same as using their ranks (since there typically are ties).

As the individual contributions $d_{ij}^{(k)}$ are in $[0, 1]$, the dissimilarity d_{ij} will remain in this range.

If all weights $w_k \delta_{ij}^{(k)}$ are zero, the dissimilarity is set to NA.

Value

an object of class "dissimilarity" containing the dissimilarities among the rows of `x`. This is typically the input for the functions `pam`, `fanny`, `agnes` or `diana`. For more details, see [dissimilarity.object](#).

Background

Dissimilarities are used as inputs to cluster analysis and multidimensional scaling. The choice of metric may have a large impact.

Author(s)

Anja Struyf, Mia Hubert, and Peter and Rousseeuw, for the original version.
 Martin Maechler improved the NA handling and type specification checking, and extended functionality to `metric = "gower"` and the optional `weights` argument.

References

- Gower, J. C. (1971) A general coefficient of similarity and some of its properties, *Biometrics* **27**, 857–874.
- Kaufman, L. and Rousseeuw, P.J. (1990) *Finding Groups in Data: An Introduction to Cluster Analysis*. Wiley, New York.
- Struyf, A., Hubert, M. and Rousseeuw, P.J. (1997) Integrating Robust Clustering Techniques in S-PLUS, *Computational Statistics and Data Analysis* **26**, 17–37.

See Also

[dissimilarity.object](#), [dist](#), [pam](#), [fanny](#), [clara](#), [agnes](#), [diana](#).

Examples

```
data(agriculture)
## Example 1 in ref:
## Dissimilarities using Euclidean metric and without standardization
d.agr <- daisy(agriculture, metric = "euclidean", stand = FALSE)
d.agr
as.matrix(d.agr)[,"DK"] # via as.matrix.dist(.)
## compare with
as.matrix(daisy(agriculture, metric = "gower"))

data(flower)
## Example 2 in ref
summary(df11 <- daisy(flower, type = list(asymm = 3)))
summary(df12 <- daisy(flower, type = list(asymm = c(1, 3), ordratio = 7)))
## this failed earlier:
summary(df13 <- daisy(flower,
  type = list(asymm = c("V1", "V3"), symm= 2,
    ordratio= 7, logratio= 8)))
```

diana

Divisive ANALysis Clustering

Description

Computes a divisive hierarchical clustering of the dataset returning an object of class `diana`.

Usage

```
diana(x, diss = inherits(x, "dist"), metric = "euclidean", stand = FALSE,
      keep.diss = n < 100, keep.data = !diss)
```

Arguments

| | |
|-----------------------------------|--|
| <code>x</code> | <p>data matrix or data frame, or dissimilarity matrix or object, depending on the value of the <code>diss</code> argument.</p> <p>In case of a matrix or data frame, each row corresponds to an observation, and each column corresponds to a variable. All variables must be numeric. Missing values (NAs) are allowed.</p> <p>In case of a dissimilarity matrix, <code>x</code> is typically the output of <code>daisy</code> or <code>dist</code>. Also a vector of length $n*(n-1)/2$ is allowed (where n is the number of observations), and will be interpreted in the same way as the output of the above-mentioned functions. Missing values (NAs) are <i>not</i> allowed.</p> |
| <code>diss</code> | <p>logical flag: if TRUE (default for <code>dist</code> or dissimilarity objects), then <code>x</code> will be considered as a dissimilarity matrix. If FALSE, then <code>x</code> will be considered as a matrix of observations by variables.</p> |
| <code>metric</code> | <p>character string specifying the metric to be used for calculating dissimilarities between observations.</p> <p>The currently available options are "euclidean" and "manhattan". Euclidean distances are root sum-of-squares of differences, and manhattan distances are the sum of absolute differences. If <code>x</code> is already a dissimilarity matrix, then this argument will be ignored.</p> |
| <code>stand</code> | <p>logical; if true, the measurements in <code>x</code> are standardized before calculating the dissimilarities. Measurements are standardized for each variable (column), by subtracting the variable's mean value and dividing by the variable's mean absolute deviation. If <code>x</code> is already a dissimilarity matrix, then this argument will be ignored.</p> |
| <code>keep.diss, keep.data</code> | <p>logicals indicating if the dissimilarities and/or input data <code>x</code> should be kept in the result. Setting these to FALSE can give much smaller results and hence even save memory allocation <i>time</i>.</p> |

Details

`diana` is fully described in chapter 6 of Kaufman and Rousseeuw (1990). It is probably unique in computing a divisive hierarchy, whereas most other software for hierarchical clustering is agglomerative. Moreover, `diana` provides (a) the divisive coefficient (see `diana.object`) which measures the amount of clustering structure found; and (b) the banner, a novel graphical display (see `plot.diana`).

The `diana`-algorithm constructs a hierarchy of clusterings, starting with one large cluster containing all n observations. Clusters are divided until each cluster contains only a single observation. At each stage, the cluster with the largest diameter is selected. (The diameter of a cluster is the largest dissimilarity between any two of its observations.)

To divide the selected cluster, the algorithm first looks for its most disparate observation (i.e., which

has the largest average dissimilarity to the other observations of the selected cluster). This observation initiates the "splinter group". In subsequent steps, the algorithm reassigns observations that are closer to the "splinter group" than to the "old party". The result is a division of the selected cluster into two new clusters.

Value

an object of class "diana" representing the clustering; this class has methods for the following generic functions: `print`, `summary`, `plot`.

Further, the class "diana" inherits from "twins". Therefore, the generic function `pltree` can be used on a diana object, and an [as.hclust](#) method is available.

A legitimate diana object is a list with the following components:

| | |
|------------------------|--|
| <code>order</code> | a vector giving a permutation of the original observations to allow for plotting, in the sense that the branches of a clustering tree will not cross. |
| <code>order.lab</code> | a vector similar to <code>order</code> , but containing observation labels instead of observation numbers. This component is only available if the original observations were labelled. |
| <code>height</code> | a vector with the diameters of the clusters prior to splitting. |
| <code>dc</code> | the divisive coefficient, measuring the clustering structure of the dataset. For each observation i , denote by $d(i)$ the diameter of the last cluster to which it belongs (before being split off as a single observation), divided by the diameter of the whole dataset. The <code>dc</code> is the average of all $1 - d(i)$. It can also be seen as the average width (or the percentage filled) of the banner plot. Because <code>dc</code> grows with the number of observations, this measure should not be used to compare datasets of very different sizes. |
| <code>merge</code> | an $(n-1)$ by 2 matrix, where n is the number of observations. Row i of <code>merge</code> describes the split at step $n-i$ of the clustering. If a number j in row r is negative, then the single observation $ j $ is split off at stage $n-r$. If j is positive, then the cluster that will be splitted at stage $n-j$ (described by row j), is split off at stage $n-r$. |
| <code>diss</code> | an object of class "dissimilarity", representing the total dissimilarity matrix of the dataset. |
| <code>data</code> | a matrix containing the original or standardized measurements, depending on the <code>stand</code> option of the function <code>agnes</code> . If a dissimilarity matrix was given as input structure, then this component is not available. |

See Also

[agnes](#) also for background and references; [cutree](#) (and [as.hclust](#)) for grouping extraction; [daisy](#), [dist](#), [plot.diana](#), [twins.object](#).

Examples

```
data(votes.repub)
dv <- diana(votes.repub, metric = "manhattan", stand = TRUE)
print(dv)
```

```

plot(dv)

## Cut into 2 groups:
dv2 <- cutree(as.hclust(dv), k = 2)
table(dv2) # 8 and 42 group members
rownames(votes.repub)[dv2 == 1]

## For two groups, does the metric matter ?
dv0 <- diana(votes.repub, stand = TRUE) # default: Euclidean
dv.2 <- cutree(as.hclust(dv0), k = 2)
table(dv2 == dv.2)## identical group assignments

data(agriculture)
## Plot similar to Figure 8 in ref
## Not run: plot(diana(agriculture), ask = TRUE)

```

dissimilarity.object *Dissimilarity Matrix Object*

Description

Objects of class "dissimilarity" representing the dissimilarity matrix of a dataset.

Value

The dissimilarity matrix is symmetric, and hence its lower triangle (column wise) is represented as a vector to save storage space. If the object, is called *do*, and *n* the number of observations, i.e., *n* <- attr(*do*, "Size"), then for $i < j \leq n$, the dissimilarity between (row) *i* and *j* is *do*[*n**(*i*-1) - *i**(*i*-1)/2 + *j*-*i*]. The length of the vector is $n * (n - 1) / 2$, i.e., of order n^2 .

"dissimilarity" objects also inherit from class `dist` and can use `dist` methods, in particular, `as.matrix`, such that d_{ij} from above is just `as.matrix(do)[i, j]`.

The object has the following attributes:

| | |
|------------|--|
| Size | the number of observations in the dataset. |
| Metric | the metric used for calculating the dissimilarities. Possible values are "euclidean", "manhattan", "mixed" (if variables of different types were present in the dataset), and "unspecified". |
| Labels | optionally, contains the labels, if any, of the observations of the dataset. |
| NA.message | optionally, if a dissimilarity could not be computed, because of too many missing values for some observations of the dataset. |
| Types | when a mixed metric was used, the types for each variable as one-letter codes (as in the book, e.g. p.54): A Asymmetric binary S Symmetric binary N Nominal (factor) |

- O** Ordinal (ordered factor)
- I** Interval scaled (numeric)
- T** raTio to be log transformed (positive numeric)
- .

GENERATION

[daisy](#) returns this class of objects. Also the functions [pam](#), [clara](#), [fanny](#), [agnes](#), and [diana](#) return a dissimilarity object, as one component of their return objects.

METHODS

The "dissimilarity" class has methods for the following generic functions: `print`, `summary`.

See Also

[daisy](#), [dist](#), [pam](#), [clara](#), [fanny](#), [agnes](#), [diana](#).

ellipsoidhull

Compute the Ellipsoid Hull or Spanning Ellipsoid of a Point Set

Description

Compute the "ellipsoid hull" or "spanning ellipsoid", i.e. the ellipsoid of minimal volume ('area' in 2D) such that all given points lie just inside or on the boundary of the ellipsoid.

Usage

```
ellipsoidhull(x, tol=0.01, maxit=5000,
              ret.wt = FALSE, ret.sqdist = FALSE, ret.pr = FALSE)
## S3 method for class 'ellipsoid'
print(x, digits = max(1, getOption("digits") - 2), ...)
```

Arguments

- `x` the n p -dimensional points as numeric $n \times p$ matrix.
- `tol` convergence tolerance for Titterton's algorithm. Setting this to much smaller values may drastically increase the number of iterations needed, and you may want to increase `maxit` as well.
- `maxit` integer giving the maximal number of iteration steps for the algorithm.
- `ret.wt`, `ret.sqdist`, `ret.pr` logicals indicating if additional information should be returned, `ret.wt` specifying the *weights*, `ret.sqdist` the *squared distances* and `ret.pr` the final **probabilities** in the algorithms.
- `digits, ...` the usual arguments to [print](#) methods.

Details

The “spanning ellipsoid” algorithm is said to stem from Titterton(1976), in Pison et al(1999) who use it for `clusplot.default`.

The problem can be seen as a special case of the “Min.Vol.” ellipsoid of which a more flexible and general implementation is `cov.mve` in the MASS package.

Value

an object of class “ellipsoid”, basically a `list` with several components, comprising at least

| | |
|-------------------------|--|
| <code>cov</code> | $p \times p$ covariance matrix description the ellipsoid. |
| <code>loc</code> | p -dimensional location of the ellipsoid center. |
| <code>d2</code> | average squared radius. Further, $d2 = t^2$, where t is “the value of a t-statistic on the ellipse boundary” (from <code>ellipse</code> in the <code>ellipse</code> package), and hence, more usefully, $d2 = qchisq(alpha, df = p)$, where $alpha$ is the confidence level for p -variate normally distributed data with location and covariance <code>loc</code> and <code>cov</code> to lie inside the ellipsoid. |
| <code>wt</code> | the vector of weights iff <code>ret.wt</code> was true. |
| <code>sqdist</code> | the vector of squared distances iff <code>ret.sqdist</code> was true. |
| <code>prob</code> | the vector of algorithm probabilities iff <code>ret.pr</code> was true. |
| <code>it</code> | number of iterations used. |
| <code>tol, maxit</code> | just the input argument, see above. |
| <code>eps</code> | the achieved tolerance which is the maximal squared radius minus p . |
| <code>ierr</code> | error code as from the algorithm; 0 means <i>ok</i> . |
| <code>conv</code> | logical indicating if the converged. This is defined as <code>it < maxit && ierr == 0</code> . |

Author(s)

Martin Maechler did the present class implementation; Rousseeuw et al did the underlying code.

References

Pison, G., Struyf, A. and Rousseeuw, P.J. (1999) Displaying a Clustering with CLUSPLOT, *Computational Statistics and Data Analysis*, **30**, 381–392.

A version of this is available as technical report from <http://www.agoras.ua.ac.be/abstract/Disclu99.htm>

D.M. Titterton (1976) Algorithms for computing D-optimal design on finite design spaces. In *Proc.\ of the 1976 Conf.\ on Information Science and Systems*, 213–216; John Hopkins University.

See Also

`predict.ellipsoid` which is also the `predict` method for ellipsoid objects. `volume.ellipsoid` for an example of ‘manual’ ellipsoid object construction;

further `ellipse` from package `ellipse` and `ellipsePoints` from package `sfsmisc`.

`chull` for the convex hull, `clusplot` which makes use of this; `cov.mve`.

Examples

```
x <- rnorm(100)
xy <- unname(cbind(x, rnorm(100) + 2*x + 10))
exy <- ellipsoidhull(xy)
exy # >> calling print.ellipsoid()

plot(xy)
lines(predict(exy))
points(rbind(exy$loc), col = "red", cex = 3, pch = 13)

exy <- ellipsoidhull(xy, tol = 1e-7, ret.wt = TRUE, ret.sq = TRUE)
str(exy) # had small 'tol', hence many iterations
(ii <- which(zapsmall(exy $ wt) > 1e-6)) # only about 4 to 6 points
round(exy$wt[ii],3); sum(exy$wt[ii]) # sum to 1
```

fanny

Fuzzy Analysis Clustering

Description

Computes a fuzzy clustering of the data into k clusters.

Usage

```
fanny(x, k, diss = inherits(x, "dist"), memb.exp = 2,
      metric = c("euclidean", "manhattan", "SqEuclidean"),
      stand = FALSE, iniMem.p = NULL, cluster.only = FALSE,
      keep.diss = !diss && !cluster.only && n < 100,
      keep.data = !diss && !cluster.only,
      maxit = 500, tol = 1e-15, trace.lev = 0)
```

Arguments

- | | |
|------|---|
| x | data matrix or data frame, or dissimilarity matrix, depending on the value of the <code>diss</code> argument. In case of a matrix or data frame, each row corresponds to an observation, and each column corresponds to a variable. All variables must be numeric. Missing values (NAs) are allowed. In case of a dissimilarity matrix, <code>x</code> is typically the output of daisy or dist . Also a vector of length $n*(n-1)/2$ is allowed (where n is the number of observations), and will be interpreted in the same way as the output of the above-mentioned functions. Missing values (NAs) are not allowed. |
| k | integer giving the desired number of clusters. It is required that $0 < k < n/2$ where n is the number of observations. |
| diss | logical flag: if TRUE (default for <code>dist</code> or dissimilarity objects), then <code>x</code> is assumed to be a dissimilarity matrix. If FALSE, then <code>x</code> is treated as a matrix of observations by variables. |

| | |
|----------------------|--|
| memb.exp | number r strictly larger than 1 specifying the <i>membership exponent</i> used in the fit criterion; see the ‘Details’ below. Default: 2 which used to be hardwired inside FANNY. |
| metric | character string specifying the metric to be used for calculating dissimilarities between observations. Options are "euclidean" (default), "manhattan", and "SqEuclidean". Euclidean distances are root sum-of-squares of differences, and manhattan distances are the sum of absolute differences, and "SqEuclidean", the <i>squared</i> euclidean distances are sum-of-squares of differences. Using this last option is equivalent (but somewhat slower) to computing so called “fuzzy C-means”. If x is already a dissimilarity matrix, then this argument will be ignored. |
| stand | logical; if true, the measurements in x are standardized before calculating the dissimilarities. Measurements are standardized for each variable (column), by subtracting the variable’s mean value and dividing by the variable’s mean absolute deviation. If x is already a dissimilarity matrix, then this argument will be ignored. |
| iniMem.p | numeric $n \times k$ matrix or NULL (by default); can be used to specify a starting membership matrix, i.e., a matrix of non-negative numbers, each row summing to one. |
| cluster.only | logical; if true, no silhouette information will be computed and returned, see details. |
| keep.diss, keep.data | logicals indicating if the dissimilarities and/or input data x should be kept in the result. Setting these to FALSE can give smaller results and hence also save memory allocation <i>time</i> . |
| maxit, tol | maximal number of iterations and default tolerance for convergence (relative convergence of the fit criterion) for the FANNY algorithm. The defaults <code>maxit</code> = 500 and <code>tol</code> = 1e-15 used to be hardwired inside the algorithm. |
| trace.lev | integer specifying a trace level for printing diagnostics during the C-internal algorithm. Default 0 does not print anything; higher values print increasingly more. |

Details

In a fuzzy clustering, each observation is “spread out” over the various clusters. Denote by u_{iv} the membership of observation i to cluster v .

The memberships are nonnegative, and for a fixed observation i they sum to 1. The particular method `fanny` stems from chapter 4 of Kaufman and Rousseeuw (1990) (see the references in [daisy](#)) and has been extended by Martin Maechler to allow user specified `memb.exp`, `iniMem.p`, `maxit`, `tol`, etc.

Fanny aims to minimize the objective function

$$\sum_{v=1}^k \frac{\sum_{i=1}^n \sum_{j=1}^n u_{iv}^r u_{jv}^r d(i, j)}{2 \sum_{j=1}^n u_{jv}^r}$$

where n is the number of observations, k is the number of clusters, r is the membership exponent `memb.exp` and $d(i, j)$ is the dissimilarity between observations i and j .

Note that $r \rightarrow 1$ gives increasingly crisper clusterings whereas $r \rightarrow \infty$ leads to complete fuzzyness. K&R(1990), p.191 note that values too close to 1 can lead to slow convergence. Further note that even the default, $r = 2$ can lead to complete fuzzyness, i.e., memberships $u_{iv} \equiv 1/k$. In that case a warning is signalled and the user is advised to chose a smaller `memb.exp` ($= r$).

Compared to other fuzzy clustering methods, `fanny` has the following features: (a) it also accepts a dissimilarity matrix; (b) it is more robust to the spherical cluster assumption; (c) it provides a novel graphical display, the silhouette plot (see [plot.partition](#)).

Value

an object of class "fanny" representing the clustering. See [fanny.object](#) for details.

See Also

[agnes](#) for background and references; [fanny.object](#), [partition.object](#), [plot.partition](#), [daisy](#), [dist](#).

Examples

```
## generate 10+15 objects in two clusters, plus 3 objects lying
## between those clusters.
x <- rbind(cbind(rnorm(10, 0, 0.5), rnorm(10, 0, 0.5)),
           cbind(rnorm(15, 5, 0.5), rnorm(15, 5, 0.5)),
           cbind(rnorm( 3,3.2,0.5), rnorm( 3,3.2,0.5)))
fannyx <- fanny(x, 2)
## Note that observations 26:28 are "fuzzy" (closer to # 2):
fannyx
summary(fannyx)
plot(fannyx)

(fan.x.15 <- fanny(x, 2, memb.exp = 1.5)) # 'crispier' for obs. 26:28
(fanny(x, 2, memb.exp = 3))               # more fuzzy in general

data(ruspini)
f4 <- fanny(ruspini, 4)
stopifnot(rle(f4$clustering)$lengths == c(20,23,17,15))
plot(f4, which = 1)
## Plot similar to Figure 6 in Stryuf et al (1996)
plot(fanny(ruspini, 5))
```

fanny.object

Fuzzy Analysis (FANNY) Object

Description

The objects of class "fanny" represent a fuzzy clustering of a dataset.

Value

A legitimate fanny object is a list with the following components:

| | |
|-------------|---|
| membership | matrix containing the memberships for each pair consisting of an observation and a cluster. |
| memb.exp | the membership exponent used in the fitting criterion. |
| coeff | Dunn's partition coefficient $F(k)$ of the clustering, where k is the number of clusters. $F(k)$ is the sum of all <i>squared</i> membership coefficients, divided by the number of observations. Its value is between $1/k$ and 1. The normalized form of the coefficient is also given. It is defined as $(F(k) - 1/k)/(1 - 1/k)$, and ranges between 0 and 1. A low value of Dunn's coefficient indicates a very fuzzy clustering, whereas a value close to 1 indicates a near-crisp clustering. |
| clustering | the clustering vector of the nearest crisp clustering, see partition.object . |
| k.crisp | integer ($\leq k$) giving the number of <i>crisp</i> clusters; can be less than k , where it's recommended to decrease memb.exp. |
| objective | named vector containing the minimal value of the objective function reached by the FANNY algorithm and the relative convergence tolerance tol used. |
| convergence | named vector with iterations, the number of iterations needed and converged indicating if the algorithm converged (in maxit iterations within convergence tolerance tol). |
| diss | an object of class "dissimilarity", see partition.object . |
| call | generating call, see partition.object . |
| silinfo | list with silhouette information of the nearest crisp clustering, see partition.object . |
| data | matrix, possibly standardized, or NULL, see partition.object . |

GENERATION

These objects are returned from [fanny](#).

METHODS

The "fanny" class has methods for the following generic functions: print, summary.

INHERITANCE

The class "fanny" inherits from "partition". Therefore, the generic functions plot and clusplot can be used on a fanny object.

See Also

[fanny](#), [print.fanny](#), [dissimilarity.object](#), [partition.object](#), [plot.partition](#).

flower

*Flower Characteristics***Description**

8 characteristics for 18 popular flowers.

Usage

```
data(flower)
```

Format

A data frame with 18 observations on 8 variables:

| | | |
|-----------|---------|------------|
| [, "V1"] | factor | winters |
| [, "V2"] | factor | shadow |
| [, "V3"] | factor | tubers |
| [, "V4"] | factor | color |
| [, "V5"] | ordered | soil |
| [, "V6"] | ordered | preference |
| [, "V7"] | numeric | height |
| [, "V8"] | numeric | distance |

V1 winters, is binary and indicates whether the plant may be left in the garden when it freezes.

V2 shadow, is binary and shows whether the plant needs to stand in the shadow.

V3 tubers, is asymmetric binary and distinguishes between plants with tubers and plants that grow in any other way.

V4 color, is nominal and specifies the flower's color (1 = white, 2 = yellow, 3 = pink, 4 = red, 5 = blue).

V5 soil, is ordinal and indicates whether the plant grows in dry (1), normal (2), or wet (3) soil.

V6 preference, is ordinal and gives someone's preference ranking going from 1 to 18.

V7 height, is interval scaled, the plant's height in centimeters.

V8 distance, is interval scaled, the distance in centimeters that should be left between the plants.

Source

The reference below.

References

Anja Struyf, Mia Hubert & Peter J. Rousseeuw (1996): Clustering in an Object-Oriented Environment. *Journal of Statistical Software*, **1**. <http://www.stat.ucla.edu/journals/jss/>

Examples

```
data(flower)
## Example 2 in ref
daisy(flower, type = list(asymm = 3))
daisy(flower, type = list(asymm = c(1, 3), ordratio = 7))
```

`lower.to.upper.tri.inds`*Permute Indices for Triangular Matrices*

Description

Compute index vectors for extracting or reordering of lower or upper triangular matrices that are stored as contiguous vectors.

Usage

```
lower.to.upper.tri.inds(n)
upper.to.lower.tri.inds(n)
```

Arguments

`n` integer larger than 1.

Value

integer vector containing a permutation of $1:N$ where $N = n(n-1)/2$.

Note

these functions are mainly for internal use in the cluster package, and may not remain available (unless we see a good reason).

See Also

[upper.tri](#), [lower.tri](#) with a related purpose.

Examples

```
m5 <- matrix(NA,5,5)
m <- m5; m[lower.tri(m)] <- upper.to.lower.tri.inds(5); m
m <- m5; m[upper.tri(m)] <- lower.to.upper.tri.inds(5); m

stopifnot(lower.to.upper.tri.inds(2) == 1,
           lower.to.upper.tri.inds(3) == 1:3,
           upper.to.lower.tri.inds(3) == 1:3,
           sort(upper.to.lower.tri.inds(5)) == 1:10,
           sort(lower.to.upper.tri.inds(6)) == 1:15)
```

mona

*MONothetic Analysis Clustering of Binary Variables***Description**

Returns a list representing a divisive hierarchical clustering of a dataset with binary variables only.

Usage

```
mona(x)
```

Arguments

x data matrix or data frame in which each row corresponds to an observation, and each column corresponds to a variable. All variables must be binary. A limited number of missing values (NAs) is allowed. Every observation must have at least one value different from NA. No variable should have half of its values missing. There must be at least one variable which has no missing values. A variable with all its non-missing values identical, is not allowed.

Details

mona is fully described in chapter 7 of Kaufman and Rousseeuw (1990). It is "monothetic" in the sense that each division is based on a single (well-chosen) variable, whereas most other hierarchical methods (including agnes and diana) are "polythetic", i.e. they use all variables together.

The mona-algorithm constructs a hierarchy of clusterings, starting with one large cluster. Clusters are divided until all observations in the same cluster have identical values for all variables.

At each stage, all clusters are divided according to the values of one variable. A cluster is divided into one cluster with all observations having value 1 for that variable, and another cluster with all observations having value 0 for that variable.

The variable used for splitting a cluster is the variable with the maximal total association to the other variables, according to the observations in the cluster to be splitted. The association between variables f and g is given by $a(f,g)*d(f,g) - b(f,g)*c(f,g)$, where $a(f,g)$, $b(f,g)$, $c(f,g)$, and $d(f,g)$ are the numbers in the contingency table of f and g . [That is, $a(f,g)$ (resp. $d(f,g)$) is the number of observations for which f and g both have value 0 (resp. value 1); $b(f,g)$ (resp. $c(f,g)$) is the number of observations for which f has value 0 (resp. 1) and g has value 1 (resp. 0).] The total association of a variable f is the sum of its associations to all variables.

This algorithm does not work with missing values, therefore the data are revised, e.g. all missing values are filled in. To do this, the same measure of association between variables is used as in the algorithm. When variable f has missing values, the variable g with the largest absolute association to f is looked up. When the association between f and g is positive, any missing value of f is replaced by the value of g for the same observation. If the association between f and g is negative, then any missing value of f is replaced by the value of $1-g$ for the same observation.

Value

an object of class "mona" representing the clustering. See mona.object for details.

See Also

[agnes](#) for background and references; [mona.object](#), [plot.mona](#).

Examples

```
data(animals)
ma <- mona(animals)
ma
## Plot similar to Figure 10 in Struyf et al (1996)
plot(ma)
```

mona.object

Monothetic Analysis (MONA) Object

Description

The objects of class "mona" represent the divisive hierarchical clustering of a dataset with only binary variables (measurements). This class of objects is returned from [mona](#).

Value

A legitimate mona object is a list with the following components:

| | |
|-----------|---|
| data | matrix with the same dimensions as the original data matrix, but with factors coded as 0 and 1, and all missing values replaced. |
| order | a vector giving a permutation of the original observations to allow for plotting, in the sense that the branches of a clustering tree will not cross. |
| order.lab | a vector similar to order, but containing observation labels instead of observation numbers. This component is only available if the original observations were labelled. |
| variable | vector of length n-1 where n is the number of observations, specifying the variables used to separate the observations of order. |
| step | vector of length n-1 where n is the number of observations, specifying the separation steps at which the observations of order are separated. |

METHODS

The "mona" class has methods for the following generic functions: print, summary, plot.

See Also

[mona](#) for examples etc, [plot.mona](#).

Description

Partitioning (clustering) of the data into k clusters “around medoids”, a more robust version of K-means.

Usage

```
pam(x, k, diss = inherits(x, "dist"), metric = "euclidean",
    medoids = NULL, stand = FALSE, cluster.only = FALSE,
    do.swap = TRUE,
    keep.diss = !diss && !cluster.only && n < 100,
    keep.data = !diss && !cluster.only, trace.lev = 0)
```

Arguments

| | |
|---------|--|
| x | <p>data matrix or data frame, or dissimilarity matrix or object, depending on the value of the <code>diss</code> argument.</p> <p>In case of a matrix or data frame, each row corresponds to an observation, and each column corresponds to a variable. All variables must be numeric. Missing values (NAs) are allowed—as long as every pair of observations has at least one case not missing.</p> <p>In case of a dissimilarity matrix, <code>x</code> is typically the output of <code>daisy</code> or <code>dist</code>. Also a vector of length $n*(n-1)/2$ is allowed (where n is the number of observations), and will be interpreted in the same way as the output of the above-mentioned functions. Missing values (NAs) are <i>not</i> allowed.</p> |
| k | positive integer specifying the number of clusters, less than the number of observations. |
| diss | logical flag: if TRUE (default for <code>dist</code> or dissimilarity objects), then <code>x</code> will be considered as a dissimilarity matrix. If FALSE, then <code>x</code> will be considered as a matrix of observations by variables. |
| metric | <p>character string specifying the metric to be used for calculating dissimilarities between observations.</p> <p>The currently available options are "euclidean" and "manhattan". Euclidean distances are root sum-of-squares of differences, and manhattan distances are the sum of absolute differences. If <code>x</code> is already a dissimilarity matrix, then this argument will be ignored.</p> |
| medoids | NULL (default) or length- k vector of integer indices (in $1:n$) specifying initial medoids instead of using the ‘ <i>build</i> ’ algorithm. |
| stand | logical; if true, the measurements in <code>x</code> are standardized before calculating the dissimilarities. Measurements are standardized for each variable (column), by subtracting the variable’s mean value and dividing by the variable’s mean absolute deviation. If <code>x</code> is already a dissimilarity matrix, then this argument will be ignored. |

| | |
|-----------------------------------|--|
| <code>cluster.only</code> | logical; if true, only the clustering will be computed and returned, see details. |
| <code>do.swap</code> | logical indicating if the swap phase should happen. The default, TRUE, correspond to the original algorithm. On the other hand, the swap phase is much more computer intensive than the build one for large n , so can be skipped by <code>do.swap = FALSE</code> . |
| <code>keep.diss, keep.data</code> | logicals indicating if the dissimilarities and/or input data x should be kept in the result. Setting these to FALSE can give much smaller results and hence even save memory allocation <i>time</i> . |
| <code>trace.lev</code> | integer specifying a trace level for printing diagnostics during the build and swap phase of the algorithm. Default 0 does not print anything; higher values print increasingly more. |

Details

`pam` is fully described in chapter 2 of Kaufman and Rousseeuw (1990). Compared to the `k-means` approach in `kmeans`, the function `pam` has the following features: (a) it also accepts a dissimilarity matrix; (b) it is more robust because it minimizes a sum of dissimilarities instead of a sum of squared euclidean distances; (c) it provides a novel graphical display, the silhouette plot (see `plot.partition`) (d) it allows to select the number of clusters using `mean(silhouette(pr))` on the result `pr <- pam(..)`, or directly its component `pr$silinfo$avg.width`, see also [pam.object](#).

When `cluster.only` is true, the result is simply a (possibly named) integer vector specifying the clustering, i.e.,

`pam(x,k, cluster.only=TRUE)` is the same as
`pam(x,k)$clustering` but computed more efficiently.

The `pam`-algorithm is based on the search for k representative objects or medoids among the observations of the dataset. These observations should represent the structure of the data. After finding a set of k medoids, k clusters are constructed by assigning each observation to the nearest medoid. The goal is to find k representative objects which minimize the sum of the dissimilarities of the observations to their closest representative object.

By default, when medoids are not specified, the algorithm first looks for a good initial set of medoids (this is called the **build** phase). Then it finds a local minimum for the objective function, that is, a solution such that there is no single switch of an observation with a medoid that will decrease the objective (this is called the **swap** phase).

When the medoids are specified, their order does *not* matter; in general, the algorithms have been designed to not depend on the order of the observations.

Value

an object of class "pam" representing the clustering. See [?pam.object](#) for details.

Note

For large datasets, `pam` may need too much memory or too much computation time since both are $O(n^2)$. Then, [clara\(\)](#) is preferable, see its documentation.

See Also

[agnes](#) for background and references; [pam.object](#), [clara](#), [daisy](#), [partition.object](#), [plot.partition](#), [dist](#).

Examples

```
## generate 25 objects, divided into 2 clusters.
x <- rbind(cbind(rnorm(10,0,0.5), rnorm(10,0,0.5)),
           cbind(rnorm(15,5,0.5), rnorm(15,5,0.5)))
pamx <- pam(x, 2)
pamx
summary(pamx)
plot(pamx)
## use obs. 1 & 16 as starting medoids -- same result (typically)
(p2m <- pam(x, 2, medoids = c(1,16)))

p3m <- pam(x, 3, trace = 2)
## rather stupid initial medoids:
(p3m. <- pam(x, 3, medoids = 3:1, trace = 1))

pam(daisy(x, metric = "manhattan"), 2, diss = TRUE)

data(ruspini)
## Plot similar to Figure 4 in Stryuf et al (1996)
## Not run: plot(pam(ruspini, 4), ask = TRUE)
```

pam.object

Partitioning Around Medoids (PAM) Object

Description

The objects of class "pam" represent a partitioning of a dataset into clusters.

Value

A legitimate pam object is a list with the following components:

| | |
|------------|---|
| medoids | the medoids or representative objects of the clusters. If a dissimilarity matrix was given as input to pam, then a vector of numbers or labels of observations is given, else medoids is a matrix with in each row the coordinates of one medoid. |
| id.med | integer vector of <i>indices</i> giving the medoid observation numbers. |
| clustering | the clustering vector, see partition.object . |
| objective | the objective function after the first and second step of the pam algorithm. |

| | |
|-----------|---|
| isolation | vector with length equal to the number of clusters, specifying which clusters are isolated clusters (L- or L*-clusters) and which clusters are not isolated. A cluster is an L*-cluster iff its diameter is smaller than its separation. A cluster is an L-cluster iff for each observation i the maximal dissimilarity between i and any other observation of the cluster is smaller than the minimal dissimilarity between i and any observation of another cluster. Clearly each L*-cluster is also an L-cluster. |
| clusinfo | matrix, each row gives numerical information for one cluster. These are the cardinality of the cluster (number of observations), the maximal and average dissimilarity between the observations in the cluster and the cluster's medoid, the diameter of the cluster (maximal dissimilarity between two observations of the cluster), and the separation of the cluster (minimal dissimilarity between an observation of the cluster and an observation of another cluster). |
| silinfo | list with silhouette width information, see partition.object . |
| diss | dissimilarity (maybe NULL), see partition.object . |
| call | generating call, see partition.object . |
| data | (possibly standardized) see partition.object . |

GENERATION

These objects are returned from [pam](#).

METHODS

The "pam" class has methods for the following generic functions: print, summary.

INHERITANCE

The class "pam" inherits from "partition". Therefore, the generic functions plot and clusplot can be used on a pam object.

See Also

[pam](#), [dissimilarity.object](#), [partition.object](#), [plot.partition](#).

Examples

```
## Use the silhouette widths for assessing the best number of clusters,
## following a one-dimensional example from Christian Hennig :
##
x <- c(rnorm(50), rnorm(50,mean=5), rnorm(30,mean=15))
asw <- numeric(20)
## Note that "k=1" won't work!
for (k in 2:20)
  asw[k] <- pam(x, k) $ silinfo $ avg.width
k.best <- which.max(asw)
cat("silhouette-optimal number of clusters:", k.best, "\n")

plot(1:20, asw, type= "h", main = "pam() clustering assessment",
```

```
xlab= "k (# clusters)", ylab = "average silhouette width")
axis(1, k.best, paste("best",k.best,sep="\n"), col = "red", col.axis = "red")
```

| | |
|------------------|----------------------------|
| partition.object | <i>Partitioning Object</i> |
|------------------|----------------------------|

Description

The objects of class "partition" represent a partitioning of a dataset into clusters.

Value

a "partition" object is a list with the following (and typically more) components:

| | |
|------------|---|
| clustering | the clustering vector. An integer vector of length n , the number of observations, giving for each observation the number ('id') of the cluster to which it belongs. |
| call | the matched call generating the object. |
| silinfo | <p>a list with all <i>silhouette</i> information, only available when the number of clusters is non-trivial, i.e., $1 < k < n$ and then has the following components, see silhouette</p> <p>widths an ($n \times 3$) matrix, as returned by silhouette(), with for each observation i the cluster to which i belongs, as well as the neighbor cluster of i (the cluster, not containing i, for which the average dissimilarity between its observations and i is minimal), and the silhouette width $s(i)$ of the observation.</p> <p>clus.avg.widths the average silhouette width per cluster.</p> <p>avg.width the average silhouette width for the dataset, i.e., simply the average of $s(i)$ over all observations i.</p> <p>This information is also needed to construct a <i>silhouette plot</i> of the clustering, see plot.partition.</p> <p>Note that avg.width can be maximized over different clusterings (e.g. with varying number of clusters) to choose an <i>optimal</i> clustering.</p> |
| objective | value of criterion maximized during the partitioning algorithm, may more than one entry for different stages. |
| diss | an object of class "dissimilarity", representing the total dissimilarity matrix of the dataset (or relevant subset, e.g. for clara). |
| data | a matrix containing the original or standardized data. This might be missing to save memory or when a dissimilarity matrix was given as input structure to the clustering method. |

GENERATION

These objects are returned from pam, clara or fanny.

METHODS

The "partition" class has a method for the following generic functions: plot, clusplot.

INHERITANCE

The following classes inherit from class "partition" : "pam", "clara" and "fanny".

See [pam.object](#), [clara.object](#) and [fanny.object](#) for details.

See Also

[pam](#), [clara](#), [fanny](#).

| | |
|-------------|----------------------------------|
| plantTraits | <i>Plant Species Traits Data</i> |
|-------------|----------------------------------|

Description

This dataset constitutes a description of 136 plant species according to biological attributes (morphological or reproductive)

Usage

```
data(plantTraits)
```

Format

A data frame with 136 observations on the following 31 variables.

pdias Diaspore mass (mg)

longindex Seed bank longevity

durflow Flowering duration

height Plant height, an ordered factor with levels 1 < 2 < ... < 8.

begflow Time of first flowering, an ordered factor with levels 1 < 2 < 3 < 4 < 5 < 6 < 7 < 8 < 9

mycor Mycorrhizas, an ordered factor with levels 0never < 1 sometimes< 2always

vegaer aerial vegetative propagation, an ordered factor with levels 0never < 1 present but limited< 2important.

vegsout underground vegetative propagation, an ordered factor with 3 levels identical to vegaer above.

autopoll selfing pollination, an ordered factor with levels 0never < 1rare < 2 often< the rule3

insects insect pollination, an ordered factor with 5 levels 0 < ... < 4.

wind wind pollination, an ordered factor with 5 levels 0 < ... < 4.

lign a binary factor with levels 0:1, indicating if plant is woody.

piq a binary factor indicating if plant is thorny.

ros a binary factor indicating if plant is rosette.
 semiros semi-rosette plant, a binary factor (0: no; 1: yes).
 leafy leafy plant, a binary factor.
 suman summer annual, a binary factor.
 winan winter annual, a binary factor.
 monocarp monocarpic perennial, a binary factor.
 polycarp polycarpic perennial, a binary factor.
 seasaes seasonal aestival leaves, a binary factor.
 seashiv seasonal hibernal leaves, a binary factor.
 seasver seasonal vernal leaves, a binary factor.
 everalw leaves always evergreen, a binary factor.
 everparti leaves partially evergreen, a binary factor.
 elaio fruits with an elaiosome (dispersed by ants), a binary factor.
 endozoo endozoochorous fruits, a binary factor.
 epizoo epizoochorous fruits, a binary factor.
 aquat aquatic dispersal fruits, a binary factor.
 windgl wind dispersed fruits, a binary factor.
 unsp unspecialized mechanism of seed dispersal, a binary factor.

Details

Most of factor attributes are not disjunctive. For example, a plant can be usually pollinated by insects but sometimes self-pollination can occurred.

Source

Vallet, Jeanne (2005) *Structuration de communautés végétales et analyse comparative de traits biologiques le long d'un gradient d'urbanisation*. Mémoire de Master 2 'Ecologie-Biodiversité-Evolution'; Université Paris Sud XI, 30p.+ annexes (in french)

Examples

```

data(plantTraits)

## Calculation of a dissimilarity matrix
library(cluster)
dai.b <- daisy(plantTraits,
              type = list(ordratio = 4:11, symm = 12:13, asymm = 14:31))

## Hierarchical classification
agn.trts <- agnes(dai.b, method="ward")
plot(agn.trts, which.plots = 2, cex= 0.6)
plot(agn.trts, which.plots = 1)
cutree6 <- cutree(agn.trts, k=6)
cutree6

```

```
## Principal Coordinate Analysis
cmds dai.b <- cmdscale(dai.b, k=6)
plot(cmdsdai.b[, 1:2], asp = 1, col = cutree6)
```

plot.agnes

*Plots of an Agglomerative Hierarchical Clustering***Description**

Creates plots for visualizing an agnes object.

Usage

```
## S3 method for class 'agnes'
plot(x, ask = FALSE, which.plots = NULL, main = NULL,
      sub = paste("Agglomerative Coefficient = ", round(x$ac, digits = 2)),
      adj = 0, nmax.lab = 35, max.strlen = 5, xax.pretty = TRUE, ...)
```

Arguments

| | |
|-------------|--|
| x | an object of class "agnes", typically created by agnes(.) . |
| ask | logical; if true and which.plots is NULL, plot.agnes operates in interactive mode, via menu . |
| which.plots | integer vector or NULL (default), the latter producing both plots. Otherwise, which.plots must contain integers of 1 for a <i>banner</i> plot or 2 for a dendrogram or "clustering tree". |
| main, sub | main and sub title for the plot, with convenient defaults. See documentation for these arguments in plot.default . |
| adj | for label adjustment in bannerplot() . |
| nmax.lab | integer indicating the number of labels which is considered too large for single-name labelling the banner plot. |
| max.strlen | positive integer giving the length to which strings are truncated in banner plot labeling. |
| xax.pretty | logical or integer indicating if pretty(*, n = xax.pretty) should be used for the x axis. xax.pretty = FALSE is for back compatibility. |
| ... | graphical parameters (see par) may also be supplied and are passed to bannerplot() or pltree() (see pltree.twins), respectively. |

Details

When `ask = TRUE`, rather than producing each plot sequentially, `plot.agnes` displays a menu listing all the plots that can be produced. If the menu is not desired but a pause between plots is still wanted one must set `par(ask= TRUE)` before invoking the plot command.

The banner displays the hierarchy of clusters, and is equivalent to a tree. See Rousseeuw (1986) or chapter 5 of Kaufman and Rousseeuw (1990). The banner plots distances at which observations and clusters are merged. The observations are listed in the order found by the agnes algorithm, and the numbers in the height vector are represented as bars between the observations.

The leaves of the clustering tree are the original observations. Two branches come together at the distance between the two clusters being merged.

For more customization of the plots, rather call `bannerplot` and `pltree()`, i.e., its method `pltree.twins`, respectively.

directly with corresponding arguments, e.g., `xlab` or `ylab`.

Side Effects

Appropriate plots are produced on the current graphics device. This can be one or both of the following choices:

Banner
Clustering tree

Note

In the banner plot, observation labels are only printed when the number of observations is limited less than `nmax.lab` (35, by default), for readability. Moreover, observation labels are truncated to maximally `max.strlen` (5) characters.

For the dendrogram, more flexibility than via `pltree()` is provided by `dg <- as.dendrogram(x)` and plotting `dg` via `plot.dendrogram`.

References

- Kaufman, L. and Rousseeuw, P.J. (1990) *Finding Groups in Data: An Introduction to Cluster Analysis*. Wiley, New York.
- Rousseeuw, P.J. (1986). A visual display for hierarchical classification, in *Data Analysis and Informatics 4*; edited by E. Diday, Y. Escoufier, L. Lebart, J. Pages, Y. Schektman, and R. Tomassone. North-Holland, Amsterdam, 743–748.
- Struyf, A., Hubert, M. and Rousseeuw, P.J. (1997) Integrating Robust Clustering Techniques in S-PLUS, *Computational Statistics and Data Analysis*, **26**, 17-37.

See Also

`agnes` and `agnes.object`; `bannerplot`, `pltree.twins`, and `par`.

Examples

```
## Can also pass 'labels' to pltree() and bannerplot():
data(iris)
cS <- as.character(Sp <- iris$Species)
cS[Sp == "setosa"] <- "S"
cS[Sp == "versicolor"] <- "V"
cS[Sp == "virginica"] <- "G"
ai <- agnes(iris[, 1:4])
plot(ai, labels = cS, nmax = 150) # bannerplot labels are mess
```

plot.diana

Plots of a Divisive Hierarchical Clustering

Description

Creates plots for visualizing a diana object.

Usage

```
## S3 method for class 'diana'
plot(x, ask = FALSE, which.plots = NULL, main = NULL,
      sub = paste("Divisive Coefficient = ", round(x$dc, digits = 2)),
      adj = 0, nmax.lab = 35, max.strlen = 5, xax.pretty = TRUE, ...)
```

Arguments

| | |
|-------------|---|
| x | an object of class "diana", typically created by diana(.) . |
| ask | logical; if true and which.plots is NULL, plot.diana operates in interactive mode, via menu . |
| which.plots | integer vector or NULL (default), the latter producing both plots. Otherwise, which.plots must contain integers of 1 for a <i>banner</i> plot or 2 for a dendrogram or "clustering tree". |
| main, sub | main and sub title for the plot, each with a convenient default. See documentation for these arguments in plot.default . |
| adj | for label adjustment in bannerplot() . |
| nmax.lab | integer indicating the number of labels which is considered too large for single-name labelling the banner plot. |
| max.strlen | positive integer giving the length to which strings are truncated in banner plot labeling. |
| xax.pretty | logical or integer indicating if pretty(*, n = xax.pretty) should be used for the x axis. xax.pretty = FALSE is for back compatibility. |
| ... | graphical parameters (see par) may also be supplied and are passed to bannerplot() or pltree() , respectively. |

Details

When `ask = TRUE`, rather than producing each plot sequentially, `plot.diana` displays a menu listing all the plots that can be produced. If the menu is not desired but a pause between plots is still wanted one must set `par(ask= TRUE)` before invoking the plot command.

The banner displays the hierarchy of clusters, and is equivalent to a tree. See Rousseeuw (1986) or chapter 6 of Kaufman and Rousseeuw (1990). The banner plots the diameter of each cluster being splitted. The observations are listed in the order found by the diana algorithm, and the numbers in the height vector are represented as bars between the observations.

The leaves of the clustering tree are the original observations. A branch splits up at the diameter of the cluster being splitted.

Side Effects

An appropriate plot is produced on the current graphics device. This can be one or both of the following choices:

Banner
Clustering tree

Note

In the banner plot, observation labels are only printed when the number of observations is limited less than `nmax.lab` (35, by default), for readability. Moreover, observation labels are truncated to maximally `max.strlen` (5) characters.

References

see those in [plot.agnes](#).

See Also

[diana](#), [diana.object](#), [twins.object](#), [par](#).

Examples

```
example(diana)# -> dv <- diana(...)  
  
plot(dv, which = 1, nmax.lab = 100)  
  
## wider labels :  
op <- par(mar = par("mar") + c(0, 2, 0,0))  
plot(dv, which = 1, nmax.lab = 100, max.strlen = 12)  
par(op)
```


plot.mona

*Banner of Monothetic Divisive Hierarchical Clusterings***Description**

Creates the banner of a mona object.

Usage

```
## S3 method for class 'mona'
plot(x, main = paste("Banner of ", deparse(x$call)),
      sub = NULL, xlab = "Separation step",
      col = c(2,0), axes = TRUE, adj = 0,
      nmax.lab = 35, max.strlen = 5, ...)
```

Arguments

| | |
|-------------------------|---|
| <code>x</code> | an object of class "mona", typically created by <code>mona(.)</code> . |
| <code>main, sub</code> | main and sub titles for the plot, with convenient defaults. See documentation in plot.default . |
| <code>xlab</code> | x axis label, see title . |
| <code>col, adj</code> | graphical parameters passed to <code>bannerplot()</code> . |
| <code>axes</code> | logical, indicating if (labeled) axes should be drawn. |
| <code>nmax.lab</code> | integer indicating the number of labels which is considered too large for labeling. |
| <code>max.strlen</code> | positive integer giving the length to which strings are truncated in labeling. |
| <code>...</code> | further graphical arguments are passed to bannerplot() and text . |

Details

Plots the separation step at which clusters are splitted. The observations are given in the order found by the mona algorithm, the numbers in the step vector are represented as bars between the observations.

When a long bar is drawn between two observations, those observations have the same value for each variable. See chapter 7 of Kaufman and Rousseeuw (1990).

Side Effects

A banner is plotted on the current graphics device.

Note

In the banner plot, observation labels are only printed when the number of observations is limited less than `nmax.lab` (35, by default), for readability. Moreover, observation labels are truncated to maximally `max.strlen` (5) characters.

References

see those in [plot.agnes](#).

See Also

[mona](#), [mona.object](#), [par](#).

| | |
|----------------|--|
| plot.partition | <i>Plot of a Partition of the Data Set</i> |
|----------------|--|

Description

Creates plots for visualizing a partition object.

Usage

```
## S3 method for class 'partition'
plot(x, ask = FALSE, which.plots = NULL,
      nmax.lab = 40, max.strlen = 5, data = x$data, dist = NULL,
      cor = TRUE, stand = FALSE, lines = 2,
      shade = FALSE, color = FALSE, labels = 0, plotchar = TRUE,
      span = TRUE, xlim = NULL, ylim = NULL, main = NULL, ...)
```

Arguments

| | |
|--|--|
| x | an object of class "partition", typically created by the functions pam , clara , or fanny . |
| ask | logical; if true and which.plots is NULL, plot.partition operates in interactive mode, via menu . |
| which.plots | integer vector or NULL (default), the latter producing both plots. Otherwise, which.plots must contain integers of 1 for a <i>clusplot</i> or 2 for <i>silhouette</i> . |
| nmax.lab | integer indicating the number of labels which is considered too large for single-name labeling the silhouette plot. |
| max.strlen | positive integer giving the length to which strings are truncated in silhouette plot labeling. |
| data | numeric matrix with the scaled data; per default taken from the partition object x, but can be specified explicitly. |
| dist | when x does not have a diss component as for pam (*, keep.diss=FALSE), dist must be the dissimilarity if a <i>clusplot</i> is desired. |
| cor, stand, lines, shade, color, labels, plotchar, span, xlim, ylim, main, ... | All optional arguments available for the clusplot.default function (except for the diss one) and graphical parameters (see par) may also be supplied as arguments to this function. |

Details

When `ask= TRUE`, rather than producing each plot sequentially, `plot.partition` displays a menu listing all the plots that can be produced. If the menu is not desired but a pause between plots is still wanted, call `par(ask= TRUE)` before invoking the plot command.

The *clusplot* of a cluster partition consists of a two-dimensional representation of the observations, in which the clusters are indicated by ellipses (see [clusplot.partition](#) for more details).

The *silhouette plot* of a nonhierarchical clustering is fully described in Rousseeuw (1987) and in chapter 2 of Kaufman and Rousseeuw (1990). For each observation i , a bar is drawn, representing its silhouette width $s(i)$, see [silhouette](#) for details. Observations are grouped per cluster, starting with cluster 1 at the top. Observations with a large $s(i)$ (almost 1) are very well clustered, a small $s(i)$ (around 0) means that the observation lies between two clusters, and observations with a negative $s(i)$ are probably placed in the wrong cluster.

A clustering can be performed for several values of k (the number of clusters). Finally, choose the value of k with the largest overall average silhouette width.

Side Effects

An appropriate plot is produced on the current graphics device. This can be one or both of the following choices:

Clusplot

Silhouette plot

Note

In the silhouette plot, observation labels are only printed when the number of observations is less than `nmax.lab` (40, by default), for readability. Moreover, observation labels are truncated to maximally `max.strlen` (5) characters.

For more flexibility, use `plot(silhouette(x), ...)`, see [plot.silhouette](#).

References

Rousseeuw, P.J. (1987) Silhouettes: A graphical aid to the interpretation and validation of cluster analysis. *J. Comput. Appl. Math.*, **20**, 53–65.

Further, the references in [plot.agnes](#).

See Also

[partition.object](#), [clusplot.partition](#), [clusplot.default](#), [pam](#), [pam.object](#), [clara](#), [clara.object](#), [fanny](#), [fanny.object](#), [par](#).

Examples

```
## generate 25 objects, divided into 2 clusters.
x <- rbind(cbind(rnorm(10,0,0.5), rnorm(10,0,0.5)),
           cbind(rnorm(15,5,0.5), rnorm(15,5,0.5)))
plot(pam(x, 2))

## Save space not keeping data in clus.object, and still clusplot() it:
```

```
data(xclara)
cx <- clara(xclara, 3, keep.data = FALSE)
cx$data # is NULL
plot(cx, data = xclara)
```

pltree

Clustering Trees - Generic Function

Description

Generic function drawing a clustering tree (“dendrogram”) on the current graphics device. There is a twins method, see [pltree.twins](#) for usage and examples.

Usage

```
pltree(x, ...)
```

Arguments

| | |
|------------------|--|
| <code>x</code> | an R object (for which a <code>pltree</code> method is defined). |
| <code>...</code> | methods may have additional arguments. Graphical parameters (see par) may also be supplied as arguments to this function. |

See Also

[pltree.twins](#), [twins.object](#).

pltree.twins

Clustering Tree of a Hierarchical Clustering

Description

Draws a clustering tree (dendrogram) of a twins object, i.e., hierarchical clustering, typically resulting from [agnes\(\)](#) or [diana\(\)](#).

Usage

```
## S3 method for class 'twins'
pltree(x, main = paste("Dendrogram of ", deparse(x$call)),
       labels = NULL, ylab = "Height", ...)
```

Arguments

| | |
|---------------------|--|
| <code>x</code> | an object of class "twins", typically created by either agnes() or diana() . |
| <code>main</code> | main title with a sensible default. |
| <code>labels</code> | labels to use; the default is constructed from <code>x</code> . |
| <code>ylab</code> | label for y-axis. |
| <code>...</code> | graphical parameters (see par) may also be supplied as arguments to this function. |

Details

Creates a plot of a clustering tree given a twins object. The leaves of the tree are the original observations. In case of an agglomerative clustering, two branches come together at the distance between the two clusters being merged. For a divisive clustering, a branch splits up at the diameter of the cluster being splitted.

Note that currently the method function simply calls `plot(as.hclust(x), ...)`, which dispatches to `plot.hclust(...)`. If more flexible plots are needed, consider `xx <- as.dendrogram(as.hclust(x))` and plotting `xx`, see [plot.dendrogram](#).

Value

a NULL value is returned.

See Also

[agnes](#), [agnes.object](#), [diana](#), [diana.object](#), [hclust](#), [par](#), [plot.agnes](#), [plot.diana](#).

Examples

```
data(votes.repub)
agn <- agnes(votes.repub)
pltree(agn)

dagn <- as.dendrogram(as.hclust(agn))
dagn2 <- as.dendrogram(as.hclust(agn), hang = 0.2)
op <- par(mar = par("mar") + c(0,0,0, 2)) # more space to the right
plot(dagn2, horiz = TRUE)
plot(dagn, horiz = TRUE, center = TRUE,
      nodePar = list(lab.cex = 0.6, lab.col = "forest green", pch = NA),
      main = deparse(agn$call))
par(op)
```

| | |
|--------|---|
| pluton | <i>Isotopic Composition Plutonium Batches</i> |
|--------|---|

Description

The pluton data frame has 45 rows and 4 columns, containing percentages of isotopic composition of 45 Plutonium batches.

Usage

```
data(pluton)
```

Format

This data frame contains the following columns:

Pu238 the percentages of ^{238}Pu , always less than 2 percent.

Pu239 the percentages of ^{239}Pu , typically between 60 and 80 percent (from neutron capture of Uranium, ^{238}U).

Pu240 percentage of the plutonium 240 isotope.

Pu241 percentage of the plutonium 241 isotope.

Details

Note that the percentage of plutonium~242 can be computed from the other four percentages, see the examples.

In the reference below it is explained why it is very desirable to combine these plutonium patches in three groups of similar size.

Source

Available as 'pluton.dat' from the archive

currently <http://www.agoras.ua.ac.be/datasets/clusplot-examples.tar.gz>.

References

Rousseeuw, P.J. and Kaufman, L and Trauwaert, E. (1996) Fuzzy clustering using scatter matrices, *Computational Statistics and Data Analysis* **23**(1), 135–151.

Examples

```
data(pluton)
```

```
hist(apply(pluton,1,sum), col = "gray") # between 94% and 100%
pu5 <- pluton
pu5$Pu242 <- 100 - apply(pluton,1,sum) # the remaining isotope.
pairs(pu5)
```

| | |
|-------------------|---|
| predict.ellipsoid | <i>Predict Method for Ellipsoid Objects</i> |
|-------------------|---|

Description

Compute points on the ellipsoid boundary, mostly for drawing.

Usage

```
predict.ellipsoid(object, n.out=201, ...)
## S3 method for class 'ellipsoid'
predict(object, n.out=201, ...)
ellipsoidPoints(A, d2, loc, n.half = 201)
```

Arguments

| | |
|---------------|--|
| object | an object of class ellipsoid, typically from ellipsoidhull() ; alternatively any list-like object with proper components, see details below. |
| n.out, n.half | half the number of points to create. |
| A, d2, loc | arguments of the auxiliary ellipsoidPoints, see below. |
| ... | passed to and from methods. |

Details

Note ellipsoidPoints is the workhorse function of predict.ellipsoid a standalone function and method for ellipsoid objects, see [ellipsoidhull](#). The class of object is not checked; it must solely have valid components loc (length p), the $p \times p$ matrix cov (corresponding to A) and d2 for the center, the shape (“covariance”) matrix and the squared average radius (or distance) or [qchisq](#)(*, p) quantile.

Unfortunately, this is only implemented for $p = 2$, currently; contributions for $p \geq 3$ are *very welcome*.

Value

a numeric matrix of dimension $2 \times n.out$ times p .

See Also

[ellipsoidhull](#), [volume.ellipsoid](#).

Examples

```
## see also example(ellipsoidhull)

## Robust vs. L.S. covariance matrix
set.seed(143)
x <- rt(200, df=3)
y <- 3*x + rt(200, df=2)
plot(x,y, main="non-normal data (N=200)")
mtext("with classical and robust cov.matrix ellipsoids")
X <- cbind(x,y)
C.ls <- cov(X) ; m.ls <- colMeans(X)
d2.99 <- qchisq(0.99, df = 2)
lines(ellipsoidPoints(C.ls, d2.99, loc=m.ls), col="green")
if(require(MASS)) {
  Cxy <- cov.rob(cbind(x,y))
  lines(ellipsoidPoints(Cxy$cov, d2 = d2.99, loc=Cxy$center), col="red")
}# MASS
```

print.agnes

Print Method for AGNES Objects

Description

Prints the call, agglomerative coefficient, ordering of objects and distances between merging clusters ('Height') of an agnes object.

This is a method for the generic `print()` function for objects inheriting from class `agnes`, see [agnes.object](#).

Usage

```
## S3 method for class 'agnes'
print(x, ...)
```

Arguments

| | |
|------------------|--|
| <code>x</code> | an agnes object. |
| <code>...</code> | potential further arguments (required by generic). |

See Also

[summary.agnes](#) producing more output; [agnes](#), [agnes.object](#), [print](#), [print.default](#).

| | |
|-------------|---------------------------------------|
| print.clara | <i>Print Method for CLARA Objects</i> |
|-------------|---------------------------------------|

Description

Prints the best sample, medoids, clustering vector and objective function of clara object.

This is a method for the function [print\(\)](#) for objects inheriting from class [clara](#).

Usage

```
## S3 method for class 'clara'  
print(x, ...)
```

Arguments

| | |
|-----|---|
| x | a clara object. |
| ... | potential further arguments (require by generic). |

See Also

[summary.clara](#) producing more output; [clara](#), [clara.object](#), [print](#), [print.default](#).

| | |
|-------------|---------------------------------------|
| print.diana | <i>Print Method for DIANA Objects</i> |
|-------------|---------------------------------------|

Description

Prints the ordering of objects, diameters of splitted clusters, and divisive coefficient of a diana object.

This is a method for the function [print\(\)](#) for objects inheriting from class [diana](#).

Usage

```
## S3 method for class 'diana'  
print(x, ...)
```

Arguments

| | |
|-----|---|
| x | a diana object. |
| ... | potential further arguments (require by generic). |

See Also

[diana](#), [diana.object](#), [print](#), [print.default](#).

print.dissimilarity *Print and Summary Methods for Dissimilarity Objects*

Description

Print or summarize the distances and the attributes of a dissimilarity object.

These are methods for the functions `print()` and `summary()` for dissimilarity objects. See `print`, `print.default`, or `summary` for the general behavior of these.

Usage

```
## S3 method for class 'dissimilarity'
print(x, diag = NULL, upper = NULL,
      digits = getOption("digits"), justify = "none", right = TRUE, ...)
## S3 method for class 'dissimilarity'
summary(object,
         digits = max(3, getOption("digits") - 2), ...)
## S3 method for class 'summary.dissimilarity'
print(x, ...)
```

Arguments

| | |
|--|---|
| <code>x</code> , <code>object</code> | a dissimilarity object or a <code>summary.dissimilarity</code> one for <code>print.summary.dissimilarity()</code> . |
| <code>digits</code> | the number of digits to use, see print.default . |
| <code>diag</code> , <code>upper</code> , <code>justify</code> , <code>right</code> | optional arguments specifying how the triangular dissimilarity matrix is printed; see print.dist . |
| <code>...</code> | potential further arguments (require by generic). |

See Also

[daisy](#), [dissimilarity.object](#), [print](#), [print.default](#), [print.dist](#).

Examples

```
## See example(daisy)

sd <- summary(daisy(matrix(rnorm(100), 20,5)))
sd # -> print.summary.dissimilarity(.)
str(sd)
```

print.fanny

Print and Summary Methods for FANNY Objects

Description

Prints the objective function, membership coefficients and clustering vector of fanny object.

This is a method for the function `print()` for objects inheriting from class `fanny`.

Usage

```
## S3 method for class 'fanny'
print(x, digits = getOption("digits"), ...)
## S3 method for class 'fanny'
summary(object, ...)
## S3 method for class 'summary.fanny'
print(x, digits = getOption("digits"), ...)
```

Arguments

`x`, `object` a `fanny` object.
`digits` number of significant digits for printing, see `print.default`.
`...` potential further arguments (required by generic).

See Also

`fanny`, `fanny.object`, `print`, `print.default`.

print.mona

Print Method for MONA Objects

Description

Prints the ordering of objects, separation steps, and used variables of a mona object.

This is a method for the function `print()` for objects inheriting from class `mona`.

Usage

```
## S3 method for class 'mona'
print(x, ...)
```

Arguments

`x` a mona object.
`...` potential further arguments (require by generic).

See Also

[mona](#), [mona.object](#), [print](#), [print.default](#).

| | |
|------------------------|-------------------------------------|
| <code>print.pam</code> | <i>Print Method for PAM Objects</i> |
|------------------------|-------------------------------------|

Description

Prints the medoids, clustering vector and objective function of pam object.
This is a method for the function `print()` for objects inheriting from class `pam`.

Usage

```
## S3 method for class 'pam'  
print(x, ...)
```

Arguments

| | |
|------------------|---|
| <code>x</code> | a pam object. |
| <code>...</code> | potential further arguments (require by generic). |

See Also

[pam](#), [pam.object](#), [print](#), [print.default](#).

| | |
|----------------------|---------------------|
| <code>ruspini</code> | <i>Ruspini Data</i> |
|----------------------|---------------------|

Description

The Ruspini data set, consisting of 75 points in four groups that is popular for illustrating clustering techniques.

Usage

```
data(ruspini)
```

Format

A data frame with 75 observations on 2 variables giving the x and y coordinates of the points, respectively.

Source

E. H. Ruspini (1970): Numerical methods for fuzzy clustering. *Inform. Sci.*, **2**, 319–350.

References

Anja Stryuf, Mia Hubert & Peter J. Rousseeuw (1996): Clustering in an Object-Oriented Environment. *Journal of Statistical Software*, **1**. <http://www.stat.ucla.edu/journals/jss/>

Examples

```
data(ruspini)

## Plot similar to Figure 4 in Stryuf et al (1996)
## Not run: plot(pam(ruspini, 4), ask = TRUE)

## Plot similar to Figure 6 in Stryuf et al (1996)
plot(fanny(ruspini, 5))
```

silhouette

Compute or Extract Silhouette Information from Clustering

Description

Compute silhouette information according to a given clustering in k clusters.

Usage

```
silhouette(x, ...)
## Default S3 method:
  silhouette(x, dist, dmatrix, ...)
## S3 method for class 'partition'
silhouette(x, ...)
## S3 method for class 'clara'
silhouette(x, full = FALSE, ...)

sortSilhouette(object, ...)
## S3 method for class 'silhouette'
summary(object, FUN = mean, ...)
## S3 method for class 'silhouette'
plot(x, nmax.lab = 40, max.strlen = 5,
     main = NULL, sub = NULL, xlab = expression("Silhouette width " * s[i]),
     col = "gray", do.col.sort = length(col) > 1, border = 0,
     cex.names = par("cex.axis"), do.n.k = TRUE, do.clus.stat = TRUE, ...)
```

Arguments

| | |
|-------------------|--|
| <code>x</code> | an object of appropriate class; for the default method an integer vector with k different integer cluster codes or a list with such an <code>x\$clustering</code> component. Note that silhouette statistics are only defined if $2 \leq k \leq n - 1$. |
| <code>dist</code> | a dissimilarity object inheriting from class <code>dist</code> or coercible to one. If not specified, <code>dmatrix</code> must be. |

| | |
|-------------------------------------|---|
| <code>dmatrix</code> | a symmetric dissimilarity matrix ($n \times n$), specified instead of <code>dist</code> , which can be more efficient. |
| <code>full</code> | logical specifying if a <i>full</i> silhouette should be computed for <code>clara</code> object. Note that this requires $O(n^2)$ memory, since the full dissimilarity (see <code>daisy</code>) is needed internally. |
| <code>object</code> | an object of class <code>silhouette</code> . |
| <code>...</code> | further arguments passed to and from methods. |
| <code>FUN</code> | function used to summarize silhouette widths. |
| <code>nmax.lab</code> | integer indicating the number of labels which is considered too large for single-name labeling the silhouette plot. |
| <code>max.strlen</code> | positive integer giving the length to which strings are truncated in silhouette plot labeling. |
| <code>main, sub, xlab</code> | arguments to <code>title</code> ; have a sensible non-NULL default here. |
| <code>col, border, cex.names</code> | arguments passed <code>barplot()</code> ; note that the default used to be <code>col = heat.colors(n)</code> , <code>border = par("fg")</code> instead. col can also be a color vector of length k for clusterwise coloring, see also <code>do.col.sort</code> : |
| <code>do.col.sort</code> | logical indicating if the colors <code>col</code> should be sorted “along” the silhouette; this is useful for casewise or clusterwise coloring. |
| <code>do.n.k</code> | logical indicating if n and k “title text” should be written. |
| <code>do.clus.stat</code> | logical indicating if cluster size and averages should be written right to the silhouettes. |

Details

For each observation i , the *silhouette width* $s(i)$ is defined as follows:

Put $a(i)$ = average dissimilarity between i and all other points of the cluster to which i belongs (if i is the *only* observation in its cluster, $s(i) := 0$ without further calculations). For all *other* clusters C , put $d(i, C)$ = average dissimilarity of i to all observations of C . The smallest of these $d(i, C)$ is $b(i) := \min_C d(i, C)$, and can be seen as the dissimilarity between i and its “neighbor” cluster, i.e., the nearest one to which it does *not* belong. Finally,

$$s(i) := \frac{b(i) - a(i)}{\max(a(i), b(i))}.$$

`silhouette.default()` is now based on C code donated by Romain Francois (the R version being still available as `cluster::silhouette.default.R`).

Observations with a large $s(i)$ (almost 1) are very well clustered, a small $s(i)$ (around 0) means that the observation lies between two clusters, and observations with a negative $s(i)$ are probably placed in the wrong cluster.

Value

`silhouette()` returns an object, `sil`, of class `silhouette` which is an $[n \times 3]$ matrix with attributes. For each observation i , `sil[i,]` contains the cluster to which i belongs as well as the neighbor cluster of i (the cluster, not containing i , for which the average dissimilarity between its observations and i is minimal), and the silhouette width $s(i)$ of the observation. The `colnames` correspondingly are `c("cluster", "neighbor", "sil_width")`.

`summary(sil)` returns an object of class `summary.silhouette`, a list with components

| | |
|------------------------------|--|
| <code>si.summary</code> | numerical <code>summary</code> of the individual silhouette widths $s(i)$. |
| <code>clus.avg.widths</code> | numeric (rank 1) array of clusterwise <i>means</i> of silhouette widths where <code>mean = FUN</code> is used. |
| <code>avg.width</code> | the total mean <code>FUN(s)</code> where s are the individual silhouette widths. |
| <code>clus.sizes</code> | <code>table</code> of the k cluster sizes. |
| <code>call</code> | if available, the call creating <code>sil</code> . |
| <code>Ordered</code> | logical identical to <code>attr(sil, "Ordered")</code> , see below. |

`sortSilhouette(sil)` orders the rows of `sil` as in the silhouette plot, by cluster (increasingly) and decreasing silhouette width $s(i)$.

`attr(sil, "Ordered")` is a logical indicating if `sil` is ordered as by `sortSilhouette()`. In that case, `rownames(sil)` will contain case labels or numbers, and `attr(sil, "iOrd")` the ordering index vector.

Note

While `silhouette()` is *intrinsic* to the `partition` clusterings, and hence has a (trivial) method for these, it is straightforward to get silhouettes from hierarchical clusterings from `silhouette.default()` with `cutree()` and distance as input.

By default, for `clara()` partitions, the silhouette is just for the best random *subset* used. Use `full = TRUE` to compute (and later possibly plot) the full silhouette.

References

Rousseeuw, P.J. (1987) Silhouettes: A graphical aid to the interpretation and validation of cluster analysis. *J. Comput. Appl. Math.*, **20**, 53–65.

chapter 2 of Kaufman, L. and Rousseeuw, P.J. (1990), see the references in `plot.agnes`.

See Also

`partition.object`, `plot.partition`.

Examples

```
data(ruspini)
pr4 <- pam(ruspini, 4)
str(si <- silhouette(pr4))
(ssi <- summary(si))
```

```

plot(si) # silhouette plot
plot(si, col = c("red", "green", "blue", "purple"))# with cluster-wise coloring

si2 <- silhouette(pr4$clustering, dist(ruspini, "canberra"))
summary(si2) # has small values: "canberra"'s fault
plot(si2, nmax= 80, cex.names=0.6)

op <- par(mfrow= c(3,2), oma= c(0,0, 3, 0),
          mgp= c(1.6,.8,0), mar= .1+c(4,2,2,2))
for(k in 2:6)
  plot(silhouette(pam(ruspini, k=k)), main = paste("k = ",k), do.n.k=FALSE)
mtext("PAM(Ruspini) as in Kaufman & Rousseeuw, p.101",
      outer = TRUE, font = par("font.main"), cex = par("cex.main")); frame()

## the same with cluster-wise colours:
c6 <- c("tomato", "forest green", "dark blue", "purple2", "goldenrod4", "gray20")
for(k in 2:6)
  plot(silhouette(pam(ruspini, k=k)), main = paste("k = ",k), do.n.k=FALSE,
       col = c6[1:k])
par(op)

## clara(): standard silhouette is just for the best random subset
data(xclara)
set.seed(7)
str(xc1k <- xclara[sample(nrow(xclara), size = 1000) ,])
cl3 <- clara(xc1k, 3)
plot(silhouette(cl3))# only of the "best" subset of 46
## The full silhouette: internally needs large (36 MB) dist object:
sf <- silhouette(cl3, full = TRUE) ## this is the same as
s.full <- silhouette(cl3$clustering, daisy(xc1k))
if(paste(R.version$major, R.version$minor, sep=".") >= "2.3.0")
  stopifnot(all.equal(sf, s.full, check.attributes = FALSE, tol = 0))
## color dependent on original "3 groups of each 1000":
plot(sf, col = 2+ as.integer(names(cl3$clustering) ) %/% 1000,
     main ="plot(silhouette(clara(.), full = TRUE))")

## Silhouette for a hierarchical clustering:
ar <- agnes(ruspini)
si3 <- silhouette(cutree(ar, k = 5), # k = 4 gave the same as pam() above
                 daisy(ruspini))
plot(si3, nmax = 80, cex.names = 0.5)
## 2 groups: Agnes() wasn't too good:
si4 <- silhouette(cutree(ar, k = 2), daisy(ruspini))
plot(si4, nmax = 80, cex.names = 0.5)

```


Description

Returns the number of observations (*sample size*) corresponding to a dissimilarity like object, or equivalently, the number of rows or columns of a matrix when only the lower or upper triangular part (without diagonal) is given.

It is nothing else but the inverse function of $f(n) = n(n - 1)/2$.

Usage

```
sizeDiss(d)
```

Arguments

`d` any R object with length (typically) $n(n - 1)/2$.

Value

a number; n if `length(d) == n(n-1)/2`, NA otherwise.

See Also

[dissimilarity.object](#) and also [as.dist](#) for class dissimilarity and dist objects which have a `Size` attribute.

Examples

```
sizeDiss(1:10) # 5, since 10 == 5 * (5 - 1) / 2
sizeDiss(1:9) # NA

n <- 1:100
stopifnot(n == sapply( n*(n-1)/2, function(n) sizeDiss(logical(n))))
```

summary.agnes

Summary Method for 'agnes' Objects

Description

Returns (and prints) a summary list for an `agnes` object. Printing gives more output than the corresponding [print.agnes](#) method.

Usage

```
## S3 method for class 'agnes'
summary(object, ...)
## S3 method for class 'summary.agnes'
print(x, ...)
```

Arguments

`x`, object a [agnes](#) object.
 ... potential further arguments (require by generic).

See Also

[agnes](#), [agnes.object](#).

Examples

```
data(agriculture)
summary(agnes(agriculture))
```

summary.clara

Summary Method for 'clara' Objects

Description

Returns (and prints) a summary list for a clara object. Printing gives more output than the corresponding [print.clara](#) method.

Usage

```
## S3 method for class 'clara'
summary(object, ...)
## S3 method for class 'summary.clara'
print(x, ...)
```

Arguments

`x`, object a [clara](#) object.
 ... potential further arguments (require by generic).

See Also

[clara.object](#)

Examples

```
## generate 2000 objects, divided into 5 clusters.
set.seed(47)
x <- rbind(cbind(rnorm(400, 0,4), rnorm(400, 0,4)),
           cbind(rnorm(400,10,8), rnorm(400,40,6)),
           cbind(rnorm(400,30,4), rnorm(400, 0,4)),
           cbind(rnorm(400,40,4), rnorm(400,20,2)),
           cbind(rnorm(400,50,4), rnorm(400,50,4))
)
clx5 <- clara(x, 5)
```

```
## Mis'classification' table:

table(rep(1:5, rep(400,5)), clx5$clust) # -> 1 "error"
summary(clx5)

## Graphically:
par(mfrow = c(3,1), mgp = c(1.5, 0.6, 0), mar = par("mar") - c(0,0,2,0))

plot(x, col = rep(2:6, rep(400,5)))
plot(clx5)
```

| | |
|---------------|---|
| summary.diana | <i>Summary Method for 'diana' Objects</i> |
|---------------|---|

Description

Returns (and prints) a summary list for a diana object.

Usage

```
## S3 method for class 'diana'
summary(object, ...)
## S3 method for class 'summary.diana'
print(x, ...)
```

Arguments

`x, object` a [diana](#) object.
`...` potential further arguments (require by generic).

See Also

[diana](#), [diana.object](#).

| | |
|--------------|--|
| summary.mona | <i>Summary Method for 'mona' Objects</i> |
|--------------|--|

Description

Returns (and prints) a summary list for a mona object.

Usage

```
## S3 method for class 'mona'
summary(object, ...)
## S3 method for class 'summary.mona'
print(x, ...)
```

Arguments

`x, object` a [mona](#) object.
`...` potential further arguments (require by generic).

See Also

[mona](#), [mona.object](#).

`summary.pam`

Summary Method for PAM Objects

Description

Summarize a [pam](#) object and return an object of class `summary.pam`. There's a [print](#) method for the latter.

Usage

```
## S3 method for class 'pam'
summary(object, ...)
## S3 method for class 'summary.pam'
print(x, ...)
```

Arguments

`x, object` a [pam](#) object.
`...` potential further arguments (require by generic).

See Also

[pam](#), [pam.object](#).

`twins.object`

Hierarchical Clustering Object

Description

The objects of class "twins" represent an agglomerative or divisive (polythetic) hierarchical clustering of a dataset.

Value

See [agnes.object](#) and [diana.object](#) for details.

GENERATION

This class of objects is returned from `agnes` or `diana`.

METHODS

The "twins" class has a method for the following generic function: `pltree`.

INHERITANCE

The following classes inherit from class "twins": "agnes" and "diana".

See Also

[agnes](#), [diana](#).

volume.ellipsoid

Compute the Volume of Planar Object

Description

Compute the volume of a planar object. This is a generic function and a method for `ellipsoid` objects.

Usage

```
## S3 method for class 'ellipsoid'
volume(object)
```

Arguments

`object` an R object the volume of which is wanted; for the `ellipsoid` method, an object of that class (see [ellipsoidhull](#) or the example below).

Value

a number, the volume of the given object.

See Also

[ellipsoidhull](#) for spanning ellipsoid computation.

Examples

```
## example(ellipsoidhull) # which defines 'ellipsoid' object <namefoo>

myEl <- structure(list(cov = rbind(c(3,1),1:2), loc = c(0,0), d2 = 10),
                  class = "ellipsoid")
volume(myEl) # i.e. "area" here (d = 2)
myEl # also mentions the "volume"
```

votes.repub

Votes for Republican Candidate in Presidential Elections

Description

A data frame with the percents of votes given to the republican candidate in presidential elections from 1856 to 1976. Rows represent the 50 states, and columns the 31 elections.

Usage

```
data(votes.repub)
```

Source

S. Peterson (1973): *A Statistical History of the American Presidential Elections*. New York: Frederick Ungar Publishing Co.

Data from 1964 to 1976 is from R. M. Scammon, *American Votes 12*, Congressional Quarterly.

xclara

Bivariate Data Set with 3 Clusters

Description

An artificial data set consisting of 3000 points in 3 well-separated clusters of size 1000 each.

Usage

```
data(xclara)
```

Format

A data frame with 3000 observations on 2 numeric variables giving the x and y coordinates of the points, respectively.

Source

Sample data set accompanying the reference below, obtained from <http://www.stat.ucla.edu/journals/jss/v01/i04/data/>.

References

Anja Struyf, Mia Hubert & Peter J. Rousseeuw (1996): Clustering in an Object-Oriented Environment. *Journal of Statistical Software*, **1**. <http://www.stat.ucla.edu/journals/jss/>

Index

- *Topic **arith**
 - sizeDiss, 64
- *Topic **array**
 - lower.to.upper.tri.inds, 35
- *Topic **cluster**
 - agnes, 3
 - agnes.object, 5
 - bannerplot, 9
 - clara, 11
 - clara.object, 14
 - clusplot, 15
 - clusplot.default, 16
 - coef.hclust, 20
 - daisy, 21
 - diana, 24
 - dissimilarity.object, 27
 - fanny, 30
 - fanny.object, 32
 - mona, 36
 - mona.object, 37
 - pam, 38
 - pam.object, 40
 - partition.object, 42
 - plot.agnes, 45
 - plot.diana, 47
 - plot.mona, 49
 - plot.partition, 50
 - pltree, 52
 - pltree.twins, 52
 - print.agnes, 56
 - print.clara, 57
 - print.diana, 57
 - print.dissimilarity, 58
 - print.fanny, 59
 - print.mona, 59
 - print.pam, 60
 - silhouette, 61
 - summary.agnes, 65
 - summary.clara, 66
 - summary.diana, 67
 - summary.mona, 67
 - summary.pam, 68
 - twins.object, 68
- *Topic **datasets**
 - agriculture, 7
 - animals, 8
 - chorSub, 10
 - flower, 34
 - plantTraits, 43
 - pluton, 54
 - ruspini, 60
 - votes.repub, 70
 - xclara, 70
- *Topic **dplot**
 - ellipsoidhull, 28
 - predict.ellipsoid, 55
- *Topic **hplot**
 - bannerplot, 9
 - clusplot, 15
 - clusplot.default, 16
 - ellipsoidhull, 28
 - plot.agnes, 45
 - plot.diana, 47
 - plot.mona, 49
 - plot.partition, 50
 - pltree, 52
 - pltree.twins, 52
- *Topic **print**
 - print.agnes, 56
 - print.clara, 57
 - print.diana, 57
 - print.dissimilarity, 58
 - print.fanny, 59
 - print.mona, 59
 - print.pam, 60
 - summary.agnes, 65
 - summary.clara, 66
 - summary.diana, 67

- summary.mona, 67
- *Topic **utilities**
 - bannerplot, 9
 - lower.to.upper.tri.inds, 35
 - predict.ellipsoid, 55
 - sizeDiss, 64
 - volume.ellipsoid, 69
- agnes, 3, 6, 7, 13, 21, 24, 26, 28, 32, 37, 40, 45, 46, 52, 53, 56, 66, 69
- agnes.object, 4, 5, 5, 21, 46, 53, 56, 66, 68
- agriculture, 7
- animals, 8
- as.dendrogram, 46, 53
- as.dist, 65
- as.hclust, 6, 26, 53
- as.matrix, 27
- bannerplot, 9, 45–47, 49
- barplot, 9, 62
- call, 42
- chorizon, 10, 11
- chorSub, 10
- chull, 29
- clara, 4, 11, 14–17, 19, 24, 28, 39, 40, 43, 50, 51, 57, 62, 63, 66
- clara.object, 12, 13, 14, 16, 43, 51, 57, 66
- clusplot, 12, 15, 29
- clusplot.default, 15, 16, 16, 29, 50, 51
- clusplot.partition, 19, 51
- cmdscale, 18, 19
- coef.hclust, 20
- coef.twins (coef.hclust), 20
- colnames, 63
- cov.mve, 19, 29
- cutree, 26, 63
- daisy, 3, 5, 7, 17–19, 21, 25, 26, 28, 30–32, 38, 40, 58, 62
- diana, 4–7, 21, 24, 24, 28, 47, 48, 52, 53, 57, 67, 69
- diana.object, 21, 48, 53, 57, 67, 68
- dissimilarity.object, 6, 15, 23, 24, 27, 33, 41, 58, 65
- dist, 3, 5, 17, 22, 24–28, 30, 32, 38, 40, 61
- ellipse, 29
- ellipsePoints, 29
- ellipsoidhull, 28, 55, 69
- ellipsoidPoints (predict.ellipsoid), 55
- fanny, 4, 15–17, 24, 28, 30, 33, 43, 50, 51, 59
- fanny.object, 16, 32, 32, 43, 51, 59
- flower, 34
- hclust, 5, 6, 21, 53
- identify, 17, 19
- list, 29
- lower.to.upper.tri.inds, 35
- lower.tri, 35
- menu, 45, 47, 50
- mona, 4, 36, 37, 49, 50, 59, 60, 68
- mona.object, 37, 37, 50, 60, 68
- NA, 17, 22–25, 38
- names, 18
- pam, 4, 12, 13, 15–17, 19, 24, 28, 38, 41, 43, 50, 51, 60, 68
- pam.object, 16, 39, 40, 40, 43, 51, 60, 68
- par, 10, 15, 16, 18, 19, 45–48, 50–53
- partition, 63
- partition (partition.object), 42
- partition.object, 13–16, 32, 33, 40, 41, 42, 51, 63
- plantTraits, 43
- plot.agnes, 4–6, 10, 45, 48, 50, 51, 53, 63
- plot.default, 18, 45, 47, 49
- plot.dendrogram, 46, 53
- plot.diana, 10, 26, 47, 53
- plot.hclust, 53
- plot.mona, 10, 37, 49
- plot.partition, 13, 15, 32, 33, 40–42, 50, 63
- plot.silhouette, 51
- plot.silhouette (silhouette), 61
- pltree, 6, 47, 52
- pltree.twins, 45, 46, 52, 52
- pluton, 54
- predict, 29
- predict.ellipsoid, 29, 55
- pretty, 10, 45, 47
- princomp, 18, 19
- print, 28, 56–60, 68
- print.agnes, 56, 65
- print.clara, 57, 66

print.default, 56–60
print.diana, 57
print.dissimilarity, 58
print.dist, 58
print.ellipsoid (ellipsoidhull), 28
print.fanny, 33, 59
print.mona, 59
print.pam, 60
print.summary.agnes (summary.agnes), 65
print.summary.clara (summary.clara), 66
print.summary.diana (summary.diana), 67
print.summary.dissimilarity
 (print.dissimilarity), 58
print.summary.fanny (print.fanny), 59
print.summary.mona (summary.mona), 67
print.summary.pam (summary.pam), 68
print.summary.silhouette (silhouette),
 61

qchisq, 55

range, 22
ruspini, 60

set.seed, 13
silhouette, 39, 42, 51, 61
sizeDiss, 64
sortSilhouette (silhouette), 61
summary, 63
summary.agnes, 56, 65
summary.clara, 57, 66
summary.diana, 67
summary.dissimilarity
 (print.dissimilarity), 58
summary.fanny (print.fanny), 59
summary.mona, 67
summary.pam, 68
summary.silhouette (silhouette), 61

table, 63
text, 49
title, 9, 18, 49, 62
twins (twins.object), 68
twins.object, 5, 6, 26, 48, 52, 68

upper.to.lower.tri.inds
 (lower.to.upper.tri.inds), 35
upper.tri, 35

volume (volume.ellipsoid), 69
volume.ellipsoid, 29, 55, 69
votes.repub, 70
xclara, 70