Package ‘fpc’

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Fixed point clustering. Linear regression clustering. Clustering by merging Gaussian mixture components. Symmetric and asymmetric discriminant projections for visualisation of the separation of groupings. Cluster validation statistics for distance based clustering including corrected Rand index. Standardisation of cluster validation statistics by random clusterings and comparison between many clustering methods and numbers of clusters based on this.
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Description

Here is a list of the main functions in package fpc. Most other functions are auxiliary functions for these.

Clustering methods

- **dbscan** Computes DBSCAN density based clustering as introduced in Ester et al. (1996).
- **fixmahal** Mahalanobis Fixed Point Clustering, Hennig and Christlieb (2002), Hennig (2005).
- **fixreg** Regression Fixed Point Clustering, Hennig (2003).
- **flexmixedruns** This fits a latent class model to data with mixed type continuous/nominal variables. Actually it calls a method for **flexmix**.
- **mergenormals** Clustering by merging components of a Gaussian mixture, see Hennig (2010).
- **regmix** ML-fit of a mixture of linear regression models, see DeSarbo and Cron (1988).

Cluster validity indexes and estimation of the number of clusters

- **cluster.stats** This computes several cluster validity statistics from a clustering and a dissimilarity matrix including the Calinski-Harabasz index, the adjusted Rand index and other statistics explained in Gordon (1999) as well as several characterising measures such as average between cluster and within cluster dissimilarity and separation. See also **calinhara**, **dudahart2** for specific indexes, and a new version **cqcluster.stats** that computes some more indexes and statistics used for computing them. There’s also **distrsimilarity**, which computes within-cluster dissimilarity to the Gaussian and uniform distribution.
- **prediction.strength** Estimates the number of clusters by computing the prediction strength of a clustering of a dataset into different numbers of components for various clustering methods, see Tibshirani and Walther (2005). In fact, this is more flexible than what is in the original paper, because it can use point classification schemes that work better with clustering methods other than k-means.
- **nselectboot** Estimates the number of clusters by bootstrap stability selection, see Fang and Wang (2012). This is quite flexible regarding clustering methods and point classification schemes and also allows for dissimilarity data.
- **clusterbenchstats** This runs many clustering methods (to be specified by the user) with many numbers of clusters on a dataset and produces standardised and comparable versions of many cluster validity indexes (see Hennig 2019, Akhanli and Hennig 2020). This is done by means of producing random clusterings on the given data, see **stupidkcentroids** and **stupidknn**. It allows to compare many clusterings based on many different potential desirable features of a clustering. **print.valstat** allows to compute an aggregated index with user-specified weights.
Cluster visualisation and validation

**clucols** Sets of colours and symbols useful for cluster plotting.

**clusterboot** Cluster-wise stability assessment of a clustering. Clusterings are performed on resampled data to see for every cluster of the original dataset how well this is reproduced. See Hennig (2007) for details.

**cluster.varstats** Extracts variable-wise information for every cluster in order to help with cluster interpretation.

**plotcluster** Visualisation of a clustering or grouping in data by various linear projection methods that optimise the separation between clusters, or between a single cluster and the rest of the data according to Hennig (2004) including classical methods such as discriminant coordinates. This calls the function `discrproj`, which is a bit more flexible but doesn’t produce a plot itself.

**ridgeline.diagnosis** Plots and diagnostics for assessing modality of Gaussian mixtures, see Ray and Lindsay (2005).

**weightplots** Plots to diagnose component separation in Gaussian mixtures, see Hennig (2010).

**localshape** Local shape matrix, can be used for finding clusters in connection with function `ics` in package ICS, see Hennig’s discussion and rejoinder of Tyler et al. (2009).

Useful wrapper functions for clustering methods

**kmeansCBI** This and other "CBI"-functions (see the `kmeansCBI`-help page) are unified wrappers for various clustering methods in R that may be useful because they do in one step for what you normally may need to do a bit more in R (for example fitting a Gaussian mixture with noise component in package mclust).

**kmeansruns** This calls `kmeans` for the k-means clustering method and includes estimation of the number of clusters and finding an optimal solution from several starting points.

**pamk** This calls `pam` and `clara` for the partitioning around medoids clustering method (Kaufman and Rousseeuw, 1990) and includes two different ways of estimating the number of clusters.

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References


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**adcoord**  
*Asymmetric discriminant coordinates*

**Description**

Asymmetric discriminant coordinates as defined in Hennig (2003). Asymmetric discriminant projection means that there are two classes, one of which is treated as the homogeneous class (i.e., it should appear homogeneous and separated in the resulting projection) while the other may be heterogeneous. The principle is to maximize the ratio between the projection of a between classes separation matrix and the projection of the covariance matrix within the homogeneous class.

**Usage**

```
adcoord(xd, clvecd, clnum=1)
```

**Arguments**

- `xd`  
  the data matrix; a numerical object which can be coerced to a matrix.

- `clvecd`  
  integer vector of class numbers; length must equal `nrow(xd)`.

- `clnum`  
  integer. Number of the homogeneous class.
Details

The square root of the homogeneous classes covariance matrix is inverted by use of \texttt{tdecomp}, which can be expected to give reasonable results for singular within-class covariance matrices.

Value

List with the following components

- \texttt{ev}: eigenvalues in descending order.
- \texttt{units}: columns are coordinates of projection basis vectors. New points x can be projected onto the projection basis vectors by $x \times \texttt{units}$.
- \texttt{proj}: projections of $xd$ onto \texttt{units}.

Author(s)

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References


See Also

- \texttt{plotcluster} for straightforward discriminant plots. \texttt{discrproj} for alternatives. \texttt{rFace} for generation of the example data used below.

Examples

```r
set.seed(4634)
face <- rFace(600,dMoNo=2,dNoEy=0)
grface <- as.integer(attr(face,“grouping”))
adcf <- adcoord(face,grface==2)
adcf2 <- adcoord(face,grface==4)
plot(adcf$proj,col=1+(grface==2))
plot(adcf2$proj,col=1+(grface==4))
# ...done in one step by function plotcluster.
```
Asymmetric neighborhood based discriminant coordinates as defined in Hennig (2003). Asymmetric discriminant projection means that there are two classes, one of which is treated as the homogeneous class (i.e., it should appear homogeneous and separated in the resulting projection) while the other may be heterogeneous. The principle is to maximize the ratio between the projection of a between classes covariance matrix, which is defined by averaging the between classes covariance matrices in the neighborhoods of the points of the homogeneous class and the projection of the covariance matrix within the homogeneous class.

Usage

```r
ancoord(xd, clvecd, clnum=1, nn=50, method="mcd", countmode=1000, ...)
```

Arguments

- `xd`: the data matrix; a numerical object which can be coerced to a matrix.
- `clvecd`: integer vector of class numbers; length must equal `nrow(xd)`.
- `clnum`: integer. Number of the homogeneous class.
- `nn`: integer. Number of points which belong to the neighborhood of each point (including the point itself).
- `method`: one of "mve", "mcd" or "classical". Covariance matrix used within the homogeneous class. "mcd" and "mve" are robust covariance matrices as implemented in `cov.rob`. "classical" refers to the classical covariance matrix.
- `countmode`: optional positive integer. Every `countmode` algorithm runs `ancoord` shows a message.
- `...`: no effect

Details

The square root of the homogeneous classes covariance matrix is inverted by use of `tdecomp`, which can be expected to give reasonable results for singular within-class covariance matrices.

Value

List with the following components

- `ev`: eigenvalues in descending order.
- `units`: columns are coordinates of projection basis vectors. New points `x` can be projected onto the projection basis vectors by `x %*% units`.
- `proj`: projections of `xd` onto `units`.
**awcoord**

*Asymmetric weighted discriminant coordinates*

**Description**

Asymmetric weighted discriminant coordinates as defined in Hennig (2003). Asymmetric discriminant projection means that there are two classes, one of which is treated as the homogeneous class (i.e., it should appear homogeneous and separated in the resulting projection) while the other may be heterogeneous. The principle is to maximize the ratio between the projection of a between classes separation matrix and the projection of the covariance matrix within the homogeneous class. Points are weighted according to their (robust) Mahalanobis distance to the homogeneous class.

**Usage**

```
awcoord(xd, clvecd, clnum=1, mahal="square", method="classical",
        clweight=switch(method,classical=FALSE,TRUE),
        alpha=0.99, subsample=0, countmode=1000, ...)```

**Author(s)**

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**References**


**See Also**

`plotcluster` for straight forward discriminant plots. `discrproj` for alternatives. `rFace` for generation of the example data used below.

**Examples**

```
set.seed(4634)
face <- rFace(600,dMoNo=2,dNoEy=0)
grface <- as.integer(attr(face,"grouping"))
ancf2 <- ancoord(face,grface==4)
plot(ancf2$proj,col=1+(grface==4))
# ...done in one step by function plotcluster.
```
Arguments

- **xd**: the data matrix; a numerical object which can be coerced to a matrix.
- **clvecd**: integer vector of class numbers; length must equal `nrow(xd)`.
- **clnum**: integer. Number of the homogeneous class.
- **mahal**: "md" or "square". If "md", the points are weighted by the square root of the alpha-quantile of the corresponding chi squared distribution over the roots of their Mahalanobis distance to the homogeneous class, unless this is smaller than 1. If "square" (which is recommended), the (originally squared) Mahalanobis distance and the unrooted quantile is used.
- **method**: one of "mve", "mcd" or "classical". Covariance matrix used within the homogeneous class and for the computation of the Mahalanobis distances. "mcd" and "mve" are robust covariance matrices as implemented in `cov.rob`. "classical" refers to the classical covariance matrix.
- **clweight**: logical. If FALSE, only the points of the heterogeneous class are weighted. This, together with `method="classical"`, computes AWC as defined in Hennig (2003). If TRUE, all points are weighted. This, together with `method="mcd"`, computes ARC as defined in Hennig (2003).
- **alpha**: numeric between 0 and 1. The corresponding quantile of the chi squared distribution is used for the downweighting of points. Points with a smaller Mahalanobis distance to the homogeneous class get full weight.
- **subsample**: integer. If 0, all points are used. Else, only a subsample of `subsample` of the points is used.
- **countmode**: optional positive integer. Every `countmode` algorithm runs `awcoord` shows a message.
- ... no effect

Details

The square root of the homogeneous classes covariance matrix is inverted by use of `tdecomp`, which can be expected to give reasonable results for singular within-class covariance matrices.

Value

List with the following components

- **ev**: eigenvalues in descending order.
- **units**: columns are coordinates of projection basis vectors. New points `x` can be projected onto the projection basis vectors by `x %*% units`
- **proj**: projections of `xd` onto `units`.

Author(s)

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References


See Also

plotcluster for straight forward discriminant plots. discrproj for alternatives. rFace for generation of the example data used below.

Examples

```r
set.seed(4634)
face <- rFace(600,dMoNo=2,dNoEy=0)
grface <- as.integer(attr(face,"grouping"))
awcf <- awcoord(face, grface==1)
# awcf2 <- ancoord(face, grface==1, method="mcd")
plot(awcf$proj, col=1+(grface==1))
# plot(awcf2$proj, col=1+(grface==1))
# ...done in one step by function plotcluster.
```

---

**batcoord**

**Bhattacharyya discriminant projection**

Description

Computes Bhattacharyya discriminant projection coordinates as described in Fukunaga (1990), p. 455 ff.

Usage

```r
batcoord(xd, clvecd, clnum=1, dom="mean")
batvarcoord(xd, clvecd, clnum=1)
```

Arguments

- **xd**
  - the data matrix; a numerical object which can be coerced to a matrix.
- **clvecd**
  - integer or logical vector of class numbers; length must equal nrow(xd).
- **clnum**
  - integer, one of the values of clvecd, if this is an integer vector. Bhattacharyya projections can only be computed if there are only two classes in the dataset. clnum is the number of one of the two classes. All the points indicated by other values of clvecd are interpreted as the second class.
dom string. dom="mean" means that the discriminant coordinate for the group means is computed as the first projection direction by discrcoord (option pool="equal"; both classes have the same weight for computing the within-class covariance matrix). Then the data is projected into a subspace orthogonal (w.r.t. the within-class covariance) to the discriminant coordinate, and the projection coordinates to maximize the differences in variance are computed. dom="variance" means that the projection coordinates maximizing the difference in variances are computed. Then they are ordered with respect to the Bhattacharyya distance, which takes also the mean differences into account. Both procedures are implemented as described in Fukunaga (1990).

Details

batvarcoord computes the optimal projection coordinates with respect to the difference in variances. batcoord combines the differences in mean and variance as explained for the argument dom.

Value

batcoord returns a list with the components ev, rev, units, proj. batvarcoord returns a list with the components ev, rev, units, proj, W, S1, S2.

ev vector of eigenvalues. If dom="mean", then first eigenvalue from discrcoord. Further eigenvalues are of $S_i^{-1}S_j$, where $S_i$ is the covariance matrix of class i. For batvarcoord or if dom="variance", all eigenvalues come from $S_i^{-1}S_j$ and are ordered by rev.


units columns are coordinates of projection basis vectors. New points x can be projected onto the projection basis vectors by x %*% units.

proj projections of xd onto units.

W matrix $S_i^{-1}S_j$.

S1 covariance matrix of the first class.

S2 covariance matrix of the second class.

Author(s)

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References

bhattacharyya.dist

See Also

- `plotcluster` for straight forward discriminant plots.
- `discrcoord` for discriminant coordinates.
- `rFace` for generation of the example data used below.

Examples

```r
set.seed(4634)
face <- rFace(600, dMoNo=2, dNoEy=0)
grface <- as.integer(attr(face, "grouping"))
bcf2 <- batcoord(face, grface==2)
plot(bcf2$proj, col=1+(grface==2))
bcfv2 <- batcoord(face, grface==2, dom="variance")
plot(bcfv2$proj, col=1+(grface==2))
bcfvv2 <- batvarcoord(face, grface==2)
plot(bcfvv2$proj, col=1+(grface==2))
```

bhattacharyya.dist  Bhattacharyya distance between Gaussian distributions

Description

Computes Bhattacharyya distance between two multivariate Gaussian distributions. See Fukunaga (1990).

Usage

```r
bhattacharyya.dist(mu1, mu2, Sigma1, Sigma2)
```

Arguments

- `mu1` mean vector of component 1.
- `mu2` mean vector of component 2.
- `Sigma1` covariance matrix of component 1.
- `Sigma2` covariance matrix of component 2.

Value

The Bhattacharyya distance between the two Gaussian distributions.

Note

Thanks to David Pinto for improving this function.

Author(s)

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bhattacharyya.matrix

References


Examples

```r
round(bhattacharyya.dist(c(1,1),c(2,5),diag(2),diag(2)),digits=2)
```

bhattacharyya.matrix  Matrix of pairwise Bhattacharyya distances

Description

Computes Bhattachryya distances for pairs of components given the parameters of a Gaussian mixture.

Usage

```r
bhattacharyya.matrix(muarray,Sigmaarray,ipairs="all", misclassification.bound=TRUE)
```

Arguments

- **muarray**: matrix of component means (different components are in different columns).
- **Sigmaarray**: three dimensional array with component covariance matrices (the third dimension refers to components).
- **ipairs**: “all” or list of vectors of two integers. If `ipairs="all"`, computations are carried out for all pairs of components. Otherwise, ipairs gives the pairs of components for which computations are carried out.
- **misclassification.bound**: logical. If `TRUE`, upper bounds for misclassification probabilities $\exp(-b)$ are given out instead of the original Bhattacharyya distances $b$.

Value

A matrix with Bhattacharyya distances (or derived misclassification bounds, see above) between pairs of Gaussian distributions with the provided parameters. If `ipairs!="all"`, the Bhattacharyya distance and the misclassification bound are given as `NA` for pairs not included in `ipairs`.

Author(s)

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References


See Also

bhattacharyya.dist

Examples

muarray <- cbind(c(0,0),c(0,0.1),c(10,10))
sigmaarray <- array(c(diag(2),diag(2),diag(2)),dim=c(2,2,3))
bhattacharyya.matrix(muarray,sigmaarray,ipairs=list(c(1,2),c(2,3)))

calinhara(x,clustering,cn=max(clustering))

Arguments

x data matrix or data frame.

clustering vector of integers. Clustering.

cn integer. Number of clusters.

Value

Calinski-Harabasz statistic, which is \((n-cn)*sum(diag(B))/((cn-1)*sum(diag(W))))\). B being the between-cluster means, and W being the within-clusters covariance matrix.

Author(s)

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References


See Also

cluster.stats

Examples

```r
set.seed(98765)
iriss <- iris[sample(150,20),-5]
km <- kmeans(iriss,3)
round(calinhara(iriss,km$cluster),digits=2)
```

Description

Generates tuning constants ca for fixreg dependent on the number of points and variables of the dataset.

Only thought for use in fixreg.

Usage

`can(n, p)`

Arguments

- `n` positive integer. Number of points.
- `p` positive integer. Number of independent variables.

Details

The formula is $3 + 33/((n * 2^{-(p-1)/2})^{1/3} + 2900000/(n * 2^{-(p-1)/2})^{3}$. For justification cf. Hennig (2002).

Value

A number.

Author(s)

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Recodes a dataset with nominal variables so that the nominal variables are replaced by binary variables for the categories.

Usage

```r
cat2bin(x, categorical=NULL)
```

Arguments

- `x`: data matrix or data frame. The data need to be organised case-wise, i.e., if there are categorical variables only, and 15 cases with values c(1,1,2) on the 3 variables, the data matrix needs 15 rows with values 1 1 2. (Categorical variables could take numbers or strings or anything that can be coerced to factor levels as values.)

- `categorical`: vector of numbers of variables to be recoded.

Value

A list with components

- `data`: data matrix with variables specified in `categorical` replaced by 0-1 variables, one for each category.

- `variableinfo`: list of lists. One list for every variable in the original dataset, with four components each, namely type ("categorical" or "not recoded"), levels (levels of nominal recoded variables in order of binary variable in output dataset), `ncat` (number of categories for recoded variables), `varnum` (number of variables in output dataset belonging to this original variable).

Examples

```r
can(429,3)
```
Author(s)

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See Also
discrete.recode

Examples

```r
set.seed(776655)
v1 <- rnorm(20)
v2 <- rnorm(20)
d1 <- sample(1:5,20,replace=TRUE)
d2 <- sample(1:4,20,replace=TRUE)
ldata <-cbind(v1,v2,d1,d2)
lc <- cat2bin(ldata,categorical=3:4)
```

cdbw

---

CDbw-index for cluster validation

Description

CDbw-index for cluster validation, as defined in Halkidi and Vazirgiannis (2008), Halkidi et al. (2015).

Usage

```r
cdbw(x,clustering,r=10,s=seq(0.1,0.8,by=0.1),
    clusterstdev=TRUE,trace=FALSE)
```

Arguments

- `x` something that can be coerced into a numerical matrix. Euclidean dataset.
- `clustering` vector of integers with length =nrow(x); indicating the cluster for each observation.
- `r` integer. Number of cluster border representatives.
- `s` numerical vector of shrinking factors (between 0 and 1).
- `clusterstdev` logical. If TRUE, the neighborhood radius for intra-cluster density is the within-cluster estimated squared distance from the mean of the cluster; otherwise it is the average of these over all clusters.
- `trace` logical. If TRUE, results are printed for the steps to compute the index.
**Value**

List with components (see Halkidi and Vazirgiannis (2008), Halkidi et al. (2015) for details)

- **cdbw**: value of CDbw index (the higher the better).
- **cohesion**: cohesion.
- **compactness**: compactness.
- **sep**: separation.

**Author(s)**

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**References**


**Examples**

```r
options(digits=3)
iriss <- as.matrix(iris[c(1:5,51:55,101:105),-5])
irisc <- as.numeric(iris[c(1:5,51:55,101:105),5])
cdbw(iriss,irisc)
```

**Description**

Standardises cluster validity statistics as produced by `clustatsum` relative to results that were achieved by random clusterings on the same data by `randomclustsim`. The aim is to make differences between values comparable between indexes, see Hennig (2019), Akhanli and Hennig (2020).

This is mainly for use within `clusterbenchstats`.

**Usage**

```r
cgrestandard(clusum,clusim,G,percentage=FALSE,
             useallmethods=FALSE,
             useallg=FALSE, othernc=list())
```
Arguments

clusum: object of class "valstat", see clusterbenchstats.
clusim: list; output object of randomclustersim, see there.
G: vector of integers. Numbers of clusters to consider.
percentage: logical. If FALSE, standardisation is done to mean zero and standard deviation 1 using the random clusterings. If TRUE, the output is the percentage of simulated values below the result (more precisely, this number plus one divided by the total plus one).
useallmethods: logical. If FALSE, only random clustering results from clusim are used for standardisation. If TRUE, also clustering results from other methods as given in clusum are used.
useallg: logical. If TRUE, standardisation uses results from all numbers of clusters in G. If FALSE, standardisation of results for a specific number of cluster only uses results from that number of clusters.
othernc: list of integer vectors of length 2. This allows the incorporation of methods that bring forth other numbers of clusters than those in G, for example because a method may have automatically estimated a number of clusters. The first number is the number of the clustering method (the order is determined by argument clustermethod in clusterbenchstats), the second number is the number of clusters. Results specified here are only standardised in useallg=TRUE.

Details

cgrestandard will add a statistic named dmode to the input set of validation statistics, which is defined as 0.75*dindex+0.25*highdgap, aggregating these two closely related statistics, see clustatsum.

Value

List of class "valstat", see valstat.object, with standardised results as explained above.

Author(s)

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References


see Also

\texttt{valstat.object, clusterbenchstats, stupidkcentroids, stupidknn, stupidkfn, stupidkaven, clustatsum}

Examples

```r
set.seed(20000)
options(digits=3)
face <- rFace(10,dMoNo=2,dNoEy=0,p=2)
dif <- dist(face)
clusum <- list()
clusum[[2]] <- list()
c12 <- kmeansCBI(face,2)
c13 <- kmeansCBI(face,3)
c12 <- claraCBI(face,2)
c123 <- claraCBI(face,2)
ccl12 <- clustatsum(dif,cl12$partition)
ccl13 <- clustatsum(dif,cl13$partition)
ccl22 <- clustatsum(dif,cl22$partition)
ccl23 <- clustatsum(dif,cl23$partition)
clusum[[1]] <- list()
clusum[[1]][[2]] <- ccl12
clusum[[1]][[3]] <- ccl13
clusum[[2]][[2]] <- ccl22
clusum[[2]][[3]] <- ccl23
clusum$maxG <- 3
clusum$minG <- 2
clusum$method <- c("kmeansCBI","claraCBI")
clusum$name <- c("kmeansCBI","claraCBI")
clusim <- randomclustersim(dist(face),G=2:3,nnruns=1,kmruns=1,
fnruns=1,avenruns=1,monitor=FALSE)
cgr <- cgrestandard(clusum,clusim,2:3)
cgr2 <- cgrestandard(clusum,clusim,2:3,useallg=TRUE)
cgr3 <- cgrestandard(clusum,clusim,2:3,percentage=TRUE)
print(str(cgr))
print(str(cgr2))
print(cgr3[[1]][[2]])
```

\texttt{classifdist}  
\textit{Classification of unclustered points}

Description

Various methods for classification of unclustered points from clustered points for use within functions \texttt{nselectboot} and \texttt{prediction.strength}.
Usage

```r
classifdist(cdist, clustering, 
method = "averagedist", 
centroids = NULL, nnk = 1)

classifnp(data, clustering, 
method = "centroid", cdist = NULL, 
centroids = NULL, nnk = 1)
```

Arguments

cdist  
dissimilarity matrix or dist-object. Necessary for classifdist but optional for classifnp and there only used if method = "averagedist" (if not provided, dist is applied to data).

data  
something that can be coerced into a an n*p-data matrix.

clustering integer vector. Gives the cluster number (between 1 and k for k clusters) for clustered points and should be -1 for points to be classified.

method one of "averagedist", "centroid", "qda", "knn". See details.

centroids for classifnp a k times p matrix of cluster centroids. For classifdist a vector of numbers of centroid objects as provided by pam. Only used if method = "centroid"; in that case mandatory for classifdist but optional for classifnp, where cluster mean vectors are computed if centroids = NULL.

nnk  
number of nearest neighbours if method = "knn".

Details

classifdist is for data given as dissimilarity matrix, classifnp is for data given as n times p data matrix. The following methods are supported:

"centroid" assigns observations to the cluster with closest cluster centroid as specified in argument centroids (this is associated to k-means and pam/clara-clustering).

"qda" only in classifnp. Classifies by quadratic discriminant analysis (this is associated to Gaussian clusters with flexible covariance matrices), calling qda with default settings. If qda gives an error (usually because a class was too small), lda is used.

"lda" only in classifnp. Classifies by linear discriminant analysis (this is associated to Gaussian clusters with equal covariance matrices), calling lda with default settings.

"averagedist" assigns to the cluster to which an observation has the minimum average dissimilarity to all points in the cluster (this is associated with average linkage clustering).

"knn" classifies by nnk nearest neighbours (for nnk=1, this is associated with single linkage clustering). Calls knn in classifnp.

"fn" classifies by the minimum distance to the farthest neighbour. This is associated with complete linkage clustering).

Value

An integer vector giving cluster numbers for all observations; those for the observations already clustered in the input are the same as in the input.
### clucols

**Sets of colours and symbols for cluster plotting**

**Description**

`clucols` gives out a vector of different random colours. `clugrey` gives out a vector of equidistant grey scales. `clusym` is a vector of different symbols starting from "1", "2",....

**Usage**

```r
clucols(i, seed=NULL)  
clugrey(i, max=0.9)  
clusym
```

**Arguments**

- `i` : integer. Length of output vector (number of clusters).
- `seed` : integer. Random seed.
- `max` : between 0 and 1. Maximum grey scale value, see `grey` (close to 1 is bright).

---

**Examples**

```r
set.seed(20000)
x1 <- rnorm(50)
y <- rnorm(100)
x2 <- rnorm(40,mean=20)
x3 <- rnorm(10,mean=25,sd=100)
x <- cbind(c(x1,x2,x3),y)
truec <- c(rep(1,50),rep(2,40),rep(3,10))
topredict <- c(1,2,51,52,91)
clumin <- truec
clumin[topredict] <- -1

classifnp(x,clumin, method="averagedist")  
classifnp(x,clumin, method="qda")  
classifdist(dist(x),clumin, centroids=c(3,53,93), method="centroid")  
classifdist(dist(x),clumin, method="knn")
```
Value

clucols gives out a vector of different random colours. clugrey gives out a vector of equidistant grey scales. clusym is a vector of different characters starting from "1", "2"... 

Author(s)

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Examples

```r
set.seed(112233)
require(MASS)
require(flexmix)
data(Cars93)
Cars934 <- Cars93[,c(3,5,8,10)]
cc <-
  discrete.recode(Cars934,xvarsorted=FALSE,continuous=c(2,3),discrete=c(1,4))
fcc <- flexmix(cc$data~1,k=3,
  model=lcmixed(continuous=2,discrete=2,ppdim=c(6,3),diagonal=TRUE))
plot(Cars934[,c(2,3)],col=clucols(3)[fcc@cluster],pch=clusym[fcc@cluster])
```

---

clujaccard

_Jaccard similarity between logical vectors_

Description

Jaccard similarity between logical or 0-1 vectors: \( \frac{\text{sum}(c_1 \& c_2)}{\text{sum}(c_1 \mid c_2)} \).

Usage

```r
clujaccard(c1,c2,zerobyzero=NA)
```

Arguments

- `c1` logical or 0-1-vector.
- `c2` logical or 0-1-vector (same length).
- `zerobyzero` result if \( \text{sum}(c_1 \mid c_2)=0 \).

Value

Numeric between 0 and 1.

Author(s)

Christian Hennig <christian.hennig@unibo.it> https://www.unibo.it/sitoweb/christian.hennig/en/
Examples

```r
c1 <- rep(TRUE,10)
c2 <- c(FALSE,rep(TRUE,9))
clujaccard(c1,c2)
```

Description

A rough approximation of the expectation of the number of times a well separated fixed point cluster (FPC) of size \( n \) is found in \( ir \) fixed point iterations of `fixreg`.

Usage

```r
clusexpect(n, p, cn, ir)
```

Arguments

- \( n \): positive integer. Total number of points.
- \( p \): positive integer. Number of independent variables.
- \( cn \): positive integer smaller or equal to \( n \). Size of the FPC.
- \( ir \): positive integer. Number of fixed point iterations.

Details

The approximation is based on the assumption that a well separated FPC is found iff all \( p+2 \) points of the initial configuration come from the FPC. The value is \( ir \) times the probability for this. For a discussion of this assumption cf. Hennig (2002).

Value

A number.

Author(s)

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References


See Also

- `fixreg`
Examples

```
round(clusexpect(500,4,150,2000), digits = 2)
```

---

**clustatsum**

*Compute and format cluster validation statistics*

**Description**

`clustatsum` computes cluster validation statistics by running `cqcluster.stats`, and potentially `distrsimilarity`, and collecting some key statistics values with a somewhat different nomenclature.

This was implemented as a helper function for use inside of `clusterbenchstats` and `cgrestandard`.

**Usage**

```
clustatsum(datadist = NULL, clustering, noisecluster = FALSE, 
datanp = NULL, npstats = FALSE, useboot = FALSE, 
bootclassif = NULL, 
bootmethod = "nselectboot", 
bootruns = 25, cbmethod = NULL, methodpars = NULL, 
distmethod = NULL, dnnk = 2, 
pamcrit = TRUE, ...)
```

**Arguments**

- `datadist`: distances on which validation-measures are based, dist object or distance matrix. If NULL, this is computed from datanp; at least one of datadist and datanp must be specified.
- `clustering`: an integer vector of length of the number of cases, which indicates a clustering. The clusters have to be numbered from 1 to the number of clusters.
- `noisecluster`: logical. If TRUE, it is assumed that the largest cluster number in clustering denotes a ‘noise class’, i.e. points that do not belong to any cluster. These points are not taken into account for the computation of all functions of within and between cluster distances including the validation indexes.
- `datanp`: optional observations times variables data matrix, see npstats.
- `npstats`: logical. If TRUE, `distrsimilarity` is called and the two statistics computed there are added to the output. These are based on datanp and require datanp to be specified.
- `useboot`: logical. If TRUE, a stability index (either nselectboot or prediction.strength) will be involved.
- `bootclassif`: If useboot=TRUE, a string indicating the classification method to be used with the stability index, see the classification argument of nselectboot and prediction.strength.
bootmethod either "nselectboot" or "prediction.strength"; stability index to be used if useboot=TRUE.

bootruns integer. Number of resampling runs. If useboot=TRUE, passed on as B to nselectboot or M to prediction.strength.

cbmethod CBI-function (see kmeansCBI); clustering method to be used for stability assessment if useboot=TRUE.

methodpars parameters to be passed on to cbmethod.

distmethod logical. In case of useboot=TRUE indicates whether cbmethod will interpret data as distances.

dnnk nnk-argument to be passed on to distrsimilarity.

pamcrit pamcrit-argument to be passed on to cqcluster.stats.

... further arguments to be passed on to cqcluster.stats.

Value

clustatsum returns a list. The components, as listed below, are outputs of summary.cquality with default parameters, which means that they are partly transformed versions of those given out by cqcluster.stats, i.e., their range is between 0 and 1 and large values are good. Those from distrsimilarity are computed with largeisgood=TRUE, correspondingly.

avewithin average distance within clusters (reweighted so that every observation, rather than every distance, has the same weight).

mnnd average distance to n nkth nearest neighbour within cluster.

cvnnd coefficient of variation of dissimilarities to n nkth nearest within-cluster neighbour, measuring uniformity of within-cluster densities, weighted over all clusters, see Sec. 3.7 of Hennig (2019).

maxdiameter maximum cluster diameter.

widestgap widest within-cluster gap or average of cluster-wise widest within-cluster gap, depending on parameter averagegap.

sindex separation index, see argument sepindex.

minsep minimum cluster separation.

asw average silhouette width. See silhouette.

dindex this index measures to what extent the density decreases from the cluster mode to the outskirts; I-densdec in Sec. 3.6 of Hennig (2019).

denscut this index measures whether cluster boundaries run through density valleys; I-densbound in Sec. 3.6 of Hennig (2019).

highdgap this measures whether there is a large within-cluster gap with high density on both sides; I-highdgap in Sec. 3.6 of Hennig (2019).

pearsongamma correlation between distances and a 0-1-vector where 0 means same cluster, 1 means different clusters. "Normalized gamma" in Halkidi et al. (2001).

withinss a generalisation of the within clusters sum of squares (k-means objective function), which is obtained if d is a Euclidean distance matrix. For general distance measures, this is half the sum of the within cluster squared dissimilarities divided by the cluster size.
clustatsum

entropy entropy of the distribution of cluster memberships, see Meila(2007).
panc average distance to cluster centroid.
kdnorm Kolmogorov distance between distribution of within-cluster Mahalanobis distances and appropriate chi-squared distribution, aggregated over clusters (I am grateful to Agustin Mayo-Iscar for the idea).
kdunif Kolmogorov distance between distribution of distances to nnkth nearest within-cluster neighbor and appropriate Gamma-distribution, see Byers and Raftery (1998), aggregated over clusters.
boot if useboot=TRUE, stability value; stabk for method nselectboot; mean.pred for method prediction.strength.

Author(s)

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References


See Also
cqcluster.stats,distrsimilarity

Examples

set.seed(20000)
options(digits=3)
face <- rFace(20,dMoNo=2,dNoEy=0,p=2)
dface <- dist(face)
complete3 <- cutree(hclust(dface),3)
clustatsum(dface,complete3)
Run many clustering methods on many numbers of clusters

Description

Runs a user-specified set of clustering methods (CBI-functions, see kmeansCBI with several numbers of clusters on a dataset with unified output.

Usage

cluster.magazine(data,G,diss = inherits(data, "dist"),
    scaling=TRUE, clustermethod,
    distmethod=rep(TRUE,length(clustermethod)),
    ncinput=rep(TRUE,length(clustermethod)),
    clustermethodpars,
    trace=TRUE)

Arguments

data data matrix or dist-object.
G vector of integers. Numbers of clusters to consider.
diss logical. If TRUE, the data matrix is assumed to be a distance/dissimilarity matrix, otherwise it’s observations times variables.
scaling either a logical or a numeric vector of length equal to the number of columns of data. If FALSE, data won’t be scaled, otherwise scaling is passed on to scale as argumentscale.
clustermethod vector of strings specifying names of CBI-functions (see kmeansCBI). These are the clustering methods to be applied.
distmethod vector of logicals, of the same length as clustermethod. TRUE means that the clustering method operates on distances. If diss=TRUE, all entries have to be TRUE. Otherwise, if an entry is true, the corresponding method will be applied on dist(data).
ncinput vector of logicals, of the same length as clustermethod. TRUE indicates that the corresponding clustering method requires the number of clusters as input and will not estimate the number of clusters itself.
clustermethodpars list of the same length as clustermethod. Specifies parameters for all involved clustering methods. Its jth entry is passed to clustermethod number k. Can be an empty entry in case all defaults are used for a clustering method. The number of clusters does not need to be specified here.
trace logical. If TRUE, some runtime information is printed.
Value

List of lists comprising:

- **output**: Two-dimensional list. The first list index i is the number of the clustering method (ordering as specified in *clustermethod*), the second list index j is the number of clusters. This stores the full output of *clustermethod* i run on number of clusters j.

- **clustering**: Two-dimensional list. The first list index i is the number of the clustering method (ordering as specified in *clustermethod*), the second list index j is the number of clusters. This stores the clustering integer vector (i.e., the partition-component of the CBI-function, see *kmeansCBI*) of *clustermethod* i run on number of clusters j.

- **noise**: Two-dimensional list. The first list index i is the number of the clustering method (ordering as specified in *clustermethod*), the second list index j is the number of clusters. List entries are single logicals. If TRUE, the clustering method estimated some noise, i.e., points not belonging to any cluster, which in the clustering vector are indicated by the highest number (number of clusters plus one in case that the number of clusters was fixed).

- **othernc**: List of integer vectors of length 2. The first number is the number of the clustering method (the order is determined by argument *clustermethod*), the second number is the number of clusters for those methods that estimate the number of clusters themselves and estimate a number that is smaller than min(G) or larger than max(G).

Author(s)

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References


See Also

- clusterbenchstats, kmeansCBI

Examples

```r
set.seed(20000)
options(digits=3)
face <- rFace(10,dMoNo=2,dNoEy=0,p=2)
clustermethod=c("kmeansCBI","hclustCBI","hclustCBI")
# A clustering method can be used more than once, with different parameters
clustermethodpars <- list()
```
cluster.stats <- cluster.stats(d = NULL, clustering, alt.clustering = NULL, noisecluster=FALSE, silhouette = TRUE, G2 = FALSE, G3 = FALSE, wgap=TRUE, sepindex=TRUE, sepprob=0.1, sepwithnoise=TRUE, compareonly = FALSE, aggregateonly = FALSE)
cluster.stats

G3 logical. If TRUE, the index G3 (cf. Gordon (1999), p. 62) is computed. This executes sort on all distances and can be extremely slow.

wgap logical. If TRUE, the widest within-cluster gaps (largest link in within-cluster minimum spanning tree) are computed. This is used for finding a good number of clusters in Hennig (2013).

sepindex logical. If TRUE, a separation index is computed, defined based on the distances for every point to the closest point not in the same cluster. The separation index is then the mean of the smallest proportion sepprob of these. This allows to formalise separation less sensitive to a single or a few ambiguous points. The output component corresponding to this is sindex, not separation! This is used for finding a good number of clusters in Hennig (2013).

sepprob numerical between 0 and 1, see sepindex.

sepwithnoise logical. If TRUE and sepindex and noisecluster are both TRUE, the noise points are incorporated as cluster in the separation index (sepindex) computation. Also they are taken into account for the computation for the minimum cluster separation.

compareonly logical. If TRUE, only the corrected Rand index and Meila’s VI are computed and given out (this requires alt.clustering to be specified).

aggregateonly logical. If TRUE (and not compareonly), no clusterwise but only aggregated information is given out (this cuts the size of the output down a bit).

Value

cluster.stats returns a list containing the components n, cluster.number, cluster.size, min.cluster.size, noisen, diameter, average.distance, median.distance, separation, average.toother, separation.matrix, average.between, average.within, n.between, n.within, within.cluster.ss, clus.avg.silwidths, avg.silwidth, g2, g3, pearsongamma, dunn, entropy, wb.ratio, ch, cwidgap, widestgap, sindex, corrected.rand, vi except if compareonly=TRUE, in which case only the last two components are computed.

n number of cases.

cluster.number number of clusters.

cluster.size vector of cluster sizes (number of points).

min.cluster.size size of smallest cluster.

noisen number of noise points, see argument noisecluster (noisen=0 if noisecluster=FALSE).

diameter vector of cluster diameters (maximum within cluster distances).

average.distance vector of clusterwise within cluster average distances.

median.distance vector of clusterwise within cluster distance medians.

separation vector of clusterwise minimum distances of a point in the cluster to a point of another cluster.

average.toother vector of clusterwise average distances of a point in the cluster to the points of other clusters.
separation.matrix
matrix of separation values between all pairs of clusters.

ave.between.matrix
matrix of mean dissimilarities between points of every pair of clusters.

average.between
average distance between clusters.

average.within average distance within clusters (rewighted so that every observation, rather than every distance, has the same weight).

n.between number of distances between clusters.

n.within number of distances within clusters.

max.diameter maximum cluster diameter.

min.separation minimum cluster separation.

within.cluster.ss
a generalisation of the within clusters sum of squares (k-means objective function), which is obtained if d is a Euclidean distance matrix. For general distance measures, this is half the sum of the within cluster squared dissimilarities divided by the cluster size.

clus.avg.silwidths vector of cluster average silhouette widths. See silhouette.

avg.silwidth average silhouette width. See silhouette.

G2

G3

pearsongamma correlation between distances and a 0-1-vector where 0 means same cluster, 1 means different clusters. "Normalized gamma" in Halkidi et al. (2001).

dunn minimum separation / maximum diameter. Dunn index, see Halkidi et al. (2002).

dunn2 minimum average dissimilarity between two cluster / maximum average within cluster dissimilarity, another version of the family of Dunn indexes.

entropy entropy of the distribution of cluster memberships, see Meila(2007).

wb.ratio average.within/average.between.

CH
Calinski and Harabasz index (Calinski and Harabasz 1974, optimal in Milligan and Cooper 1985; generalised for dissimilarites in Hennig and Liao 2013).

cwidegap vector of widest within-cluster gaps.

widestgap widest within-cluster gap.

sindex separation index, see argument sepindex.

corrected.rand corrected Rand index (if alt.clustering has been specified), see Gordon (1999, p. 198).

vi variation of information (VI) index (if alt.clustering has been specified), see Meila (2007).

Note
Because cluster.stats processes a full dissimilarity matrix, it isn’t suitable for large data sets. You may consider distcritmulti in that case.
Author(s)

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References


See Also

cccluster.stats is a more sophisticated version of cluster.stats with more options. silhouette, dist, calinhara, distcritmulti. clusterboot computes clusterwise stability statistics by re-sampling.

Examples

```r
set.seed(20000)
options(digits=3)
face <- rFace(200,dMoNo=2,dNoEy=0,p=2)
dface <- dist(face)
complete3 <- cutree(hclust(dface),3)
cluster.stats(dface,complete3,
           alt.clustering=as.integer(attr(face,"grouping")))
```
cluster.varstats  Variablewise statistics for clusters

Description

This function gives some helpful variable-wise information for cluster interpretation, given a clustering and a data set. The output object contains some tables. For categorical variables, tables compare clusterwise distributions with overall distributions. Continuous variables are categorised for this.

If desired, tables, histograms, some standard statistics of continuous variables and validation plots as available through discrproj (Hennig 2004) are given out on the fly.

Usage

cluster.varstats(clustering, vardata, contdata=vardata, clusterwise=TRUE, tablevar=NULL, catvar=NULL, quantvar=NULL, catvarcats=10, proportions=FALSE, projmethod="none", minsize=ncol(contdata)+2, ask=TRUE, rangefactor=1)

## S3 method for class 'varwisetables'
print(x, digits=3, ...)

Arguments

clustering  vector of integers. Clustering (needs to be in standard coding, 1,2,...).
vardata  data matrix or data frame of which variables are summarised.
contdata  variable matrix or data frame, normally all or some variables from vardata, on which cluster visualisation by projection methods is performed unless projmethod="none". It should make sense to interpret these variables in a quantitative (interval-scaled) way.
clusterwise  logical. If FALSE, only the output tables are computed but no more detail and graphs are given on the fly.
tablevar  vector of integers. Numbers of variables treated as categorical (i.e., no histograms and statistics, just tables) if clusterwise=TRUE. Note that an error will be produced by factor type variables unless they are declared as categorical here.
catvar  vector of integers. Numbers of variables to be categorised by proportional quantiles for table computation. Recommended for all continuous variables.
quantvar  vector of integers. Variables for which means, standard deviations and quantiles should be given out if clusterwise=TRUE.
catvarcats  integer. Number of categories used for categorisation of variables specified in quantvar.
proportions logical. If TRUE, output tables contain proportions, otherwise numbers of observations.

projmethod one of "none", "dc", "bc", "vbc", "mvdc", "adc", "awc" (recommended if not "none"), "arc", "nc", "wnc", "anc". Cluster validation projection method introduced in Hennig (2004), passed on as method argument in discrproj.

minsize integer. Projection is not carried out for clusters with fewer points than this. (If this is chosen smaller, it may lead to errors with some projection methods.)

ask logical. If TRUE, par(ask=TRUE) is set in the beginning to prompt the user before plots and par(ask=FALSE) in the end.

rangefactor numeric. Factor by which to multiply the range for projection plot ranges.

x an object of class "varwisetables", output object of cluster.varstats.

digits integer. Number of digits after the decimal point to print out.

Value

An object of class "varwisetables", which is a list with a table for each variable, giving (categorised) marginal distributions by cluster.

Author(s)

Christian Hennig <christian.hennig@unibo.it> https://www.unibo.it/sitoweb/christian.hennig/en

References


Examples

set.seed(112233)
options(digits=3)
require(MASS)
require(flexmix)
data(Cars93)
Cars934 <- Cars93[,c(3,5,8,10)]
cc <-
discrete.recode(Cars934,xvarsorted=FALSE,continuous=c(2,3),discrete=c(1,4))
fcc <- flexmix(cc$data=1,k=2,
model=lcmixed(continuous=2,discrete=2,ppdim=c(6,3),diagonal=TRUE))
cv <-
cluster.varstats(fcc@cluster,Cars934, contdata=Cars934[,c(2,3)],
tablevar=c(1,4),catvar=c(2,3),quantvar=c(2,3),projmethod="awc",
ask=FALSE)
print(cv)
Description

This runs the methodology explained in Hennig (2019), Akhanli and Hennig (2020). It runs a user-specified set of clustering methods (CBI-functions, see \texttt{kmeansCBI}) with several numbers of clusters on a dataset, and computes many cluster validation indexes. In order to explore the variation of these indexes, random clusterings on the data are generated, and validation indexes are standardised by use of the random clusterings in order to make them comparable and differences between values interpretable.

The function \texttt{print.valstat} can be used to provide weights for the cluster validation statistics, and will then compute a weighted validation index that can be used to compare all clusterings.

See the examples for how to get the indexes A1 and A2 from Akhanli and Hennig (2020).

Usage

\begin{verbatim}
clusterbenchstats(data,G,diss = inherits(data, "dist"),
    scaling=TRUE, clustermethod,
    methodnames=clustermethod,
    distmethod=rep(TRUE,length(clustermethod)),
    ncinput=rep(TRUE,length(clustermethod)),
    clustermethodpars,
    npstats=FALSE,
    useboot=FALSE,
    bootclassif=NULL,
    bootmethod="nselectboot",
    bootruns=25,
    trace=TRUE,
    pamcrit=TRUE,snnk=2,
    dnnk=2,
    nnrns=100,kmrns=100,fnrns=100,avenrns=100,
    multicore=FALSE,cores=detectCores()-1,
    useallmethods=TRUE,
    useallg=FALSE,...)
\end{verbatim}

\texttt{print(x,...)}

Arguments

- **data**: data matrix or \texttt{dist}-object.
- **G**: vector of integers. Numbers of clusters to consider.
- **diss**: logical. If \texttt{TRUE}, the data matrix is assumed to be a distance/dissimilarity matrix, otherwise it’s observations times variables.
scaling: either a logical or a numeric vector of length equal to the number of columns of data. If FALSE, data won’t be scaled, otherwise scaling is passed on to scale as arguments.

clustermethod: vector of strings specifying names of CBI-functions (see `kmeansCBI`). These are the clustering methods to be applied.

methodnames: vector of strings with user-chosen names for clustering methods, one for every method in clustermethod. These can be used to distinguish different methods run by the same CBI-function but with different parameter values such as complete and average linkage for `hclustCBI`.

distmethod: vector of logicals, of the same length as clustermethod. TRUE means that the clustering method operates on distances. If diss=TRUE, all entries have to be TRUE. Otherwise, if an entry is true, the corresponding method will be applied on dist(data).

ncinput: vector of logicals, of the same length as clustermethod. TRUE indicates that the corresponding clustering method requires the number of clusters as input and will not estimate the number of clusters itself. Only methods for which this is TRUE can be used with useboot=TRUE.

clustermethodpars: list of the same length as clustermethod. Specifies parameters for all involved clustering methods. Its jth entry is passed to clustermethod number k. Can be an empty entry in case all defaults are used for a clustering method. However, the last entry is not allowed to be empty (you may just set a parameter of the last clustering method to its default value if you don’t want to specify anything else)! The number of clusters does not need to be specified here.

npsstats: logical. If TRUE, `distrsimilarity` is called and the two validity statistics computed there are added. These require diss=FALSE.

useboot: logical. If TRUE, a stability index (either nselectboot or prediction.strength) will be involved.

boottclassif: If useboot=TRUE, a vector of strings indicating the classification methods to be used with the stability index for the different methods indicated in clustermethods, see the classification argument of nselectboot and prediction.strength.

boottmethod: either "nselectboot" or "prediction.strength"; stability index to be used if useboot=TRUE.

boottruns: integer. Number of resampling runs. If useboot=TRUE, passed on as B to nselectboot or M to prediction.strength. Note that these are applied to all kmruns+nnruns+avennruns+fnruns random clusterings on top of the regular ones, which may take a lot of time if bootruns and these values are chosen large.

trace: logical. If TRUE, some runtime information is printed.

pamcrit: logical. If TRUE, the average distance of points to their respective cluster centroids is computed (criterion of the PAM clustering method, validation criterion pamc); centroids are chosen so that they minimise this criterion for the given clustering. Passed on to cqcluster.stats.

snnk: integer. Number of neighbours used in coefficient of variation of distance to nearest within cluster neighbour, the cvnnd-statistic (clusters with snnk or fewer points are ignored for this). Passed on to cqcluster.stats as argument snk.
dnnk  
integer. Number of nearest neighbors to use for dissimilarity to the uniform in case that npstats=TRUE; nnk-argument to be passed on to distrsimilarity.

nnruns  
integer. Number of runs of stupidknn (random clusterings). With useboot=TRUE one may want to choose this lower than the default for reasons of computation time.

kmruns  
integer. Number of runs of stupidcentroids (random clusterings). With useboot=TRUE one may want to choose this lower than the default for reasons of computation time.

fnruns  
integer. Number of runs of stupidkfn (random clusterings). With useboot=TRUE one may want to choose this lower than the default for reasons of computation time.

avenruns  
integer. Number of runs of stupidkaven (random clusterings). With useboot=TRUE one may want to choose this lower than the default for reasons of computation time.

multicore  
logical. If TRUE, parallel computing is used through the function mclapply from package parallel; read warnings there if you intend to use this; it won’t work on Windows.

cores  
integer. Number of cores for parallelisation.

useallmethods  
logical, to be passed on to cgrestandard. If FALSE, only random clustering results are used for standardisation. If TRUE, clustering results from all methods are used.

useallg  
logical to be passed on to cgrestandard. If TRUE, standardisation uses results from all numbers of clusters in G. If FALSE, standardisation of results for a specific number of clusters only uses results from that number of clusters.

...  
further arguments to be passed on to cqcluster.stats through clustatsum (no effect in print.clusterbenchstats).

x  
one object of class "clusterbenchstats".

Value

The output of clusterbenchstats is a big list of lists comprising lists cm, stat, sim, qstat, sstat

- cm  
output object of cluster.magazine, see there for details. Clustering of all methods and numbers of clusters on the dataset data.

- stat  
one object of class "valstat", see valstat.object for details. Unstandardised cluster validation statistics.

- sim  
output object of randomclustersim, see there. Validity indexes from random clusterings used for standardisation of validation statistics on data.

- qstat  
one object of class "valstat", see valstat.object for details. Cluster validation statistics standardised by random clusterings, output of cgrestandard based on percentages, i.e., with percentage=TRUE.
sstat object of class "valstat", see valstat.object for details. Cluster validation statistics standardised by random clusterings, output of cgrestandard based on mean and standard deviation (called Z-score standardisation in Akhanli and Hennig (2020), i.e., with percentage=FALSE.

Note

This may require a lot of computing time and also memory for datasets that are not small, as most indexes require computation and storage of distances.

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References


See Also

valstat.object, cluster.magazine, kmeansCBI, cqcluster.stats, clustatsum, cgrestandard

Examples

set.seed(20000)
options(digits=3)
face <- rFace(10,dMoNo=2,dNoEy=0,p=2)
clustermethod=c("kmeansCBI","hclustCBI")
# A clustering method can be used more than once, with different parameters
clustermethodpars <- list()
clustermethodpars[[2]] <- list()
clustermethodpars[[2]]$method <- "average"
# Last element of clustermethodpars needs to have an entry!
methodname <- c("kmeans","average")
cbs <- clusterbenchstats(face,G=2:3,clustermethod=clustermethod,
methodname=methodname,distmethod=rep(FALSE,2),
clustermethodpars=clustermethodpars,nnruns=1,kmruns=1,fnruns=1,avenruns=1)
print(cbs)
print(cbs$qstat,aggregate=TRUE,weights=c(1,0,0,0,1,0,1,0,1,0,0,0,1,1))
# The weights are weights for the validation statistics ordered as in
cbs$qstat$statistics for computation of an aggregated index, see
# ?print.valstat.
# Now using bootstrap stability assessment as in Akhanli and Hennig (2020):
cb <- clusterbenchstats(face,G=2:3,clustermethod=clustermethod,
methodname=methodname,distmethod=rep(FALSE,2),
clustermethodpars=clustermethodpars,
useboot=TRUE,bootclassif=bootclassif,bootmethod="nselectboot",
bootruns=2,nnruns=1,kmruns=1,fnruns=1,avenruns=1,useallg=TRUE)
print(cbsboot)
## Not run:
# Index A1 in Akhanli and Hennig (2020) (need these weights choices):
print(cbsboot$sstat,aggregate=TRUE,weights=c(1,0,0,0,0,0,0,0,1,0,0,0,1,0,0,1,0))
# Index A2 in Akhanli and Hennig (2020) (need these weights choices):
print(cbsboot$sstat,aggregate=TRUE,weights=c(0,0,0,0,1,1,0,0,0,0,0,0,1,0,0,1,0))
## End(Not run)
# Results from nselectboot:
plot(cbsboot$stat,cbsboot$sim,statistic="boot")

---

**Description**

Assessment of the clusterwise stability of a clustering of data, which can be cases*variables or dissimilarity data. The data is resampled using several schemes (bootstrap, subsetting, jittering, replacement of points by noise) and the Jaccard similarities of the original clusters to the most similar clusters in the resampled data are computed. The mean over these similarities is used as an index of the stability of a cluster (other statistics can be computed as well). The methods are described in Hennig (2007).

clusterboot is an integrated function that computes the clustering as well, using interface functions for various clustering methods implemented in R (several interface functions are provided, but you can implement further ones for your favourite clustering method). See the documentation of the input parameter clustermethod below.

Quite general clustering methods are possible, i.e. methods estimating or fixing the number of clusters, methods producing overlapping clusters or not assigning all cases to clusters (but declaring them as "noise"). Fuzzy clusterings cannot be processed and have to be transformed to crisp clusterings by the interface function.

**Usage**

```r
clusterboot(data,B=100, distances=(inherits(data, "dist")),
bootmethod="boot",
bscompare=TRUE,
multipleboot=FALSE,
jittertuning=0.05, noisetuning=c(0.05,4),
subtuning=floor(nrow(data)/2),
```

---
clusterboot

clustermethod,noisemethod=FALSE,count=TRUE,
showplots=FALSE,dissolution=0.5,
recover=0.75,seed=NULL,datatomatrix=TRUE,...)

## S3 method for class 'clboot'
print(x,statistics=c("mean","dissolution","recovery"),...)

## S3 method for class 'clboot'
plot(x,xlim=c(0,1),breaks=seq(0,1,by=0.05),...)

Arguments

data by default something that can be coerced into a (numerical) matrix (data frames
with non-numerical data are allowed when using datatomatrix=FALSE, see be-
low). The data matrix - either an n*p-data matrix (or data frame) or an n*n-
dissimilarity matrix (or dist-object).

B integer. Number of resampling runs for each scheme, see bootmethod.

distances logical. If TRUE, the data is interpreted as dissimilarity matrix. If data is a
dist-object, distances=TRUE automatically, otherwise distances=FALSE by
default. This means that you have to set it to TRUE manually if data is a dissim-
ilarity matrix.

bootmethod vector of strings, defining the methods used for resampling. Possible methods:
"boot": nonparametric bootstrap (precise behaviour is controlled by parameters
bscompare and multipleboot).
"subset": selecting random subsets from the dataset. Size determined by
subtuning.
"noise": replacing a certain percentage of the points by random noise, see
noisetuning.
"jitter": add random noise to all points, see jittertuning. (This didn't per-
form well in Hennig (2007), but you may want to get your own experience.)
"bojit" nonparametric bootstrap first, and then adding noise to the points, see
jittertuning.

Important: only the methods "boot" and "subset" work with dissimilarity

The results in Hennig (2007) indicate that "boot" is generally informative and
often quite similar to "subset" and "bojit", while "noise" sometimes pro-
vides different information. Therefore the default (for distances=FALSE) is to
use "boot" and "noise". However, some clustering methods may have prob-
lems with multiple points, which can be solved by using "bojit" or "subset" instead of "boot" or by multipleboot=FALSE below.

bscompare logical. If TRUE, multiple points in the bootstrap sample are taken into account to
compute the Jaccard similarity to the original clusters (which are represented by
their "bootstrap versions", i.e., the points of the original cluster which also occur
in the bootstrap sample). If a point was drawn more than once, it is in the "boot-
strap version" of the original cluster more than once, too, if bscompare=TRUE.
Otherwise multiple points are ignored for the computation of the Jaccard similar-
ities. If multipleboot=FALSE, it doesn't make a difference.
multipleboot logical. If FALSE, all points drawn more than once in the bootstrap draw are only used once in the bootstrap samples.

jittertuning positive numeric. Tuning for the "jitter"-method. The noise distribution for jittering is a normal distribution with zero mean. The covariance matrix has the same Eigenvectors as that of the original data set, but the standard deviation along the principal directions is determined by the jittertuning-quantile of the distances between neighboring points projected along these directions.

noisetuning A vector of two positive numerics. Tuning for the "noise"-method. The first component determines the probability that a point is replaced by noise. Noise is generated by a uniform distribution on a hyperrectangle along the principal directions of the original data set, ranging from -noisetuning[2] to noisetuning[2] times the standard deviation of the data set along the respective direction. Note that only points not replaced by noise are considered for the computation of Jaccard similarities.

subtuning integer. Size of subsets for "subset".

clustermethod an interface function (the function name, not a string containing the name, has to be provided!). This defines the clustering method. See the "Details"-section for a list of available interface functions and guidelines how to write your own ones.

noisemethod logical. If TRUE, the last cluster is regarded as "noise cluster", which means that for computing the Jaccard similarity, it is not treated as a cluster. The noise cluster of the original clustering is only compared with the noise cluster of the clustering of the resampled data. This means that in the clusterboot-output (and plot), if points were assigned to the noise cluster, the last cluster number refers to it, and its Jaccard similarity values refer to comparisons with estimated noise components in resampled datasets only. (Some cluster methods such as tclust and mclustBIC produce such noise components.)

count logical. If TRUE, the resampling runs are counted on the screen.

showplots logical. If TRUE, a plot of the first two dimensions of the resampled data set (or the classical MDS solution for dissimilarity data) is shown for every resampling run. The last plot shows the original data set. Ignored if datatomatrix=FALSE.

dissolution numeric between 0 and 1. If the Jaccard similarity between the resampling version of the original cluster and the most similar cluster on the resampled data is smaller or equal to this value, the cluster is considered as "dissolved". Numbers of dissolved clusters are recorded.

recover numeric between 0 and 1. If the Jaccard similarity between the resampling version of the original cluster and the most similar cluster on the resampled data is larger than this value, the cluster is considered as "successfully recovered". Numbers of recovered clusters are recorded.

seed integer. Seed for random generator (fed into set.seed) to make results reproducible. If NULL, results depend on chance.

datatomatrix logical. If TRUE, data is coerced into a (numerical) matrix at the start of clusterboot. FALSE may be chosen for mixed type data including e.g. categorical factors (assuming that the chosen clustermethod allows for this). This disables some features of clusterboot, see parameters bootmethod and showplots.
... additional parameters for the clustermethods called by clusterboot. No effect in print.clboot and plot.clboot.

x object of class clboot.

statistics specifies in print.clboot, which of the three clusterwise Jaccard similarity statistics "mean", "dissolution" (number of times the cluster has been dissolved) and "recovery" (number of times a cluster has been successfully recovered) is printed.

xlim transferred to hist.

breaks transferred to hist.

Details

Here are some guidelines for interpretation. There is some theoretical justification to consider a Jaccard similarity value smaller or equal to 0.5 as an indication of a "dissolved cluster", see Hennig (2008). Generally, a valid, stable cluster should yield a mean Jaccard similarity value of 0.75 or more. Between 0.6 and 0.75, clusters may be considered as indicating patterns in the data, but which points exactly should belong to these clusters is highly doubtful. Below average Jaccard values of 0.6, clusters should not be trusted. "Highly stable" clusters should yield average Jaccard similarities of 0.85 and above. All of this refers to bootstrap; for the other resampling schemes it depends on the tuning constants, though their default values should grant similar interpretations in most cases.

While B=100 is recommended, smaller run numbers could give quite informative results as well, if computation times become too high.

Note that the stability of a cluster is assessed, but stability is not the only important validity criterion - clusters obtained by very inflexible clustering methods may be stable but not valid, as discussed in Hennig (2007). See plotcluster for graphical cluster validation.

Information about interface functions for clustering methods:

The following interface functions are currently implemented (in the present package; note that almost all of these functions require the specification of some control parameters, so if you use one of them, look up their common help page kmeansCBI) first:

kmeansCBI an interface to the function kmeans for k-means clustering. This assumes a cases*variables matrix as input.

hclustCBI an interface to the function hclust for agglomerative hierarchical clustering with optional noise cluster. This function produces a partition and assumes a cases*variables matrix as input.

hclusttreeCBI an interface to the function hclust for agglomerative hierarchical clustering. This function produces a tree (not only a partition; therefore the number of clusters can be huge!) and assumes a cases*variables matrix as input.

disthclustCBI an interface to the function hclust for agglomerative hierarchical clustering with optional noise cluster. This function produces a partition and assumes a dissimilarity matrix as input.

noisemclustCBI an interface to the function mclustBIC for normal mixture model based clustering. This assumes a cases*variables matrix as input. Warning: mclustBIC sometimes has problems with multiple points. It is recommended to use this only together with multipleboot=FALSE.
**distnoisemclustCBI** an interface to the function `mclustBIC` for normal mixture model based clustering. This assumes a dissimilarity matrix as input and generates a data matrix by multidimensional scaling first. Warning: `mclustBIC` sometimes has problems with multiple points. It is recommended to use this only together with `multipleboot=FALSE`.

**claraCBI** an interface to the functions `pam` and `clara` for partitioning around medoids. This can be used with cases*variables as well as dissimilarity matrices as input.

**pamkCBI** an interface to the function `pamk` for partitioning around medoids. The number of cluster is estimated by the average silhouette width. This can be used with cases*variables as well as dissimilarity matrices as input.

**tclustCBI** an interface to the function `tclust` in the tclust library for trimmed Gaussian clustering. This assumes a cases*variables matrix as input. Note that this function is not currently provided because the tclust package is only available in the CRAN archives, but the code is in the Examples-section of the `kmeansCBI`-help page.

**dbscanCBI** an interface to the function `dbscan` for density based clustering. This can be used with cases*variables as well as dissimilarity matrices as input.

**mahalCBI** an interface to the function `fixmahal` for fixed point clustering. This assumes a cases*variables matrix as input.

**mergenormCBI** an interface to the function `mergenormals` for clustering by merging Gaussian mixture components.

**speccCBI** an interface to the function `specc` for spectral clustering.

You can write your own interface function. The first argument of an interface function should preferably be a data matrix (of class "matrix", but it may be a symmetrical dissimilarity matrix). It can be a data frame, but this restricts some of the functionality of `clusterboot`, see above. Further arguments can be tuning constants for the clustering method. The output of an interface function should be a list containing (at least) the following components:

- **result** clustering result, usually a list with the full output of the clustering method (the precise format doesn’t matter); whatever you want to use later.
- **nc** number of clusters. If some points don’t belong to any cluster but are declared as "noise", `nc` includes the noise cluster, and there should be another component `nc1`, being the number of clusters not including the noise cluster (note that it is not mandatory to define a noise component if not all points are assigned to clusters, but if you do it, the stability of the noise cluster is assessed as well.)
- **clusterlist** this is a list consisting of a logical vectors of length of the number of data points (n) for each cluster, indicating whether a point is a member of this cluster (TRUE) or not. If a noise cluster is included, it should always be the last vector in this list.
- **partition** an integer vector of length n, partitioning the data. If the method produces a partition, it should be the clustering. This component is only used for plots, so you could do something like `rep(1,n)` for non-partitioning methods. If a noise cluster is included, `nc=nc1+1` and the noise cluster is cluster no. `nc`.
- **clustermethod** a string indicating the clustering method.

**Value**

`clusterboot` returns an object of class "clboot", which is a list with components `result`, `partition`, `nc`, `clustermethod`, `B`, `noisemethod`, `bootmethod`, `multipleboot`, `dissolution`, `recover`, `bootresult`,...
bootmean, bootbrd, bootrecover, jitterresult, jittermean, jitterbrd, jitterrecover, 
subsetresult, subsetmean, subsetbrd, subsetrecover, bojitresult, bojitmean, bojitbrd, 
bojitrecover, noiseresult, noisemean, noisebrd, noiserecover.

result: clustering result; full output of the selected clustermethod for the original data set.
partition: partition parameter of the selected clustermethod (note that this is only meaningful for partitioning clustering methods).
nc: number of clusters in original data (including noise component if noisemethod=TRUE).
nccl: number of clusters in original data (not including noise component if noisemethod=TRUE).
clustermethod, B, noisemethod, bootmethod, multipleboot, dissolution, recover
input parameters, see above.
bootresult: matrix of Jaccard similarities for bootmethod="boot". Rows correspond to clusters in the original data set. Columns correspond to bootstrap runs.
bootmean: clusterwise means of the bootresult.
bootbrd: clusterwise number of times a cluster has been dissolved.
bootrecover: clusterwise number of times a cluster has been successfully recovered.
subsetresult, subsetmean, etc.: same as bootresult, bootmean, etc., but for the other resampling methods.

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References

See Also
dist, interface functions: kmeansCBI, hclustCBI, hclusttreeCBI, disthclustCBI, noisemclustCBI, distnoisemclustCBI, claraCBI, pamkCBI, dbscanCBI, mahalCBI

Examples
options(digits=3)
set.seed(20000)
face <- rFace(50,dMoNo=2,dNoEy=0,p=2)
cl <- clusterboot(face,B=3,bootmethod=
c("boot","noise","jitter"),clustermethod=kmeansCBI,
krange=5,seed=15555)

print(cl)
plot(cf1)

cf2 <- clusterboot(dist(face),B=3,bootmethod="subset",clustermethod=disthclustCBI,
k=5, cut="number", method="average", showplots=TRUE, seed=15555)
print(cf2)
d1 <- c("a", "b", "a", "c")
d2 <- c("a", "a", "a", "b")
dx <- as.data.frame(cbind(d1,d2))
cpx <- clusterboot(dx,k=2,B=10,clustermethod=claraCBI,
multipleboot=TRUE,usepam=TRUE,datatomatrix=FALSE)
print(cpx)

```r

Description

Generates tuning constants \( c_a \) for `fixmahal` dependent on the number of points and variables of the current fixed point cluster (FPC).

This is experimental and only thought for use in `fixmahal`.

Usage

```r

```c

Arguments

- `n`, `p`, `nmin`, `cmin`, `nc1`, `c1 = cmin`, `q = 1`

Details

Some experiments suggest that the tuning constant \( c_a \) should decrease with increasing FPC size and increase with increasing \( p \) in `fixmahal`. This is to prevent too small meaningless FPCs while maintaining the significant larger ones. `cmahal` with \( q=1 \) computes \( c_a \) in such a way that as long as \( c_a < c_{min} \), the decrease in \( n \) is as steep as possible in order to maintain the validity of the convergence theorem in Hennig and Christlieb (2002).`
con.comp

Value
A numeric vector of length n, giving the values for ca for all FPC sizes smaller or equal to n.

Author(s)
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References

See Also
fixmahal

Examples
plot(1:100, cmahal(100, 3, nmin=5, cmin=qchisq(0.99, 3), nc1=90),
     xlab="FPC size", ylab="cmahal")

con.comp  Connectivity components of an undirected graph

Description
Computes the connectivity components of an undirected graph from a matrix giving the edges.

Usage
con.comp(comat)

Arguments
comat a symmetric logical or 0-1 matrix, where comat[i,j]=TRUE means that there is an edge between vertices i and j. The diagonal is ignored.

Details
The "depth-first search" algorithm of Cormen, Leiserson and Rivest (1990, p. 477) is used.

Value
An integer vector, giving the number of the connectivity component for each vertex.
**confusion**

**Description**

Estimates a misclassification probability in a mixture distribution between two mixture components from estimated posterior probabilities regardless of component parameters, see Hennig (2010).

**Usage**

```r
confusion(z, pro, i, j, adjustprobs = FALSE)
```

**Arguments**

- `z`: matrix of posterior probabilities for observations (rows) to belong to mixture components (columns), so entries need to sum up to 1 for each row.
- `pro`: vector of component proportions, need to sum up to 1.
- `i`: integer. Component number.
- `adjustprobs`: logical. If `TRUE`, probabilities are initially standardised so that those for components `i` and `j` add up to one (i.e., if they were the only components).

**Examples**

```r
set.seed(1000)
x <- rnorm(20)
m <- matrix(0, nrow = 20, ncol = 20)
for(i in 1:20)
  for(j in 1:20)
    m[i, j] <- abs(x[i] - x[j])
d <- m < 0.2
c <- con.comp(d)
max(c) # number of connectivity components
plot(x, c)
# The same should be produced by
# cutree(hclust(as.dist(m), method = "single"), h = 0.2).
```
Value

Estimated probability that an observation generated by component \( j \) is classified to component \( i \) by maximum a posteriori rule.

Author(s)

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References


Examples

```r
set.seed(12345)
m <- rpois(20, lambda=5)
dim(m) <- c(5,4)
pro <- apply(m, 2, sum)
pro <- pro/sum(pro)
m <- m/apply(m, 1, sum)
round(confusion(m, pro, 1, 2), digits=2)
```

---

cov.wml | Weighted Covariance Matrices (Maximum Likelihood)

Description

Returns a list containing estimates of the weighted covariance matrix and the mean of the data, and optionally of the (weighted) correlation matrix. The covariance matrix is divided by the sum of the weights, corresponding to \( n \) and the ML-estimator in the case of equal weights, as opposed to \( n-1 \) for \texttt{cov.wt}.

Usage

```r
cov.wml(x, wt = rep(1/nrow(x), nrow(x)), cor = FALSE, center = TRUE)
```

Arguments

- **x**
  
a matrix or data frame. As usual, rows are observations and columns are variables.

- **wt**
  
a non-negative and non-zero vector of weights for each observation. Its length must equal the number of rows of \( x \).

- **cor**
  
A logical indicating whether the estimated correlation weighted matrix will be returned as well.
center  Either a logical or a numeric vector specifying the centers to be used when computing covariances. If TRUE, the (weighted) mean of each variable is used, if FALSE, zero is used. If center is numeric, its length must equal the number of columns of x.

Value

A list containing the following named components:

cov        the estimated (weighted) covariance matrix.
center     an estimate for the center (mean) of the data.
n.obs      the number of observations (rows) in x.
wt         the weights used in the estimation. Only returned if given as an argument.
cor        the estimated correlation matrix. Only returned if ‘cor’ is ‘TRUE’.

Author(s)

Christian Hennig <christian.hennig@unibo.it> https://www.unibo.it/sitoweb/christian.hennig/en/

See Also

cov.wt, cov, var

Examples

x <- c(1,2,3,4,5,6,7,8,9,10)
y <- c(1,2,3,8,7,6,5,8,9,10)
cov.wml(cbind(x,y),wt=c(0,0,0,1,1,1,1,1,0,0))
cov.wt(cbind(x,y),wt=c(0,0,0,1,1,1,1,1,0,0))

cqcluster.stats  Cluster validation statistics (version for use with clusterbenchstats)

Description

This is a more sophisticated version of cluster.stats for use with clusterbenchstats, see Hennig (2017). Computes a number of distance-based statistics, which can be used for cluster validation, comparison between clusterings and decision about the number of clusters: cluster sizes, cluster diameters, average distances within and between clusters, cluster separation, biggest within cluster gap, average silhouette widths, the Calinski and Harabasz index, a Pearson version of Hubert’s gamma coefficient, the Dunn index, further statistics introduced in Hennig (2017) and two indexes to assess the similarity of two clusterings, namely the corrected Rand index and Meila’s VI.
Usage

cqcluster.stats(d = NULL, clustering, alt.clustering = NULL,
  noisecluster = FALSE,
  silhouette = TRUE, G2 = FALSE, G3 = FALSE, wgap = TRUE, sepindex = TRUE,
  sepprob = 0.1, sepwithnoise = TRUE, compareonly = FALSE,
  aggregateonly = FALSE,
  averagegap=FALSE, pamcrit=TRUE,
  dquantile=0.1,
  nnkdist=TRUE, nnk=2, standardisation="max", sepall=TRUE, maxk=10,
  cvstan=sqrt(length(clustering)))

## S3 method for class 'cquality'
summary(object,stanbound=TRUE,largeisgood=TRUE, ...)

## S3 method for class 'summary.cquality'
print(x, ...)

Arguments

d a distance object (as generated by dist) or a distance matrix between cases.
clustering an integer vector of length of the number of cases, which indicates a clustering.
The clusters have to be numbered from 1 to the number of clusters.
alt.clustering an integer vector such as for clustering, indicating an alternative clustering.
  If provided, the corrected Rand index and Meila's VI for clustering vs.
  alt.clustering are computed.
noisecluster logical. If TRUE, it is assumed that the largest cluster number in clustering
denotes a 'noise class', i.e. points that do not belong to any cluster. These points
are not taken into account for the computation of all functions of within and
between cluster distances including the validation indexes.
silhouette logical. If TRUE, the silhouette statistics are computed, which requires package
cluster.
is computed. This executes lots of sorting algorithms and can be very slow (it
has been improved by R. Francois - thanks!)
G3 logical. If TRUE, the index G3 (cf. Gordon (1999), p. 62) is computed. This
executes sort on all distances and can be extremely slow.
wgap logical. If TRUE, the widest within-cluster gaps (largest link in within-cluster
minimum spanning tree) are computed. This is used for finding a good number
of clusters in Hennig (2013). See also parameter averagegap.
sepindex logical. If TRUE, a separation index is computed, defined based on the distances
for every point to the closest point not in the same cluster. The separation index
is then the mean of the smallest proportion sepprob of these. This allows to
formalise separation less sensitive to a single or a few ambiguous points. The
output component corresponding to this is sindex, not separation! This is
used for finding a good number of clusters in Hennig (2013). See also parameter sepall.

sepprob
  numerical between 0 and 1, see sepindex.

sepwithnoise
  logical. If TRUE and sepindex and noisecluster are both TRUE, the noise points are incorporated as cluster in the separation index (sepindex) computation. Also they are taken into account for the computation for the minimum cluster separation.

compareonly
  logical. If TRUE, only the corrected Rand index and Meila's VI are computed and given out (this requires alt.clustering to be specified).

aggregateonly
  logical. If TRUE (and not compareonly), no clusterwise but only aggregated information is given out (this cuts the size of the output down a bit).

averagegap
  logical. If TRUE, the average of the widest within-cluster gaps over all clusters is given out; if FALSE, the maximum is given out.

pamcrit
  logical. If TRUE, the average distance of points to their respective cluster centroids is computed (criterion of the PAM clustering method); centroids are chosen so that they minimise this criterion for the given clustering.

dquantile
  numerical between 0 and 1; quantile used for kernel density estimator for density indexes, see Hennig (2019), Sec. 3.6.

nndist
  logical. If TRUE, average distance to nnkth nearest neighbour within cluster is computed.

nnk
  integer. Number of neighbours used in average and coefficient of variation of distance to nearest within cluster neighbour (clusters with nnk or fewer points are ignored for this).

standardisation
  "none", "max", "ave", "q90", or a number. See details.

sepall
  logical. If TRUE, a fraction of smallest sepprob distances to other clusters is used from every cluster. Otherwise, a fraction of smallest sepprob distances overall is used in the computation of sindex.

maxk
  numeric. Parsimony is defined as the number of clusters divided by maxk.

cvstan
  numeric. cvnnd is standardised by cvstan if there is standardisation, see Details.

object
  object of class cquality, output of cqcluster.stats.

x
  object of class cquality, output of cqcluster.stats.

stanbound
  logical. If TRUE, all index values larger than 1 will be set to 1, and all values smaller than 0 will be set to 0. This is for preparation in case of largeisgood=TRUE (if values are already suitably standardised within cqcluster.stats, it won't do harm and can do good).

largeisgood
  logical. If TRUE, indexes x are transformed to 1-x in case that before transformation smaller values indicate a better clustering (that's average.within, mnd, widestgap, within.cluster.ss, dindex, denscut, pamc, max.diameter, highdgap, cvnnd. For this to make sense, cqcluster.stats should be run with standardisation="max" and summary.cquality with stanbound=TRUE.

... no effect.
Details

The standardisation-parameter governs the standardisation of the index values. standardisation="none" means that unstandardised raw values of indexes are given out. Otherwise, entropy will be standardised by the maximum possible value for the given number of clusters; within.cluster.ss and between.cluster.ss will be standardised by the overall sum of squares; mnn will be standardised by the maximum distance to the nnk nearest neighbour within cluster; pearsongamma will be standardised by adding 1 and dividing by 2; cvnn will be standardised by cvstan (the default is the possible maximum).

standardisation allows options for the standardisation of average.within, sindex, wgap, pamcrit, max.diameter, min.separation and can be "max" (maximum distance), "ave" (average distance), q90 (0.9-quantile of distances), or a positive number. "max" is the default and standardises all the listed indexes into the range [0,1].

Value

cqcluster.stats with compareonly=FALSE and aggregateonly=FALSE returns a list of type cquality containing the components n, cluster.number, cluster.size, min.cluster.size, noisen, diameter, average.distance, median.distance, separation, average.toother, separation.matrix, ave.between.matrix, average.between, average.within, n.between, n.within, max.diameter, min.separation, within.cluster.ss, clus.avg sillwidths, avg sillwidth, g2, g3, pearsongamma, dunn, dunn2, entropy, wb.ratio, ch, cwidegap, widestgap, corrected.rand, vi, sindex, svec, psep, stan, nnk, mnn, pamc, pamcentroids, dindex, denscut, highdgap, npenalty, dpenalty, withindensp, densoc, pdistto, pclsetomode, distto, percdens, percndensoc, parsimony, cvnnd, cvnndc. Some of these are standardised, see Details. If compareonly=TRUE, only corrected.rand, vi are given out. If aggregateonly=TRUE, only n, cluster.number, min.cluster.size, noisen, diameter, average.between, average.within, max.diameter, min.separation, within.cluster.ss, clus.avg sillwidth, avg sillwidth, g2, g3, pearsongamma, dunn, dunn2, entropy, wb.ratio, ch, cwidegap, widestgap, corrected.rand, vi, sindex, svec, psep, stan, nnk, mnn, pamc, pamcentroids, dindex, denscut, highdgap, parsimony, cvnnd, cvnndc are given out.

summary.cquality returns a list of type summary.cquality with components average.within, nnk, mnn, avg sillwidth, widestgap, sindex, pearsongamma, entropy, pamc, within.cluster.ss, dindex, denscut, highdgap, parsimony, max.diameter, min.separation, cvnnd. These are as documented below for cqcluster.stats, but after transformation by stanbound and largeisgood, see arguments.

n
number of points.

cluster.number
number of clusters.

cluster.size
vector of cluster sizes (number of points).

min.cluster.size
size of smallest cluster.

noisen
number of noise points, see argument noisecluster (noisen=0 if noisecluster=FALSE).

diameter
vector of cluster diameters (maximum within cluster distances).

average.distance
vector of clusterwise within cluster average distances.

median.distance
vector of clusterwise within cluster distance medians.
separation vector of clusterwise minimum distances of a point in the cluster to a point of another cluster.

average.toother vector of clusterwise average distances of a point in the cluster to the points of other clusters.

separation.matrix matrix of separation values between all pairs of clusters.

ave.between.matrix matrix of mean dissimilarities between points of every pair of clusters.

avebetween average distance between clusters.

avewithin average distance within clusters (reweighted so that every observation, rather than every distance, has the same weight).

n.between number of distances between clusters.

n.within number of distances within clusters.

maxdiameter maximum cluster diameter.

minsep minimum cluster separation.

withinss a generalisation of the within clusters sum of squares (k-means objective function), which is obtained if d is a Euclidean distance matrix. For general distance measures, this is half the sum of the within cluster squared dissimilarities divided by the cluster size.

clus.avg.silwidths vector of cluster average silhouette widths. See silhouette.

asw average silhouette width. See silhouette.


g3 G3 coefficient. See Gordon (1999, p. 62).

pearsongamma correlation between distances and a 0-1-vector where 0 means same cluster, 1 means different clusters. "Normalized gamma" in Halkidi et al. (2001).

dunn minimum separation / maximum diameter. Dunn index, see Halkidi et al. (2002).

dunn2 minimum average dissimilarity between two cluster / maximum average within cluster dissimilarity, another version of the family of Dunn indexes.

entropy entropy of the distribution of cluster memberships, see Meila(2007).

wb.ratio average.within/average.between.

ch Calinski and Harabasz index (Calinski and Harabasz 1974, optimal in Milligan and Cooper 1985; generalised for dissimilarites in Hennig and Liao 2013).

cwidegap vector of widest within-cluster gaps.

widestgap widest within-cluster gap or average of cluster-wise widest within-cluster gap, depending on parameter averagegap.

corrected.rand corrected Rand index (if alt.clustering has been specified), see Gordon (1999, p. 198).

vi variation of information (VI) index (if alt.clustering has been specified), see Meila (2007).
sindex: separation index, see argument sepindex.

svec: vector of smallest closest distances of points to next cluster that are used in the computation of sindex if sepall=TRUE.

psep: vector of all closest distances of points to next cluster.

stan: value by which som statistics were standardised, see Details.

nnk: value of input parameter nnk.

mnd: average distance to nnkth nearest neighbour within cluster.

pamc: average distance to cluster centroid.

pamcentroids: index numbers of cluster centroids.

dindex: this index measures to what extent the density decreases from the cluster mode to the outskirts; I-densdec in Sec. 3.6 of Hennig (2019); low values are good.

denscut: this index measures whether cluster boundaries run through density valleys; I-densbound in Sec. 3.6 of Hennig (2019); low values are good.

highdgap: this measures whether there is a large within-cluster gap with high density on both sides; I-highdgap in Sec. 3.6 of Hennig (2019); low values are good.

npenalty: vector of penalties for all clusters that are used in the computation of denscut, see Hennig (2019) (these are sums of penalties over all points in the cluster).

depenalty: vector of penalties for all clusters that are used in the computation of dindex, see Hennig (2019) (these are sums of several penalties for density increase when going from the mode outward in the cluster).

withindensp: distance-based kernel density values for all points as computed in Sec. 3.6 of Hennig (2019).

densoc: contribution of points from other clusters than the one to which a point is assigned to the density, for all points; called h_o in Sec. 3.6 of Hennig (2019).

pdistto: list that for all clusters has a sequence of point numbers. These are the points already incorporated in the sequence of points constructed in the algorithm in Sec. 3.6 of Hennig (2019) to which the next point to be joined is connected.

pclosetomode: list that for all clusters has a sequence of point numbers. Sequence of points to be incorporated in the sequence of points constructed in the algorithm in Sec. 3.6 of Hennig (2019).

distto: list that for all clusters has a sequence of differences between the standardised densities (see percwdens) at the new point added and the point to which it is connected (if this is positive, the penalty is this to the square), in the algorithm in Sec. 3.6 of Hennig (2019).

percwdens: this is withindensp divided by its maximum.

percdensoc: this is densoc divided by the maximum of withindensp, called h_o^* in Sec. 3.6 of Hennig (2019).

parsimony: number of clusters divided by maxk.

cvnn: coefficient of variation of dissimilarities to nnkth nearest within-cluster neighbour, measuring uniformity of within-cluster densities, weighted over all clusters, see Sec. 3.7 of Hennig (2019).

cvnnec: vector of cluster-wise coefficients of variation of dissimilarities to nnkth nearest within-cluster neighbour as required in computation of cvnn.
Note
Because `cqcluster.stats` processes a full dissimilarity matrix, it isn’t suitable for large data sets. You may consider `distcritmulti` in that case.

Author(s)
Christian Hennig <christian.hennig@unibo.it> https://www.unibo.it/sitoweb/christian.hennig/en/

References

See Also
`cluster.stats`, `silhouette`, `dist`, `calinhara`, `distcritmulti`. `clusterboot` computes clusterwise stability statistics by resampling.

Examples
```r
set.seed(20000)
options(digits=3)
```
cvnn <- rFace(200, dMoNo=2, dNoEy=0, p=2)
dface <- dist(face)
complete3 <- cutree(hclust(dface), 3)
cqcluster.stats(dface, complete3, 
    alt.clustering=as.integer(attr(face, "grouping")))

---

### cvnn

**Cluster validation based on nearest neighbours**

### Description

Cluster validity index based on nearest neighbours as defined in Liu et al. (2013) with a correction explained in Halkidi et al. (2015).

### Usage

```r
cvnn(d=NULL, clusterings, k=5)
```

### Arguments

- **d**: dissimilarity matrix or `dist`-object.
- **clusterings**: list of vectors of integers with length `nrow(d)`; indicating the cluster for each observation for several clusterings (list elements) to be compared.
- **k**: integer. Number of nearest neighbours.

### Value

List with components (see Liu et al. (2013), Halkidi et al. (2015) for details)

- **cvnnindex**: vector of index values for the various clusterings, see Liu et al. (2013), the lower the better.
- **sep**: vector of separation values.
- **comp**: vector of compactness values.

### Author(s)

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### References


cweight

Examples

options(digits=3)
iriss <- as.matrix(iris[c(1:10,51:55,101:105),-5])
irisc <- as.numeric(iris[c(1:10,51:55,101:105),5])
print(cvnn(dist(iriss),list(irisc,rep(1:4,5))))

cweight

Weight function for AWC

Description

For use in awcoord only.

Usage

cweight(x, ca)

Arguments

x numerical.
ca numerical.

Value

cia/x if smaller than 1, else 1.

Author(s)

Christian Hennig <christian.hennig@unibo.it> https://www.unibo.it/sitoweb/christian.
hennig/en/

See Also

awcoord

Examples

cweight(4,1)
**dbscan**  

**DBSCAN density reachability and connectivity clustering**

**Description**

Generates a density based clustering of arbitrary shape as introduced in Ester et al. (1996).

**Usage**

```r
dbscan(data, eps, MinPts = 5, scale = FALSE, method = c("hybrid", "raw", "dist"), seeds = TRUE, showplot = FALSE, countmode = NULL)
```

## S3 method for class 'dbscan'

1. `print(x, ...)`
2. `plot(x, data, ...)`
3. `predict(object, data, newdata = NULL, predict.max=1000, ...)`

**Arguments**

- **data**: data matrix, data.frame, dissimilarity matrix or dist-object. Specify method="dist" if the data should be interpreted as dissimilarity matrix or object. Otherwise Euclidean distances will be used.
- **eps**: Reachability distance, see Ester et al. (1996).
- **MinPts**: Reachability minimum no. of points, see Ester et al. (1996).
- **scale**: scale the data if TRUE.
- **method**: "dist" treats data as distance matrix (relatively fast but memory expensive), "raw" treats data as raw data and avoids calculating a distance matrix (saves memory but may be slow), "hybrid" expects also raw data, but calculates partial distance matrices (very fast with moderate memory requirements).
- **seeds**: FALSE to not include the isseed-vector in the dbscan-object.
- **showplot**: 0 = no plot, 1 = plot per iteration, 2 = plot per subiteration.
- **countmode**: NULL or vector of point numbers at which to report progress.
- **x**: object of class dbscan.
- **object**: object of class dbscan.
- **newdata**: matrix or data.frame with raw data to predict.
- **predict.max**: max. batch size for predictions.
- **...**: Further arguments transferred to plot methods.
Details

Clusters require a minimum number of points (MinPts) within a maximum distance (eps) around one of its members (the seed). Any point within eps around any point which satisfies the seed condition is a cluster member (recursively). Some points may not belong to any clusters (noise).

We have clustered a 100,000 x 2 dataset in 40 minutes on a Pentium M 1600 MHz.

print.dbscan shows a statistic of the number of points belonging to the clusters that are seeds and border points.

plot.dbscan distinguishes between seed and border points by plot symbol.

Value

predict.dbscan gives out a vector of predicted clusters for the points in newdata.

dbscan gives out an object of class 'dbscan' which is a LIST with components

cluster integer vector coding cluster membership with noise observations (singletons) coded as 0
isseed logical vector indicating whether a point is a seed (not border, not noise)
eps parameter eps
MinPts parameter MinPts

Note

this is a simplified version of the original algorithm (no K-D-trees used), thus we have \( o(n^2) \) instead of \( o(n \times \log(n)) \)

Author(s)

Jens Oehlschlaegel, based on a draft by Christian Hennig.

References


Examples

```r
set.seed(665544)
n <- 600
x <- cbind(runif(10, 0, 10)+rnorm(n, sd=0.2), runif(10, 0, 10)+rnorm(n, sd=0.2))
par(bg="grey40")
ds <- dbscan(x, 0.2)
# run with showplot=1 to see how dbscan works.
ds
plot(ds, x)
```
\begin{verbatim}
x2 <- matrix(0,nrow=4,ncol=2)
x2[1,] <- c(5,2)
x2[2,] <- c(8,3)
x2[3,] <- c(4,4)
x2[4,] <- c(9,9)
predict(ds, x, x2)

n <- 600
x <- cbind((1:3)+rnorm(n, sd=0.2), (1:3)+rnorm(n, sd=0.2))

# Not run, but results from my machine are 0.105 - 0.068 - 0.255:
# system.time(ds <- dbscan(x, 0.3, countmode=NULL, method="raw"))[3]
# system.time(dsb <- dbscan(x, 0.3, countmode=NULL, method="hybrid"))[3]
# system.time(dsc <- dbscan(dist(x), 0.3, countmode=NULL,
#     method="dist"))[3]
\end{verbatim}

dipp.tantrum

Simulates p-value for dip test

Description

Simulates p-value for dip test (see dip) in the way suggested by Tantrum, Murua and Stuetzle (2003) from the closest unimodal distribution determined by kernel density estimation with bandwidth chosen so that the density just becomes unimodal. This is less conservative (and in fact sometimes anti-conservative) than the values from dip.test.

Usage

dipp.tantrum(xdata,d,M=100)

Arguments

\textbf{xdata} numeric vector. One-dimensional dataset.
\textbf{d} numeric. Value of dip statistic.
\textbf{M} integer. Number of artificial datasets generated in order to estimate the p-value.

Value

List with components

\textbf{p.value} approximated p-value.
\textbf{bw} borderline unimodality bandwith in density with default settings.
\textbf{dv} vector of dip statistic values from simulated artificial data.

Author(s)

Christian Hennig <christian.hennig@unibo.it> https://www.unibo.it/sitoweb/christian.hennig/en/
References


Examples

```r
# not run, requires package diptest
# x <- runif(100)
# d <- dip(x)
# dt <- dipp.tantrum(x,d,M=10)
```

---

**diptest.multi**  
*Diptest for discriminant coordinate projection*

**Description**

Diptest (Hartigan and Hartigan, 1985, see `dip`) for data projected in discriminant coordinate separating optimally two class means (see `discrcoord`) as suggested by Tantrum, Murua and Stuetzle (2003).

**Usage**

```r
diptest.multi(xdata,class,pvalue="uniform",M=100)
```

**Arguments**

- `xdata`  
  matrix. Potentially multidimensional dataset.

- `class`  
  vector of integers giving class numbers for observations.

- `pvalue`  
  "uniform" or "tantrum". Defines whether the p-value is computed from a uniform null model as suggested in Hartigan and Hartigan (1985, using `dip.test`) or as suggested in Tantrum et al. (2003, using `dipp.tantrum`).

- `M`  
  integer. Number of artificial datasets generated in order to estimate the p-value if `pvalue="tantrum"`.

**Value**

The resulting p-value.

**Author(s)**

Christian Hennig <christian.hennig@unibo.it>  
discrcoord

References


Examples

```r
require(diptest)
x <- cbind(runif(100),runif(100))
partition <- 1+(x[,1]<0.5)
d1 <- diptest.multi(x,partition)
d2 <- diptest.multi(x,partition,pvalue="tantrum",M=10)
```

```
require(diptest)
x <- cbind(runif(100),runif(100))
```

---

**discrcoord**

*Discriminant coordinates/canonical variates*

**Description**

Computes discriminant coordinates, sometimes referred to as "canonical variates" as described in Seber (1984).

**Usage**

```
discrcoord(xd, clvecd, pool = "n", ...)
```

**Arguments**

- **xd**: the data matrix; a numerical object which can be coerced to a matrix.
- **clvecd**: integer vector of class numbers; length must equal nrow(xd).
- **pool**: string. Determines how the within classes covariance is pooled. "n" means that the class covariances are weighted corresponding to the number of points in each class (default). "equal" means that all classes get equal weight.
- **...**: no effect

**Details**

The matrix $T$ (see Seber (1984), p. 270) is inverted by use of `tdecomp`, which can be expected to give reasonable results for singular within-class covariance matrices.

**Value**

List with the following components

- **ev**: eigenvalues in descending order.
- **units**: columns are coordinates of projection basis vectors. New points $x$ can be projected onto the projection basis vectors by $x \times \%\% units$
- **proj**: projections of $xd$ onto units.
Author(s)

Christian Hennig <christian.hennig@unibo.it> https://www.unibo.it/sitoweb/christian.hennig/en/

References


See Also

plotcluster for straight forward discriminant plots.

batcoord for discriminating projections for two classes, so that also the differences in variance are shown (discrcoord is based only on differences in mean).

rFace for generation of the example data used below.

Examples

```r
set.seed(4634)
fce <- rFace(600,dMoNo=2,dNoEy=0)
grface <- as.integer(attr(fce,"grouping"))
dcf <- discrcoord(fce,grface)
plot(dcf$proj,col=grface)
# ...done in one step by function plotcluster.
```

---

discrete.recode  Recodes mixed variables dataset

Description

Recodes a dataset with mixed continuous and categorical variables so that the continuous variables come first and the categorical variables have standard coding 1, 2, 3,... (in lexicographical ordering of values coerced to strings).

Usage

discrete.recode(x,xvarsorted=TRUE,continuous=0,discrete)

Arguments

- **x**  data matrix or data frame. The data need to be organised case-wise, i.e., if there are categorical variables only, and 15 cases with values c(1,1,2) on the 3 variables, the data matrix needs 15 rows with values 1 1 2. (Categorical variables could take numbers or strings or anything that can be coerced to factor levels as values.)

- **xvarsorted**  logical. If TRUE, the continuous variables are assumed to be the first ones, and the categorical variables to be behind them.
continuous vector of integers giving positions of the continuous variables. If xvarsorted=TRUE, a single integer, number of continuous variables.

 discrete vector of integers giving positions of the categorical variables (the variables need to be coded in such a way that data.matrix converts them to something numeric). If xvarsorted=TRUE, a single integer, number of categorical variables.

Value

A list with components

data data matrix with continuous variables first and categorical variables in standard coding behind them.

ppdim vector of categorical variable-wise numbers of categories.

discretelevels list of levels of the categorical variables belonging to what is treated by flexmixedruns as category 1, 2, 3 etc.

continuous number of continuous variables.

discrete number of categorical variables.

Author(s)

Christian Hennig <christian.hennig@unibo.it> https://www.unibo.it/sitoweb/christian.hennig/en

See Also

lcmixed

Examples

set.seed(776655)
v1 <- rnorm(20)
v2 <- rnorm(20)
d1 <- sample(c(2,4,6,8),20,replace=TRUE)
d2 <- sample(1:4,20,replace=TRUE)
data <- cbind(v1,d1,v2,d2)
lc <-
discrete.recode(data,xvarsorted=FALSE,continuous=c(1,3),discrete=c(2,4))
require(MASS)
data(Cars93)
Cars934 <- Cars93[,c(3,5,8,10)]
cc <- discrete.recode(Cars934,xvarsorted=FALSE,continuous=c(2,3),discrete=c(1,4))
Linear dimension reduction for classification

Description
An interface for ten methods of linear dimension reduction in order to separate the groups optimally in the projected data. Includes classical discriminant coordinates, methods to project differences in mean and covariance structure, asymmetric methods (separation of a homogeneous class from a heterogeneous one), local neighborhood-based methods and methods based on robust covariance matrices.

Usage

discrproj(x, clvecd, method="dc", clnum=NULL, ignorepoints=FALSE, ignorenum=0, ...)  

Arguments

- `x`: the data matrix; a numerical object which can be coerced to a matrix.
- `clvecd`: vector of class numbers which can be coerced into integers; length must equal `nrow(xd)`.
- `method`: one of 
  - "dc" usual discriminant coordinates, see `discrcoord`, 
  - "bc" Bhattacharyya coordinates, first coordinate showing mean differences, second showing covariance matrix differences, see `batcoord`, 
  - "vbc" variance dominated Bhattacharyya coordinates, see `batcoord`, 
  - "mvdc" added meana and variance differences optimizing coordinates, see `mvdcoord`, 
  - "adc" asymmetric discriminant coordinates, see `adcoord`, 
  - "awc" asymmetric discriminant coordinates with weighted observations, see `awcoord`, 
  - "arc" asymmetric discriminant coordinates with weighted observations and robust MCD-covariance matrix, see `awcoord`, 
  - "nc" neighborhood based coordinates, see `ncoord`, 
  - "wnc" neighborhood based coordinates with weighted neighborhoods, see `ncoord`, 
  - "anc" asymmetric neighborhood based coordinates, see `ancoord`. 

Note that "bc", "vbc", "adc", "awc", "arc" and "anc" assume that there are only two classes.

- `clnum`: integer. Number of the class which is attempted to plot homogeneously by "asymmetric methods", which are the methods assuming that there are only two classes, as indicated above.

- `ignorepoints`: logical. If TRUE, points with label `ignorenum` in `clvecd` are ignored in the computation for `method` and are only projected afterwards onto the resulting units. If `pch=NULL`, the plot symbol for these points is "N".
ignorenum  one of the potential values of the components of clvecd. Only has effect if
ignorepoints=TRUE, see above.
...
additional parameters passed to the projection methods.

Value
discrproj returns the output of the chosen projection method, which is a list with at least the com-
ponents ev, units, proj. For detailed informations see the help pages of the projection methods.
ev      eigenvalues in descending order, usually indicating portion of information in the
        corresponding direction.
units  columns are coordinates of projection basis vectors. New points x can be pro-
        jected onto the projection basis vectors by x %*% units
proj     projections of xd onto units.

Author(s)
Christian Hennig <christian.hennig@unibo.it> https://www.unibo.it/sitoweb/christian.
hennig/en/

References
tional and Graphical Statistics 13, 930-945.
Press.

See Also
discrcoord, batcoord, mvdcoord, adcoord, awcoord, ncoord, ancoord.
rFace for generation of the example data used below.

Examples
set.seed(4634)
face <- rFace(300,dMoNo=2,dNoEy=0,p=3)
grface <- as.integer(attr(face,"grouping"))

# The abs in the following is there to unify the output,
# because eigenvectors are defined only up to their sign.
# Statistically it doesn't make sense to compute absolute values.
round(abs(discrproj(face,grface, method="nc")$units),digits=2)
round(abs(discrproj(face,grface, method="wnc")$units),digits=2)
round(abs(discrproj(face,grface, clnum=1, method="arc")$units),digits=2)
distancefactor

**Factor for dissimilarity of mixed type data**

**Description**

Computes a factor that can be used to standardise ordinal categorical variables and binary dummy variables coding categories of nominal scaled variables for Euclidean dissimilarity computation in mixed type data. See Hennig and Liao (2013).

**Usage**

```r
distancefactor(cat, n=NULL, catsizes=NULL, type="categorical", normfactor=2, qfactor=ifelse(type=="categorical", 1/2, 1/(1+1/(cat-1))))
```

**Arguments**

- `cat` integer. Number of categories of the variable to be standardised. Note that for type="categorical" the number of categories of the original variable is required, although the distancefactor is used to standardise dummy variables for the categories.
- `n` integer. Number of data points.
- `catsizes` vector of integers giving numbers of observations per category. One of `n` and `catsizes` must be supplied. If `catsizes=NULL`, `rep(round(n/cat), cat)` is used (this may be appropriate as well if numbers of observations of categories are unequal, if the researcher decides that the dissimilarity measure should not be influenced by empirical category sizes.
- `type` "categorical" if the factor is used for dummy variables belonging to a nominal variable, "ordinal" if the factor is used for an ordinal variable and standard Likert coding.
- `normfactor` numeric. Factor on which standardisation is based. As a default, this is \(E(X_1-X_2)^2=2\) for independent unit variance variables.
- `qfactor` numeric. Factor q in Hennig and Liao (2013) to adjust for clumping effects due to discreteness.

**Value**

A factor by which to multiply the variable in order to make it comparable to a unit variance continuous variable when aggregated in Euclidean fashion for dissimilarity computation, so that expected effective difference between two realisations of the variable equals `qfactor*normfactor`.

**Author(s)**

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References


See Also

lcmixed, pam

Examples

```r
set.seed(776655)
d1 <- sample(1:5,20,replace=TRUE)
d2 <- sample(1:4,20,replace=TRUE)
data <- cbind(d1,d2)
lc <- cat2bin(data,categorical=1)$data
lc[,1:5] <- lc[,1:5]*distancefactor(5,20,type="categorical")
lc[,6] <- lc[,6]*distancefactor(4,20,type="ordinal")
```

distcritmulti *Distance based validity criteria for large data sets*

Description

Approximates average silhouette width or the Pearson version of Hubert’s gamma criterion by hacking the dataset into pieces and averaging the subset-wise values, see Hennig and Liao (2013).

Usage

```r
distcritmulti(x,clustering,part=NULL,ns=10,criterion="asw", fun="dist",metric="euclidean", count=FALSE,seed=NULL, ...)
```

Arguments

- **x**: cases times variables data matrix.
- **clustering**: vector of integers indicating the clustering.
- **part**: vector of integer subset sizes; sum should be smaller or equal to the number of cases of x. If NULL, subset sizes are chosen approximately equal.
- **ns**: integer. Number of subsets, only used if part==NULL.
- **criterion**: "asw" or "pearsongamma", specifies whether the average silhouette width or the Pearson version of Hubert’s gamma is computed.
- **fun**: "dist" or "daisy", specifies which function is used for computing dissimilarities.
- **metric**: passed on to dist (as argument method) or daisy to determine which dissimilarity is used.
**distcritmulti**

- **count**: logical. If TRUE, the subset number just processed is printed.
- **seed**: integer, random seed. (If NULL, result depends on random numbers.)
- **...**: further arguments to be passed on to `dist` or `daisy`.

**Value**

A list with components `crit.overall`, `crit.sub`, `crit.sd`, `part`.

- **crit.overall**: value of criterion.
- **crit.sub**: vector of subset-wise criterion values.
- **crit.sd**: standard deviation of `crit.sub`, can be used to assess stability.
- **subsets**: list of case indexes in subsets.

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**References**


**See Also**

`cluster.stats`, `silhouette`

**Examples**

```r
set.seed(20000)
options(digits=3)
face <- rFace(50,dMoNo=2,dNoEy=0,p=2)
clustering <- as.integer(attr(face,"grouping"))
distcritmulti(face,clustering,ns=3,seed=100000,criterion="pearsongamma")
```
distrsimilarity

Similarity of within-cluster distributions to normal and uniform

Description

Two measures of dissimilarity between the within-cluster distributions of a dataset and normal or uniform distribution. For the normal it’s the Kolmogorov dissimilarity between the Mahalanobis distances to the center and a chi-squared distribution. For the uniform it is the Kolmogorov distance between the distance to the kth nearest neighbour and a Gamma distribution (this is based on Byers and Raftery (1998)). The clusterwise values are aggregated by weighting with the cluster sizes.

Usage

distrsimilarity(x,clustering,noisecluster = FALSE, distribution=c("normal","uniform"),nnk=2, largeisgood=FALSE,messages=FALSE)

Arguments

x 
the data matrix; a numerical object which can be coerced to a matrix.

clustering 
integer vector of class numbers; length must equal nrow(x), numbers must go from 1 to the number of clusters.

noisecluster 
logical. If TRUE, the cluster with the largest number is ignored for the computations.

distribution 
vector of "normal", "uniform" or both. Indicates which of the two dissimilarities is/are computed.

nnk 
integer. Number of nearest neighbors to use for dissimilarity to the uniform.

largeisgood 
logical. If TRUE, dissimilarities are transformed to 1-d (this means that larger values indicate a better fit).

messages 
logical. If TRUE, warnings are given if within-cluster covariance matrices are not invertible (in which case all within-cluster Mahalanobis distances are set to zero).

Value

List with the following components

kdnorm 
Kolmogorov distance between distribution of within-cluster Mahalanobis distances and appropriate chi-squared distribution, aggregated over clusters (I am grateful to Agustin Mayo-Iscar for the idea).

kdunif 
Kolmogorov distance between distribution of distances to nnkth nearest within-cluster neighbor and appropriate Gamma-distribution, see Byers and Raftery (1998), aggregated over clusters.

kdnormc 
vector of cluster-wise Kolmogorov distances between distribution of within-cluster Mahalanobis distances and appropriate chi-squared distribution.
kdunifc  
vector of cluster-wise Kolmogorov distances between distribution of distances to \( nnk \)th nearest within-cluster neighbor and appropriate Gamma-distribution.

xmahal  
vector of Mahalanobs distances to the respective cluster center.

xdknn  
vector of distance to \( nnk \)th nearest within-cluster neighbor.

**Note**

It is very hard to capture similarity to a multivariate normal or uniform in a single value, and both used here have their shortcomings. Particularly, the dissimilarity to the uniform can still indicate a good fit if there are holes or it’s a uniform distribution concentrated on several not connected sets.

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**References**


**See Also**

cqcluster.stats, cluster.stats for more cluster validity statistics.

**Examples**

```r
set.seed(20000)
options(digits=3)
face <- rFace(200,dMoNo=2,dNoEy=0,p=2)
km3 <- kmeans(face,3)
distrsimilarity(face,km3$cluster)
```

---

**dridgeline**  
*Density along the ridgeline*

**Description**

Computes the density of a two-component Gaussian mixture along the ridgeline (Ray and Lindsay, 2005), along which all its density extrema are located.

**Usage**

```r
dridgeline(alpha=seq(0,1,0.001), prop, mul, mu2, Sigma1, Sigma2, showplot=FALSE, ...)
```
Arguments

alpha sequence of values between 0 and 1 for which the density is computed.
prop mixture proportion of first component.
mu1 mean vector of component 1.
mu2 mean vector of component 2.
Sigma1 covariance matrix of component 1.
Sigma2 covariance matrix of component 2.
showplot logical. If TRUE, the density is plotted against alpha.
... further arguments to be passed on to plot.

Value

Vector of density values for values of alpha.

Author(s)

Christian Hennig <christian.hennig@unibo.it> https://www.unibo.it/sitoweb/christian.hennig/en/

References


Examples

```r
q <- dridgeline(seq(0,1,0.1),0.5,c(1,1),c(2,5),diag(2),diag(2))
```

---

**Duda-Hart test for splitting**

**Description**

Duda-Hart test for whether a data set should be split into two clusters.

**Usage**

```r
dudahart2(x, clustering, alpha=0.001)
```

**Arguments**

x data matrix or data frame.
clustering vector of integers. Clustering into two clusters.
alpha numeric between 0 and 1. Significance level (recommended to be small if this is used for estimating the number of clusters).
Value

A list with components

<table>
<thead>
<tr>
<th>Component</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>p.value</td>
<td>p-value against null hypothesis of homogeneity.</td>
</tr>
<tr>
<td>dh</td>
<td>Ratio of within-cluster sum of squares for two clusters and overall sum of squares.</td>
</tr>
<tr>
<td>compare</td>
<td>Critical value for dh at level alpha.</td>
</tr>
<tr>
<td>cluster1</td>
<td>TRUE/FALSE if the null hypothesis of homogeneity is rejected.</td>
</tr>
<tr>
<td>alpha</td>
<td>See above.</td>
</tr>
<tr>
<td>z</td>
<td>1-alpha-quantile of a standard Gaussian.</td>
</tr>
</tbody>
</table>

Author(s)

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References


See Also

cluster.stats

Examples

```r
options(digits=2)
set.seed(98765)
iriss <- iris[sample(150,20),-5]
km <- kmeans(iriss,2)
dudahart2(iriss,km$cluster)
```

```r
extract.mixturepars Extract parameters for certain components from mclust

Description

Extracts parameters of certain mixture components from the output of `summary.mclustBIC` and updates proportions so that they sum up to 1.

Usage

```r
extract.mixturepars(mclustsum,compproportions,noise=FALSE)
```

Arguments

- `mclustsum`: Output object of `summary.mclustBIC`.
- `compproportions`: Vector of integers. Numbers of mixture components.
- `noise`: Logical. Should be TRUE if a noise component was fitted by `mclustBIC`. 75
Value

Object as component parameters of `summary.mclustBIC`-output, but for specified components only. (Orientation information from all components is kept.)

Author(s)

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Examples

```r
set.seed(98765)
require(mclust)
iriss <- iris[sample(150,20),-5]
irisBIC <- mclustBIC(iriss,G=5,modelNames="VEV")
siris <- summary(irisBIC,iriss)
emp <- extract.mixturepars(siris,2)
emp$pro
round(emp$mean,digits=1)
emp$variance$modelName
round(emp$variance$scale,digits=2)
```

findrep

Finding representatives for cluster border

Description

Finds representative objects for the border of a cluster and the within-cluster variance as defined in the framework of the `cdbw` cluster validation index (and meant to be used in that context).

Usage

```r
findrep(x,xcen,clustering,cluster,r,p=ncol(x),n=nrow(x),
nc=sum(clustering==cluster))
```

Arguments

- `x` matrix. Euclidean dataset.
- `xcen` mean vector of cluster.
- `clustering` vector of integers with length = `nrow(x)`; indicating the cluster for each observation.
- `cluster` integer. Number of cluster to be treated.
- `r` integer. Number of representatives.
- `p` integer. Number of dimensions.
- `n` integer. Number of observations.
- `nc` integer. Number of observations in cluster.
Value

List with components

repc  vector of index of representatives (out of all observations).
repx  vector of index of representatives (out of only the observations in cluster).
maxr  number of representatives (this can be smaller than r if fewer pairwise different observations are in cluster).
wvar  estimated average within-cluster squared distance to mean.

Author(s)

Christian Hennig <christian.hennig@unibo.it> https://www.unibo.it/sitoweb/christian.hennig/en/

References


See Also
cdbw

Examples

options(digits=3)
iriss <- as.matrix(iris[c(1:5,51:55,101:105),-5])
irisc <- as.numeric(iris[c(1:5,51:55,101:105),5])
findrep(iriss,colMeans(iriss),irisc,cluster=1,r=2)

fixmahal  Mahalanobis Fixed Point Clusters

Description

Computes Mahalanobis fixed point clusters (FPCs), i.e., subsets of the data, which consist exactly of the non-outliers w.r.t. themselves, and may be interpreted as generated from a homogeneous normal population. FPCs may overlap, are not necessarily exhausting and do not need a specification of the number of clusters.

Note that while fixmahal has lots of parameters, only one (or few) of them have usually to be specified, cf. the examples. The philosophy is to allow much flexibility, but to always provide sensible defaults.
Usage

```r
fixmahal(dat, n = nrow(as.matrix(dat)), p = ncol(as.matrix(dat)),
method = "fuzzy", cgen = "fixed",
ca = NA, ca2 = NA,
calpha = ifelse(method=="fuzzy",0.95,0.99),
calpha2 = 0.995,
pointit = TRUE, subset = n,
ncl = 100+20*p,
startn = 18+p, mnc = floor(startn/2),
mer = ifelse(pointit,0.1,0),
distcut = 0.85, maxit = 5*n, iter = n*1e-5,
init.group = list(),
ind.storage = TRUE, countmode = 100,
plot = "none")
```

## S3 method for class 'mfpc'
summary(object, ...)

## S3 method for class 'summary.mfpc'
print(x, maxnc=30, ...)

## S3 method for class 'mfpc'
plot(x, dat, no, bw=FALSE, main=c("Representative FPC No. ",no),
  xlab=NULL, ylab=NULL,
pch=NULL, col=NULL, ...)

## S3 method for class 'mfpc'
fpcclusters(object, dat=NA, ca=object$ca, p=object$p, ...)

## S3 method for class 'mfpc'
fpmi(dat, n = nrow(as.matrix(dat)), p = ncol(as.matrix(dat)),
  gv, ca, ca2, method = "ml", plot,
  maxit = 5*n, iter = n*1e-6)
```

Arguments

dat something that can be coerced to a numerical matrix or vector. Data matrix, rows are points, columns are variables. `fpclusters.rfpc` does not need specification of `dat` if `fixmahal` has been run with `ind.storage=TRUE`.

n optional positive integer. Number of cases.

p optional positive integer. Number of independent variables.

method a string. method="classical" means 0-1 weighting of observations by Mahalanobis distances and use of the classical normal covariance estimator. method="ml" uses the ML-covariance estimator (division by n instead of n-1) This is used in Hennig and Christlieb (2002). method can also be "mcd" or "mve", to enforce the use of robust centers and covariance matrices, see `cov.rob`. This is experimental, not recommended at the moment, may be very slowly and requires
library lqs. The default is method="fuzzy", where weighted means and covariance matrices are used (Hennig, 2005). The weights are computed by wfu, i.e., a function that is constant 1 for arguments smaller than ca, 0 for arguments larger than ca2 and continuously linear in between. Convergence is only proven for method="ml" up to now.

cgen optional string. "fixed" means that the same tuning constant ca is used for all iterations. "auto" means that ca is generated dependently on the size of the current data subset in each iteration by cmahal. This is experimental.

cia optional positive number. Tuning constant, specifying required cluster separation. By default determined as calpha-quantile of the chisquared distribution with p degrees of freedom.

cia2 optional positive number. Second tuning constant needed if method="fuzzy". By default determined as calpha2-quantile of the chisquared distribution with p degrees of freedom.

calpha number between 0 and 1. See ca.

calpha2 number between 0 and 1, larger than calpha. See ca2.

pointit optional logical. If TRUE, subset fixed point algorithms are started from initial configurations, which are built around single points of the dataset, cf. mahalconf. Otherwise, initial configurations are only specified by init.group.

subset optional positive integer smaller or equal than n. Initial configurations for the fixed point algorithm (cf. mahalconf) are built from a subset of subset points from the data. No effect if pointit=FALSE. Default: all points.

nc1 optional positive integer. Tuning constant needed by cmahal to generate ca automatically. Only needed for cgen="auto".

startn optional positive integer. Size of the initial configurations. The default value is chosen to prevent that small meaningless FPCs are found, but it should be decreased if clusters of size smaller than the default value are of interest.

mnc optional positive integer. Minimum size of clusters to be reported.

mer optional nonnegative number. FPCs (groups of them, respectively, see details) are only reported as stable if the ratio of the number of their findings to their number of points exceeds mer. This holds under pointit=TRUE and subset=n. For subset<n, the ratio is adjusted, but for small subset, the results may extremely vary and have to be taken with care.

distcut optional value between 0 and 1. A similarity measure between FPCs, given in Hennig (2002), and the corresponding Single Linkage groups of FPCs with similarity larger than distcut are computed. A single representative FPC is selected for each group.

maxit optional integer. Maximum number of iterations per algorithm run (usually an FPC is found much earlier).

iter positive number. Algorithm stops when difference between subsequent weight vectors is smaller than iter. Only needed for method="fuzzy".

init.group optional list of logical vectors of length n. Every vector indicates a starting configuration for the fixed point algorithm. This can be used for datasets with high dimension, where the vectors of init.group indicate cluster candidates found
by graphical inspection or background knowledge, as in Hennig and Christlieb (2002).

**ind.storage**
optional logical. If TRUE, then all indicator vectors of found FPCs are given in the value of `fixmahal`. May need lots of memory, but is a bit faster.

**countmode**
optional positive integer. Every `countmode` algorithm runs `fixmahal` shows a message.

**plot**
optional string. If "start", you get a scatterplot of the first two variables to highlight the initial configuration, "iteration" generates such a plot at each iteration, "both" does both (this may be very time consuming). The default is "none".

**object**
object of class `mfpc`, output of `fixmahal`.

**x**
object of class `mfpc`, output of `fixmahal`.

**maxnc**
positive integer. Maximum number of FPCs to be reported.

**no**
positive integer. Number of the representative FPC to be plotted.

**bw**
optional logical. If TRUE, plot is black/white, FPC is indicated by different symbol. Else FPC is indicated red.

**main**
plot title.

**xlab**
label for x-axis. If NULL, a default text is used.

**ylab**
label for y-axis. If NULL, a default text is used.

**pch**
plotting symbol, see `par`. If NULL, the default is used.

**col**
plotting color, see `par`. If NULL, the default is used.

**gv**
logical vector (or, with method="fuzzy", vector of weights between 0 and 1) of length n. Indicates the initial configuration for the fixed point algorithm.

**...**
additional parameters to be passed to `plot` (no effects elsewhere).

### Details

A (crisp) Mahalanobis FPC is a data subset that reproduces itself under the following operation: Compute mean and covariance matrix estimator for the data subset, and compute all points of the dataset for which the squared Mahalanobis distance is smaller than `ca`. Fixed points of this operation can be considered as clusters, because they contain only non-outliers (as defined by the above mentioned procedure) and all other points are outliers w.r.t. the subset. The current default is to compute fuzzy Mahalanobis FPCs, where the points in the subset have a membership weight between 0 and 1 and give rise to weighted means and covariance matrices. The new weights are then obtained by computing the weight function `wfu` of the squared Mahalanobis distances, i.e., full weight for squared distances smaller than `ca`, zero weight for squared distances larger than `ca2` and decreasing weights (linear function of squared distances) in between. A fixed point algorithm is started from the whole dataset, algorithms are started from the subsets specified in `init.group`, and further algorithms are started from further initial configurations as explained under `subset` and in the function `mahalconf`. Usually some of the FPCs are unstable, and more than one FPC may correspond to the same significant pattern in the data. Therefore the number of FPCs is reduced: A similarity matrix is computed between FPCs. Similarity between sets is defined as the ratio between 2 times size of intersection and the sum of sizes of both sets. The Single Linkage clusters (groups) of level `distcut` are
computed, i.e. the connectivity components of the graph where edges are drawn between FPCs with similarity larger than distcut. Groups of FPCs whose members are found often enough (cf. parameter mer) are considered as stable enough. A representative FPC is chosen for every Single Linkage cluster of FPCs according to the maximum expectation ratio ser. ser is the ratio between the number of findings of an FPC and the number of points of an FPC, adjusted suitably if subset<n. Usually only the representative FPCs of stable groups are of interest.

Default tuning constants are taken from Hennig (2005). Generally, the default settings are recommended for fixmahal. For large datasets, the use of init.group together with pointit=FALSE is useful. Occasionally, mnc and startn may be chosen smaller than the default, if smaller clusters are of interest, but this may lead to too many clusters. Decrease of ca will often lead to too many clusters, even for homogeneous data. Increase of ca will produce only very strongly separated clusters. Both may be of interest occasionally.

Singular covariance matrices during the iterations are handled by solvecov.

summary.mfpc gives a summary about the representative FPCs of stable groups.

plot.mfpc is a plot method for the representative FPC of stable group no. no. It produces a scatterplot, where the points belonging to the FPC are highlighted, the mean is and for p<3 also the region of the FPC is shown. For p>=3, the optimal separating projection computed by batcoord is shown.

fpclusters.mfpc produces a list of indicator vectors for the representative FPCs of stable groups.

fpmi is called by fixmahal for a single fixed point algorithm and will usually not be executed alone.

Value

fixmahal returns an object of class mfpc. This is a list containing the components nc, g, means, covs, nfound, er, tsc, ncoll, skc, grto, imatrix, smatrix, stn, stfound, ser, sfpc, ssig, sto, struc, n, p, method, cgen, ca, ca2, cvec, calpha, pointit, subset, mnc, startn, mer, distcut.

summary.mfpc returns an object of class summary.mfpc. This is a list containing the components means, covs, stn, stfound, sn, ser, tskip, skc, tsc, sim, ca, ca2, calpha, pointit.

fpclusters.mfpc returns a list of indicator vectors for the representative FPCs of stable groups.

fpmi returns a list with the components mg, covg, md, gv, coll, method, ca.

nc integer. Number of FPCs.

g list of logical vectors. Indicator vectors of FPCs. FALSE if ind.storage=FALSE.

means list of numerical vectors. Means of FPCs. In summary.mfpc, only for representative FPCs of stable groups and sorted according to ser.

covs list of numerical matrices. Covariance matrices of FPCs. In summary.mfpc, only for representative FPCs of stable groups and sorted according to ser.

nfound vector of integers. Number of findings for the FPCs.

er numerical vector. Ratio of number of findings of FPCs to their size. Under pointit=TRUE, this can be taken as a measure of stability of FPCs.

tsc integer. Number of algorithm runs leading to too small or too seldom found FPCs.
ncoll integer. Number of algorithm runs where collinear covariance matrices oc-
curred.

skc integer. Number of skipped clusters.

grto vector of integers. Numbers of FPCs to which algorithm runs led, which were
started by init.group.

imatrix vector of integers. Size of intersection between FPCs. See sseg.

smatrix numerical vector. Similarities between FPCs. See sseg.

stn integer. Number of representative FPCs of stable groups. In summary.mfpc,
sorted according to ser.

stfound vector of integers. Number of findings of members of all groups of FPCs. In
summary.mfpc, sorted according to ser.

ser numerical vector. Ratio of number of findings of groups of FPCs to their size.
Under pointit=TRUE, this can be taken as a measure of stability of FPCs. In
summary.mfpc, sorted from largest to smallest.

sfpd vector of integers. Numbers of representative FPCs of all groups.

ssig vector of integers of length stn. Numbers of representative FPCs of the stable
groups.

sto vector of integers. Numbers of groups ordered according to largest ser.

struc vector of integers. Number of group an FPC belongs to.

n see arguments.

p see arguments.

method see arguments.

cgen see arguments.

dca see arguments, if cgen has been "fixed". Else numerical vector of length nc
(see below), giving the final values of ca for all FPC. In fpni, tuning constant
for the iterated FPC.

cdca see arguments.

cvec numerical vector of length n for cgen="auto". The values for the tuning con-
stant ca corresponding to the cluster sizes from 1 to n.

calpha see arguments.

pointit see arguments.

subset see arguments.

mnc see arguments.

startn see arguments.

mer see arguments.

discut see arguments.

sn vector of integers. Number of points of representative FPCs.

tskip integer. Number of algorithm runs leading to skipped FPCs.

sim vector of integers. Size of intersections between representative FPCs of stable
groups. See sseg.
fixmahal

mg mean vector.

covg covariance matrix.

md Mahalanobis distances.

gv logical (numerical, respectively, if method="fuzzy") indicator vector of iterated FPC.

coll logical. TRUE means that singular covariance matrices occurred during the iterations.

Author(s)

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References


See Also

fixreg for linear regression fixed point clusters.

mahalconf, wfu, cmahal for computation of initial configurations, weights, tuning constants.

sseg for indexing the similarity/intersection vectors computed by fixmahal.

batcoord, cov.rob, solvecov, cov.wml, plotcluster for computation of projections, (inverted) covariance matrices, plotting.

rFace for generation of example data, see below.

Examples

options(digits=2)
set.seed(20000)
face <- rFace(400,dMoNo=2,dNoEy=0, p=3)
# The first example uses grouping information via init.group.
initg <- list()
grface <- as.integer(attr(face,"grouping"))
for (i in 1:5) initg[[i]] <- (grface==i)
ff0 <- fixmahal(face, pointit=FALSE, init.group=initg)
summary(ff0)
cff0 <- fpclusters(ff0)
plot(face, col=1+cff0[[1]])
plot(face, col=1+cff0[[4]]) # Why does this come out as a cluster?
plot(ff0, face, 4) # A bit clearer...
# Without grouping information, examples need more time:
fixreg

Linear Regression Fixed Point Clusters

Description

Computes linear regression fixed point clusters (FPCs), i.e., subsets of the data, which consist exactly of the non-outliers w.r.t. themselves, and may be interpreted as generated from a homogeneous linear regression relation between independent and dependent variable. FPCs may overlap, are not necessarily exhausting and do not need a specification of the number of clusters.

Note that while fixreg has lots of parameters, only one (or few) of them have usually to be specified, cf. the examples. The philosophy is to allow much flexibility, but to always provide sensible defaults.

Usage

```r
fixreg(indep=rep(1,n), dep, n=length(dep),
   p=ncol(as.matrix(indep)),
   ca=NA, mnc=NA, mtf=3, ir=NA, irnc=NA,
   irprob=0.95, mncprob=0.5, maxir=20000, maxit=5*n,
   distcut=0.85, init.group=list(),
)```

### S3 method for class 'rfpc'

```r
summary(object, ...)```

### S3 method for class 'summary.rfpc'

```r
print(x, maxnc=30, ...)```

### S3 method for class 'rfpc'

```r
plot(x, indep=rep(1,n), dep, no, bw=TRUE,
main=c("Representative FPC No. ",no),
 xlab="Linear combination of independents",
ylab=deparse(substitute(indep)),
xlim=NULL, ylim=range(dep),
pch=NULL, col=NULL,...)
```

### S3 method for class 'rfpc'

```r
fpclusters(object, indep=NA, dep=NA, ca=object$ca, ...)
```

### Arguments

- **indep**
  - numerical matrix or vector. Independent variables. Leave out for clustering one-dimensional data. `fpclusters.rfpc` does not need specification of `indep` if `fixreg` was run with `ind.storage=TRUE`.

- **dep**
  - numerical vector. Dependent variable. `fpclusters.rfpc` does not need specification of `dep` if `fixreg` was run with `ind.storage=TRUE`.

- **n**
  - optional positive integer. Number of cases.

- **p**
  - optional positive integer. Number of independent variables.

- **ca**
  - optional positive number. Tuning constant, specifying required cluster separation. By default determined automatically as a function of `n` and `p`, see function `can`, Hennig (2002a).

- **mnc**
  - optional positive integer. Minimum size of clusters to be reported. By default determined automatically as a function of `mncprob`. See Hennig (2002a).

- **mtf**
  - optional positive integer. FPCs must be found at least `mtf` times to be reported by `summary.rfpc`.

- **ir**

- **irnc**
  - optional positive integer. Size of the smallest cluster to be found with approximated probability `irprob`.

- **irprob**
  - optional value between 0 and 1. Approximated probability for a cluster of size `irnc` to be found.
**mncprob**
optional value between 0 and 1. Approximated probability for a cluster of size mnc to be found.

**maxir**
onoptional integer. Maximum number of algorithm runs.

**maxit**
onoptional integer. Maximum number of iterations per algorithm run (usually an FPC is found much earlier).

**distcut**
onoptional value between 0 and 1. A similarity measure between FPCs, given in Hennig (2002a), and the corresponding Single Linkage groups of FPCs with similarity larger than distcut are computed. A single representative FPC is selected for each group.

**init.group**
onoptional list of logical vectors of length n. Every vector indicates a starting configuration for the fixed point algorithm. This can be used for datasets with high dimension, where the vectors of init.group indicate cluster candidates found by graphical inspection or background knowledge.

**ind.storage**
onoptional logical. If TRUE, then all indicator vectors of found FPCs are given in the value of fixreg. May need lots of memory, but is a bit faster.

**countmode**
onoptional positive integer. Every countmode algorithm runs fixreg shows a message.

**plot**
onoptional logical. If TRUE, you get a scatterplot of first independent vs. dependent variable at each iteration.

**object**
oobject of class rfpc, output of fixreg.

**x**
oobject of class rfpc, output of fixreg.

**maxnc**
positive integer. Maximum number of FPCs to be reported.

**no**
positive integer. Number of the representative FPC to be plotted.

**bw**
onoptional logical. If TRUE, plot is black/white, FPC is indicated by different symbol. Else FPC is indicated red.

**main**
plot title.

**xlab**
label for x-axis.

**ylab**
label for y-axis.

**xlim**
plotted range of x-axis. If NULL, the range of the plotted linear combination of independent variables is used.

**ylim**
plotted range of y-axis.

**pch**
plotting symbol, see par. If NULL, the default is used.

**col**
plotting color, see par. If NULL, the default is used.

**gv**
logical vector of length n. Indicates the initial configuration for the fixed point algorithm.

**...**
additional parameters to be passed to plot (no effects elsewhere).

**Details**

A linear regression FPC is a data subset that reproduces itself under the following operation: Compute linear regression and error variance estimator for the data subset, and compute all points of the dataset for which the squared residual is smaller than ca times the error variance.
Fixed points of this operation can be considered as clusters, because they contain only non-outliers (as defined by the above mentioned procedure) and all other points are outliers w.r.t. the subset.

fixreg performs $ir$ fixed point algorithms started from random subsets of size $p+2$ to look for FPCs. Additionally an algorithm is started from the whole dataset, and algorithms are started from the subsets specified in init.group.

Usually some of the FPCs are unstable, and more than one FPC may correspond to the same significant pattern in the data. Therefore the number of FPCs is reduced: FPCs with less than $mnc$ points are ignored. Then a similarity matrix is computed between the remaining FPCs. Similarity between sets is defined as the ratio between 2 times size of intersection and the sum of sizes of both sets. The Single Linkage clusters (groups) of level $distcut$ are computed, i.e. the connectivity components of the graph where edges are drawn between FPCs with similarity larger than $distcut$.

Groups of FPCs whose members are found $mtf$ times or more are considered as stable enough. A representative FPC is chosen for every Single Linkage cluster of FPCs according to the maximum expectation ratio $ser$. $ser$ is the ratio between the number of findings of an FPC and the estimated expectation of the number of findings of an FPC of this size, called expectation ratio and computed by clusexpect.

Usually only the representative FPCs of stable groups are of interest. The choice of the involved tuning constants such as $ca$ and $ir$ is discussed in detail in Hennig (2002a). Statistical theory is presented in Hennig (2003).

Generally, the default settings are recommended for fixreg. In cases where they lead to a too large number of algorithm runs (e.g., always for $p>4$), the use of init.group together with $mtf=1$ and $ir=0$ is useful. Occasionally, $irnc$ may be chosen smaller than the default, if smaller clusters are of interest, but this may lead to too many clusters and too many algorithm runs. Decrease of $ca$ will often lead to too many clusters, even for homogeneous data. Increase of $ca$ will produce only very strongly separated clusters. Both may be of interest occasionally.

rfpi is called by fixreg for a single fixed point algorithm and will usually not be executed alone. summary.rfpc gives a summary about the representative FPCs of stable groups.

plot.rfpc is a plot method for the representative FPC of stable group no. no. It produces a scatter-plot of the linear combination of independent variables determined by the regression coefficients of the FPC vs. the dependent variable. The regression line and the region of non-outliers determined by $ca$ are plotted as well.

fpclusters.rfpc produces a list of indicator vectors for the representative FPCs of stable groups.

Value

fixreg returns an object of class rfpc. This is a list containing the components $nc$, $g$, $coefs$, $vars$, $nfound$, $er$, $tsc$, $ncoll$, $grto$, $imatrix$, $smatrix$, $stn$, $stfound$, $sfpc$, $ssig$, $sto$, $struc$, $n$, $p$, $ca$, $ir$, $mnc$, $mtf$, $distcut$.

summary.rfpc returns an object of class summary.rfpc. This is a list containing the components $coefs$, $vars$, $stfound$, $stn$, $sn$, $ser$, $tsc$, $sim$, $ca$, $ir$, $mnc$, $mtf$.

fpclusters.rfpc returns a list of indicator vectors for the representative FPCs of stable groups.

rfpi returns a list with the components $coef$, $var$, $g$, $coll$, $ca$.

$nc$ integer. Number of FPCs.

$g$ list of logical vectors. Indicator vectors of FPCs. FALSE if ind. storage=FALSE.

$coefs$ list of numerical vectors. Regression coefficients of FPCs. In summary.rfpc, only for representative FPCs of stable groups and sorted according to stfound.
vars  list of numbers. Error variances of FPCs. In summary.rfpc, only for representative FPCs of stable groups and sorted according to stfound.
nfound  vector of integers. Number of findings for the FPCs.
er  numerical vector. Expectation ratios of FPCs. Can be taken as a stability measure.
tsc  integer. Number of algorithm runs leading to too small or too seldom found FPCs.
ncoll  integer. Number of algorithm runs where collinear regressor matrices occurred.
grto  vector of integers. Numbers of FPCs to which algorithm runs led, which were started by init.group.
imatrix  vector of integers. Size of intersection between FPCs. See sseg.
smatrix  numerical vector. Similarities between FPCs. See sseg.
stn  integer. Number of representative FPCs of stable groups. In summary.rfpc sorted according to stfound.
stfound  vector of integers. Number of findings of members of all groups of FPCs. In summary.rfpc sorted according to stfound.
sfpc  vector of integers. Numbers of representative FPCs.
ssig  vector of integers. As sfpc, but only for stable groups.
sto  vector of integers. Number of representative FPC of most, 2nd most, ..., often found group of FPCs.
struc  vector of integers. Number of group an FPC belongs to.
n  see arguments.
p  see arguments.
ca  see arguments.
ir  see arguments.
mnc  see arguments.
mtf  see arguments.
distcut  see arguments.
sn  vector of integers. Number of points of representative FPCs.
ser  numerical vector. Expectation ratio for stable groups.
sim  vector of integers. Size of intersections between representative FPCs of stable groups. See sseg.
coef  vector of regression coefficients.
var  error variance.
g  logical indicator vector of iterated FPC.
coll  logical. TRUE means that singular covariance matrices occurred during the iterations.

Author(s)

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References


See Also

*fixmahal* for fixed point clusters in the usual setup (non-regression).

*regmix* for clusterwise linear regression by mixture modeling ML.

*can, itnumber* for computation of the default settings.

*clusexpect* for estimation of the expected number of findings of an FPC of given size.

*itnumber* for the generation of the number of fixed point algorithms.

*minsize* for the smallest FPC size to be found with a given probability.

*sseg* for indexing the similarity/intersection vectors computed by *fixreg*.

Examples

```r
set.seed(190000)
options(digits=3)
data(tonedata)
attach(tonedata)
tonefix <- fixreg(stretchratio,tuned,mtf=1,ir=20)
summary(tonefix)
# This is designed to have a fast example; default setting would be better.
# If you want to see more (and you have a bit more time),
# try out the following:
## Not run:
set.seed(1000)
tonefix <- fixreg(stretchratio,tuned)
# Default - good for these data
summary(tonefix)
plot(tonefix,stretchratio,tuned,1)
plot(tonefix,stretchratio,tuned,2)
plot(tonefix,stretchratio,tuned,3,bw=FALSE,pch=5)
toneclus <- fpclusters(tonefix,stretchratio,tuned)
plot(stretchratio,tuned,col=1+toneclus[[2]])
tonefix2 <- fixreg(stretchratio,tuned,distcut=1,mtf=1,countmode=50)
# Every found fixed point cluster is reported,
# no matter how instable it may be.
summary(tonefix2)
tonefix3 <- fixreg(stretchratio,tuned,ca=7)
# ca defaults to 10.07 for these data.
summary(tonefix3)
subset <- c(rep(FALSE,5),rep(TRUE,24),rep(FALSE,121))
tonefix4 <- fixreg(stretchratio,tuned,
                   mtf=1,ir=0,init.group=list(subset))
summary(tonefix4)
```
flexmixedruns

**Fitting mixed Gaussian/multinomial mixtures with flexmix**

## Description

flexmixedruns fits a latent class mixture (clustering) model where some variables are continuous and modelled within the mixture components by Gaussian distributions and some variables are categorical and modelled within components by independent multinomial distributions. The fit is by maximum likelihood estimation computed with the EM-algorithm. The number of components can be estimated by the BIC.

Note that at least one categorical variable is needed, but it is possible to use data without continuous variable.

## Usage

```r
flexmixedruns(x, diagonal=TRUE, xvarsorted=TRUE, 
continuous, discrete, ppdim=NULL, initial.cluster=NULL, 
simruns=20, n.cluster=1:20, verbose=TRUE, recode=TRUE, 
allout=TRUE, control=list(minprior=0.001), silent=TRUE)
```

## Arguments

- **x**
  - data matrix or data frame. The data need to be organised case-wise, i.e., if there are categorical variables only, and 15 cases with values c(1,1,2) on the 3 variables, the data matrix needs 15 rows with values 1 1 2. (Categorical variables could take numbers or strings or anything that can be coerced to factor levels as values.)

- **diagonal**
  - logical. If TRUE, Gaussian models are fitted restricted to diagonal covariance matrices. Otherwise, covariance matrices are unrestricted. TRUE is consistent with the "within class independence" assumption for the multinomial variables.

- **xvarsorted**
  - logical. If TRUE, the continuous variables are assumed to be the first ones, and the categorical variables to be behind them.

- **continuous**
  - vector of integers giving positions of the continuous variables. If xvarsorted=TRUE, a single integer, number of continuous variables.

- **discrete**
  - vector of integers giving positions of the categorical variables. If xvarsorted=TRUE, a single integer, number of categorical variables.

- **ppdim**
  - vector of integers specifying the number of (in the data) existing categories for each categorical variable. If recode=TRUE, this can be omitted and is computed automatically.

- **initial.cluster**
  - this corresponds to the cluster parameter in flexmix and should only be specified if simruns=1 and n.cluster is a single number. Either a matrix with
**n.cluster** columns of initial cluster membership probabilities for each observation; or a factor or integer vector with the initial cluster assignments of observations at the start of the EM algorithm. Default is random assignment into **n.cluster** clusters.

**simruns** integer. Number of starts of the EM algorithm with random initialisation in order to find a good global optimum.

**n.cluster** vector of integers, numbers of components (the optimum one is found by minimising the BIC).

**verbose** logical. If TRUE, some information about the different runs of the EM algorithm is given out.

**recode** logical. If TRUE, the function `discrete.recode` is applied in order to recode categorical data so that the `lcmixed`-method can use it. Only set this to FALSE if your data already has that format (even if that case, TRUE doesn't do harm). If recode=FALSE, the categorical variables are assumed to be coded 1,2,3,...

**allout** logical. If TRUE, the regular `flexmix`-output is given out for every single number of clusters, which can create a huge output object.

**control** list of control parameters for `flexmix`, for details see the help page of [FLXcontrol-class](https://CRAN.R-project.org/package=flexmix).

**silent** logical. This is passed on to the `try`-function. If FALSE, error messages from failed runs of `flexmix` are suppressed. (The information that a `flexmix`-error occurred is still given out if verbose=TRUE).

**Details**

Sometimes `flexmix` produces errors because of degenerating covariance matrices, too small clusters etc. `flexmixedruns` tolerates these and treats them as non-optimal runs. (Higher `simruns` or different `control` may be required to get a valid solution.)

General documentation on `flexmix` can be found in Friedrich Leisch's "FlexMix: A General Framework for Finite Mixture Models and Latent Class Regression in R", [https://CRAN.R-project.org/package=flexmix](https://CRAN.R-project.org/package=flexmix)

**Value**

A list with components

- **optsummary** summary object for `flexmix` object with optimal number of components.
- **optimalk** optimal number of components.
- **errcount** vector with numbers of EM runs for each number of components that led to `flexmix` errors.
- **flexout** if allout=TRUE, list of `flexmix` output objects for all numbers of components, for details see the help page of `flexmix-class`. Slots that can be used include for example cluster and components. So if fo is the `flexmixedruns`-output object, fo$flexout[[fo$optimalk]]@cluster gives a component number vector for the observations (maximum posterior rule), and fo$flexout[[fo$optimalk]]@components gives the estimated model parameters, which for `lcmixed` and therefore `flexmixedruns` are called

  - **center** mean vector
covariance matrix

pp  list of categorical variable-wise category probabilities

If allout=FALSE, only the flexmix output object for the optimal number of components, i.e., the [[fo$optimalk]] indexing above can then be omitted.

bicvals  vector of values of the BIC for each number of components.

ppdim  vector of categorical variable-wise numbers of categories.

discretelevels  list of levels of the categorical variables belonging to what is treated by flexmixedruns as category 1, 2, 3 etc.

Author(s)

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References


See Also

lcmixed, flexmix, FLXcontrol-class, flexmix-class, discrete.recode.

Examples

```r
options(digits=3)
set.seed(776655)
v1 <- rnorm(100)
v2 <- rnorm(100)
d1 <- sample(1:5,100,replace=TRUE)
d2 <- sample(1:4,100,replace=TRUE)
data <- cbind(v1,v2,d1,d2)
fr <- flexmixedruns(data,
    continuous=2,discrete=2,simruns=2,n.cluster=2:3,allout=FALSE)
print(fr$optimalk)
print(fr$optsummary)
print(fr$flexout@cluster)
print(fr$flexout@components)
```

Description

fpclusters is a generic function which extracts the representative fixed point clusters (FPCs) from FPC objects generated by fixmahal and fixreg. For documentation and examples see fixmahal and fixreg.
itnumber

Usage

fpclusters(object, ...)

Arguments

object  object of class rfpc or mfpc.
...  further arguments depending on the method.

Value

a list of logical or numerical vectors indicating or giving the weights of the cluster memberships.

Author(s)

Christian Hennig <christian.hennig@unibo.it> https://www.unibo.it/sitoweb/christian.hennig/en/

See Also

fixmahal, fixreg

---

**itnumber**

*Number of regression fixed point cluster iterations*

---

Description

Computes the number of fixed point iterations needed by *fixreg* to find *mtf* times a fixed point cluster (FPC) of size *cn* with an approximated probability of *prob*.

Thought for use within *fixreg*.

Usage

itnumber(n, p, cn, mtf, prob = 0.95, maxir = 20000)

Arguments

n  positive integer. Total number of points.
p  positive integer. Number of independent variables.
cn  positive integer smaller or equal to *n*. Size of the FPC.
mtf  positive integer.
prob  number between 0 and 1.
maxir  positive integer. *itnumber* is set to this value if it would otherwise be larger.
jittervar

Details
The computation is based on the binomial distribution with probability given by clusexpect with ir=1.

Value
An integer.

Author(s)
Christian Hennig <christian.hennig@unibo.it> https://www.unibo.it/sitoweb/christian.hennig/en/

References

See Also
fixreg, clusexpect

Examples
itnumber(500,4,150,2)

jittervar Jitter variables in a data matrix

Description
Jitters some variables in a data matrix.

Usage
jittervar(x,jitterv=NULL,factor=1)

Arguments
x data matrix or data frame.
jitterv vector of numbers of variables to be jittered.
factor numeric. Passed on to jitter. See the documentation there. The higher, the more jittering.

Value
data matrix or data frame with jittered variables.
**kmeansCBI**

*Interface functions for clustering methods*

**Description**

These functions provide an interface to several clustering methods implemented in R, for use together with the cluster stability assessment in `clusterboot` (as parameter `clustermethod`; "CBI" stands for "clusterboot interface"). In some situations it could make sense to use them to compute a clustering even if you don’t want to run `clusterboot`, because some of the functions contain some additional features (e.g., normal mixture model based clustering of dissimilarity matrices projected into the Euclidean space by MDS or partitioning around medoids with estimated number of clusters, noise/outlier identification in hierarchical clustering).

**Usage**

```r
kmeansCBI(data, krange, k, scaling=FALSE, runs=1, criterion="ch", ...)
hclustCBI(data, k, cut="number", method, scaling=TRUE, noisecut=0, ...)
hclusttreeCBI(data, minlevel=2, method, scaling=TRUE, ...)
disthclustCBI(dmatrix, k, cut="number", method, noisecut=0, ...)
noisemclustCBI(data, G, k, modelNames, nnk, hcmodel=NULL, Vinv=NULL, summary.out=FALSE, ...)
distnoisemclustCBI(dmatrix, G, k, modelNames, nnk, ...
```

**Examples**

```r
set.seed(776655)
v1 <- rnorm(20)v2 <- rnorm(20)d1 <- sample(1:5,20,replace=TRUE)d2 <- sample(1:4,20,replace=TRUE)ldata <- cbind(v1,v2,d1,d2)jv <- jittervar(ldata,jitterv=3:4)
```
kmeansCBI

hcmodel=NULL, Vinv=NULL, mdsmethod="classical",
mdsdim=4, summary.out=FALSE, points.out=FALSE,...

claraCBI(data,k, usepam=TRUE, diss=inherits(data,"dist"),...)

pamkCBI(data,krange=2:10, k=NULL, criterion="asw", usepam=TRUE,
 scaling=FALSE, diss=inherits(data,"dist"),...)

tclustCBI(data,k,trim=0.05,...)

dbscanCBI(data,eps, MinPts, diss=inherits(data,"dist"),...)

mahalCBI(data, clustercut=0.5,...)

mergenormCBI(data, G=NULL, k=NULL, modelNames=NULL, nnk=0,
 hcmodel = NULL,
 Vinv = NULL, mergemethod="bhat",
cutoff=0.1,...)

speccCBI(data,k,...)

pdfclustCBI(data,...)

stupidkcentroidsCBI(dmatrix,k,distances=TRUE)

stupidknnCBI(dmatrix,k)

stupidkfnCBI(dmatrix,k)

stupidkavenCBI(dmatrix,k)

**Arguments**

data a numeric matrix. The data matrix - usually a cases*variables-data matrix.
claraCBI, pamkCBI and dbscanCBI work with an n*n-dissimilarity matrix as well, see parameter diss.

dmatrix a squared numerical dissimilarity matrix or a dist-object.
k numeric, usually integer. In most cases, this is the number of clusters for methods where this is fixed. For hclustCBI and disthclustCBI see parameter cut below. Some methods have a k parameter on top of a G or krange parameter for compatibility; k in these cases does not have to be specified but if it is, it is always a single number of clusters and overwrites G and krange.

scaling either a logical value or a numeric vector of length equal to the number of variables. If scaling is a numeric vector with length equal to the number of variables, then each variable is divided by the corresponding value from scaling.
If scaling is TRUE then scaling is done by dividing the (centered) variables by their root-mean-square, and if scaling is FALSE, no scaling is done before execution.

**runs** integer. Number of random initializations from which the k-means algorithm is started.

**criterion** "ch" or "asw". Decides whether number of clusters is estimated by the Calinski-Harabasz criterion or by the average silhouette width.

**cut** either "level" or "number". This determines how the tree is cut to obtain a fixed number of clusters. The parameter k specifies the number of clusters or the dissimilarity level, depending on cut.

**method** method for hierarchical clustering, see the documentation of `hclust`.

**noisecut** numeric. All clusters of size \( \leq \text{noisecut} \) in the `disthclustCBI/hclustCBI`-partition are joined and declared as noise/outliers.

**minlevel** integer. `minlevel=1` means that all clusters in the tree are given out by `hclusttreeCBI` or `disthclusttreeCBI`, including one-point clusters (but excluding the cluster with all points). `minlevel=2` excludes the one-point clusters. `minlevel=3` excludes the two-point cluster which has been merged first, and increasing the value of `minlevel` by 1 in all further steps means that the remaining earliest formed cluster is excluded.

**G** vector of integers. Number of clusters or numbers of clusters used by `mclustBIC`. If `G` has more than one entry, the number of clusters is estimated by the BIC.

**modelNames** vector of string. Models for covariance matrices, see documentation of `mclustBIC`.

**nnk** integer. Tuning constant for `NNclean`, which is used to estimate the initial noise for `noisemclustCBI` and `distnoisemclustCBI`. See parameter `k` in the documentation of `NNclean`. `nnk=0` means that no noise component is fitted.

**hcmodel** string or NULL. Determines the initialization of the EM-algorithm for `mclustBIC`. Documented in `hc`.

**Vinv** numeric. See documentation of `mclustBIC`.

**summary.out** logical. If TRUE, the result of `summary.mclustBIC` is added as component `mclustsummary` to the output of `noisemclustCBI` and `distnoisemclustCBI`.

**mdsmethod** "classical", "kruskal" or "sammon". Determines the multidimensional scaling method to compute Euclidean data from a dissimilarity matrix. See `cmdscale`, `isoMDS` and `sammon`.

**mdsdim** integer. Dimensionality of MDS solution.

**points.out** logical. If TRUE, the matrix of MDS points is added as component points to the output of `noisemclustCBI`.

**usepam** logical. If TRUE, the function `pam` is used for clustering, otherwise `clara`. `pam` is better, `clara` is faster.

**diss** logical. If TRUE, data will be considered as a dissimilarity matrix. In `claraCBI`, this requires `usepam=TRUE`.

**krange** vector of integers. Numbers of clusters to be compared.
trim numeric between 0 and 1. Proportion of data points trimmed, i.e., assigned to noise. See tclust in the tclust package.

eps numeric. The radius of the neighborhoods to be considered by dbscan.

MinPts integer. How many points have to be in a neighborhood so that a point is considered to be a cluster seed? See documentation of dbscan.

clustercut numeric between 0 and 1. If fixmahal is used for fuzzy clustering, a crisp partition is generated and points with cluster membership values above clustercut are considered as members of the corresponding cluster.

mergemethod method for merging Gaussians, passed on as method to mergenormals.

cutoff numeric between 0 and 1, tuning constant for mergenormals.

distances logical (only for stupidkcentroidsCBI). If FALSE, dmatrix is interpreted as cases&variables data matrix.

... further parameters to be transferred to the original clustering functions (not required).

Details

All these functions call clustering methods implemented in R to cluster data and to provide output in the format required by clusterboot. Here is a brief overview. For further details see the help pages of the involved clustering methods.

kmeansCBI an interface to the function kmeansruns calling kmeans for k-means clustering. (kmeansruns allows the specification of several random initializations of the k-means algorithm and estimation of k by the Calinski-Harabasz index or the average silhouette width.)

hclustCBI an interface to the function hclust for agglomerative hierarchical clustering with noise component (see parameter noisecut above). This function produces a partition and assumes a cases*variables matrix as input.

hclustreeCBI an interface to the function hclust for agglomerative hierarchical clustering. This function gives out all clusters belonging to the hierarchy (upward from a certain level, see parameter minlevel above).

disthclustCBI an interface to the function hclust for agglomerative hierarchical clustering with noise component (see parameter noisecut above). This function produces a partition and assumes a dissimilarity matrix as input.

noiseemclustCBI an interface to the function mclustBIC, for normal mixture model based clustering. Warning: mclustBIC often has problems with multiple points. In clusterboot, it is recommended to use this together with multipleboot=FALSE.

distnoiseemclustCBI an interface to the function mclustBIC for normal mixture model based clustering. This assumes a dissimilarity matrix as input and generates a data matrix by multidimensional scaling first. Warning: mclustBIC often has problems with multiple points. In clusterboot, it is recommended to use this together with multipleboot=FALSE.

claraCBI an interface to the functions pam and clara for partitioning around medoids.

pamkCBI an interface to the function pamk calling pam for partitioning around medoids. The number of clusters is estimated by the Calinski-Harabasz index or by the average silhouette width.
tclustCBI an interface to the function tclust in the tclust package for trimmed Gaussian clustering. This assumes a cases*variables matrix as input.
dbscanCBI an interface to the function dbscan for density based clustering.
mahalCBI an interface to the function fixmahal for fixed point clustering. This assumes a cases*variables matrix as input.
mergenormCBI an interface to the function mergenorms for clustering by merging Gaussian mixture components. Unlike mergenorms, mergenormCBI includes the computation of the initial Gaussian mixture. This assumes a cases*variables matrix as input.
speccCBI an interface to the function specc for spectral clustering. See the specc help page for additional tuning parameters. This assumes a cases*variables matrix as input.
pdfclustCBI an interface to the function pdfCluster for density-based clustering. See the pdfCluster help page for additional tuning parameters. This assumes a cases*variables matrix as input.
stupidkcentroidsCBI an interface to the function stupidkcentroids for random centroid-based clustering. See the stupidkcentroids help page. This can have a distance matrix as well as a cases*variables matrix as input, see parameter distances.
stupidkfnCBI an interface to the function stupidkfn for random farthest neighbour clustering. See the stupidkfn help page. This assumes a distance matrix as input.
stupidkavenCBI an interface to the function stupidkaven for random average dissimilarity clustering. See the stupidkaven help page. This assumes a distance matrix as input.

Value

All interface functions return a list with the following components (there may be some more, see summary.out and points.out above):

result clustering result, usually a list with the full output of the clustering method (the precise format doesn’t matter); whatever you want to use later.
nc number of clusters. If some points don’t belong to any cluster, these are declared “noise”. nc includes the “noise cluster”, and there should be another component nccl, being the number of clusters not including the noise cluster.
clusterlist this is a list consisting of a logical vectors of length of the number of data points (n) for each cluster, indicating whether a point is a member of this cluster (TRUE) or not. If a noise cluster is included, it should always be the last vector in this list.
partition an integer vector of length n, partitioning the data. If the method produces a partition, it should be the clustering. This component is only used for plots, so you could do something like rep(1,n) for non-partitioning methods. If a noise cluster is included, nc=nccl+1 and the noise cluster is cluster no. nc.
clustermethod a string indicating the clustering method.

The output of some of the functions has further components:

nccl see nc above.
nnk by noisemclustCBI and distnoisemclustCBI, see above.
initnoise logical vector, indicating initially estimated noise by **NNclean**, called by **noisemclustCBI** and **distnoisemclustCBI**.

noise logical. TRUE if points were classified as noise/outliers by **disthclustCBI**.

**Author(s)**

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**See Also**


**Examples**

```r
options(digits=3)
set.seed(20000)
f <- rFace(50,dMoNo=2,dNoEy=0,p=2)
dbs <- dbscanCBI(f,eps=1.5,MinPts=4)
dhc <- disthclustCBI(dist(f),method="average",k=1.5,noisecut=2)
table(dbs$partition,dhc$partition)
```

```r
dm <- mergenormCBI(f,G=10,modelNames="EEE",nnk=2)
dtc <- tclustCBI(f,6,trim=0.1,restr.fact=500)
table(dm$partition,dtc$partition)
```

---

**kmeansruns** _k-means with estimating k and initialisations_

**Description**

This calls the function **kmeans** to perform a k-means clustering, but initializes the k-means algorithm several times with random points from the data set as means. Furthermore, it is more robust against the occurrence of empty clusters in the algorithm and it estimates the number of clusters by either the Calinski Harabasz index (**calinhara**) or average silhouette width (see **pam.object**). The Duda-Hart test (**dudahart2**) is applied to decide whether there should be more than one cluster (unless 1 is excluded as number of clusters).

**Usage**

```r
kmeansruns(data,krange=2:10,criterion="ch",
iter.max=100,runs=100,
scaledata=FALSE,alpha=0.001,
criout=FALSE,plot=FALSE,...)
```
### Arguments

- **data**: A numeric matrix of data, or an object that can be coerced to such a matrix (such as a numeric vector or a data frame with all numeric columns).
- **krange**: integer vector. Numbers of clusters which are to be compared by the average silhouette width criterion. Note: average silhouette width and Calinski-Harabasz can’t estimate number of clusters \( nc=1 \). If 1 is included, a Duda-Hart test is applied and 1 is estimated if this is not significant.
- **criterion**: one of "asw" or "ch". Determines whether average silhouette width or Calinski-Harabasz is applied.
- **iter.max**: integer. The maximum number of iterations allowed.
- **runs**: integer. Number of starts of the k-means algorithm.
- **scaledata**: logical. If TRUE, the variables are centered and scaled to unit variance before execution.
- **alpha**: numeric between 0 and 1, tuning constant for dudahart2 (only used for 1-cluster test).
- **critout**: logical. If TRUE, the criterion value is printed out for every number of clusters.
- **plot**: logical. If TRUE, every clustering resulting from a run of the algorithm is plotted.
- **...**: further arguments to be passed on to kmeans.

### Value

The output of the optimal run of the kmeans-function with added components bestk and crit. A list with components

- **cluster**: A vector of integers indicating the cluster to which each point is allocated.
- **centers**: A matrix of cluster centers.
- **withinss**: The within-cluster sum of squares for each cluster.
- **size**: The number of points in each cluster.
- **bestk**: The optimal number of clusters.
- **crit**: Vector with values of the criterion for all used numbers of clusters (0 if number not tried).

### Author(s)

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### References

lcmixed

See Also

kmeans, pamk, calinhara, dudahart2)

Examples

options(digits=3)
set.seed(20000)
face <- rFace(50, dMoNo=2, dNoEy=0, p=2)
pka <- kmeansruns(face, krange=1:5, critout=TRUE, runs=2, criterion="asw")
pkc <- kmeansruns(face, krange=1:5, critout=TRUE, runs=2, criterion="ch")

Description

lcmixed is a method for the flexmix-function in package flexmix. It provides the necessary information to run an EM-algorithm for maximum likelihood estimation for a latent class mixture (clustering) model where some variables are continuous and modelled within the mixture components by Gaussian distributions and some variables are categorical and modelled within components by independent multinomial distributions. lcmixed can be called within flexmix. The function flexmixedruns is a wrapper function that can be run to apply lcmixed.

Note that at least one categorical variable is needed, but it is possible to use data without continuous variable.

There are further format restrictions to the data (see below in the documentation of continuous and discrete), which can be ignored when running lcmixed through flexmixedruns.

Usage

lcmixed( formula = .~., continuous, discrete, ppdim,
         diagonal = TRUE, pred.ordinal=FALSE, printlik=FALSE )

Arguments

formula a formula to specify response and explanatory variables. For lcmixed this always has the form x~1, where x is a matrix or data frame of all variables to be involved, because regression and explanatory variables are not implemented.

continuous number of continuous variables. Note that the continuous variables always need to be the first variables in the matrix or data frame.

discrete number of categorical variables. Always the last variables in the matrix or data frame. Note that categorical variables always must be coded as integers 1,2,3, etc. without interruption.

ppdim vector of integers specifying the number of (in the data) existing categories for each categorical variable.
\texttt{lcmixed}

- **diagonal** \texttt{logical. If TRUE, Gaussian models are fitted restricted to diagonal covariance matrices. Otherwise, covariance matrices are unrestricted. TRUE is consistent with the “within class independence” assumption for the multinomial variables.}

- **pred.\texttt{ordinal}** \texttt{logical. If FALSE, the within-component predicted value for categorical variables is the probability mode, otherwise it is the mean of the standard (1,2,3,...) scores, which may be better for ordinal variables.}

- **printlik** \texttt{logical. If TRUE, the loglikelihood is printed out whenever computed.}

\textbf{Details}

The data need to be organised case-wise, i.e., if there are categorical variables only, and 15 cases with values c(1,1,2) on the 3 variables, the data matrix needs 15 rows with values 1 1 2.

General documentation on flexmix methods can be found in Chapter 4 of Friedrich Leisch’s “FlexMix: A General Framework for Finite Mixture Models and Latent Class Regression in R”, https://CRAN.R-project.org/package=flexmix

\textbf{Value}

An object of class \texttt{FLXMC} (not documented; only used internally by \texttt{flexmix}).

\textbf{Author(s)}

Christian Hennig <christian.hennig@unibo.it> https://www.unibo.it/sitoweb/christian.hennig/en

\textbf{References}


\textbf{See Also}

\texttt{flexmixedruns, flexmix, flexmix-class, discrete.recode}, which recodes a dataset into the format required by \texttt{lcmixed}

\textbf{Examples}

```r
set.seed(112233)
options(digits=3)
require(MASS)
require(flexmix)
data(Cars93)
Cars934 <- Cars93[,c(3,5,8,10)]
cc <-
discrete.recode(Cars934,xvarsorted=FALSE,continuous=c(2,3),discrete=c(1,4))
fcc <- flexmix(cc$data~1,k=2,
model=lcmixed(continuous=2,discrete=2,ppdim=c(6,3),diagonal=TRUE))
summary(fcc)
```
localshape

Local shape matrix

Description

This computes a matrix formalising 'local shape', i.e., aggregated standardised variance/covariance in a Mahalanobis neighbourhood of the data points. This can be used for finding clusters when used as one of the covariance matrices in Invariant Coordinate Selection (function ics in package ICS), see Hennig's discussion and rejoinder of Tyler et al. (2009).

Usage

localshape(xdata, proportion=0.1, mscatter="mcd", mcdalpha=0.8, covstandard="det")

Arguments

xdata | objects times variables data matrix.
proportion | proportion of points to be considered as neighbourhood.
msscatter | "mcd" or "cov"; specified minimum covariance determinant or classical covariance matrix to be used for Mahalanobis distance computation.
mcdalpha | if mscatter="mcd", this is the alpha parameter to be used by the MCD covariance matrix, i.e. one minus the asymptotic breakdown point, see covMcd.
covstandard | one of "trace", "det" or "none", determining by what constant the pointwise neighbourhood covariance matrices are standardised. "det" makes the affine equivariant, as noted in the discussion rejoinder of Tyler et al. (2009).

Value

The local shape matrix.

Author(s)

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References


Examples

options(digits=3)
data(iris)
localshape(iris[, -5], mscatter="cov")
mahalanodisc

mahalanodisc  

**Mahalanobis for AWC**

---

**Description**

Vector of Mahalanobis distances or their root. For use in awcoord only.

**Usage**

```r
mahalanodisc(x2, mg, covg, modus="square")
```

**Arguments**

- `x2`: numerical data matrix.
- `mg`: mean vector.
- `covg`: covariance matrix.
- `modus`: "md" (roots of Mahalanobis distances) or "square" (original squared form of Mahalanobis distances).

**Details**

The covariance matrix is inverted by use of `solvecov`, which can be expected to give reasonable results for singular within-class covariance matrices.

**Value**

vector of (rooted) Mahalanobis distances.

**Author(s)**

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**See Also**

`awcoord`, `solvecov`

**Examples**

```r
options(digits=3)
x <- cbind(rnorm(50),rnorm(50))
mahalanodisc(x,c(0,0),cov(x))
mahalanodisc(x,c(0,0),matrix(0,ncol=2,nrow=2))
```
mahalanofix

Mahalanobis distances from center of indexed points

Description

Computes the vector of (classical or robust) Mahalanobis distances of all points of x to the center of the points indexed (or weighted) by gv. The latter also determine the covariance matrix.

Thought for use within fixmahal.

Usage

mahalanofix(x, n = nrow(as.matrix(x)), p = ncol(as.matrix(x)), gv = rep(1, times = n), cmax = 1e+10, method = "ml")

mahalanofuz(x, n = nrow(as.matrix(x)), p = ncol(as.matrix(x)),
          gv = rep(1, times = n), cmax = 1e+10)

Arguments

x  a numerical data matrix, rows are points, columns are variables.
n  positive integer. Number of points.
p  positive integer. Number of variables.
gv  for mahalanofix a logical or 0-1 vector of length n. For mahalanofuz a numerical vector with values between 0 and 1.
cmax  positive number. used in solvecov if covariance matrix is singular.
method  "ml", "classical", "mcd" or "mve". Method to compute the covariance matrix estimator. See cov.rob, fixmahal.

Details

solvecov is used to invert the covariance matrix. The methods "mcd" and "mve" in mahalanofix do not work properly with point constellations with singular covariance matrices!

Value

A list of the following components:

md  vector of Mahalanobis distances.
mg  mean of the points indexed by gv, weighted mean in mahalanofuz.
covg  covariance matrix of the points indexed by gv, weighted covariance matrix in mahalanofuz.
covinv  covg inverted by solvecov.
coll  logical. If TRUE, covg has been (numerically) singular.
Note

Methods "mcd" and "mve" require library lqs.

Author(s)

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See Also

fixmahal, solvecov, cov.rob

Examples

```r
x <- c(1,2,3,4,5,6,7,8,9,10)
y <- c(1,2,3,8,7,6,5,8,9,10)
mahalanofix(cbind(x,y),gv=c(0,0,0,1,1,1,0,0))
mahalanofix(cbind(x,y),gv=c(0,0,0,1,1,1,0,0,0))
mahalanofix(cbind(x,y),gv=c(0,0,0,1,1,1,0,0,0),method="mcd")
mahalanofuz(cbind(x,y),gv=c(0,0,0.5,0.5,1,1,1,0.5,0.5,0))
```

Description

Generates an initial configuration of startn points from dataset x for the fixmahal fixed point iteration.

Thought only for use within fixmahal.

Usage

```r
mahalconf(x, no, startn, covall, plot)
```

Arguments

- `x`: numerical matrix. Rows are points, columns are variables.
- `no`: integer between 1 and nrow(x). Number of the first point of the configuration.
- `startn`: integer between 1 and nrow(x).
- `covall`: covariance matrix for the computation of the first Mahalanobis distances.
- `plot`: a string. If equal to "start" or "both", the first two variables and the first ncol(x)+1 points are plotted.
Details

`mahalconf` first chooses the \( p \) (number of variables) nearest points to point no. no in terms of the Mahalanobis distance w.r.t. \( \text{covall} \), so that there are \( p + 1 \) points. In every further step, the covariance matrix of the current configuration is computed and the nearest point in terms of the new Mahalanobis distance is added. `solvecov` is used to invert singular covariance matrices.

Value

A logical vector of length \( \text{nrow}(x) \).

Author(s)

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See Also

`fixmahal`, `solvecov`

Examples

```r
set.seed(4634)
face <- rFace(600, dMoNo=2, dNoEy=0, p=2)
mahalconf(face, no=200, startn=20, covall=cov(face), plot="start")
```

---

mergenormals

*Clustering by merging Gaussian mixture components*

Description

Clustering by merging Gaussian mixture components; computes all methods introduced in Hennig (2010) from an initial `mclust` clustering. See details section for details.

Usage

```r
mergenormals(xdata, mclustsummary=NULL, clustering, probs, muarray, Sigmaarray, z, method=NULL, cutoff=NULL, by=0.005, numberstop=NULL, renumber=TRUE, M=50, ...)
```

```r
## S3 method for class 'mergenorm'
summary(object, ...)
```

```r
## S3 method for class 'summary.mergenorm'
print(x, ...)
```
Arguments

- **xdata**: data (something that can be coerced into a matrix).
- **mclustsummary**: output object from `summary.mclustBIC` for xdata. Either mclustsummary or all of clustering, probs, muarray, Sigmaarray and z need to be specified (the latter are obtained from mclustsummary if they are not provided). I am not aware of restrictions of the usage of `mclustBIC` to produce an initial clustering; covariance matrix models can be restricted and a noise component can be included if desired, although I have probably not tested all possibilities.
- **clustering**: vector of integers. Initial assignment of data to mixture components.
- **probs**: vector of component proportions (for all components; should sum up to one).
- **muarray**: matrix of component means (rows).
- **Sigmaarray**: array of component covariance matrices (third dimension refers to component number).
- **z**: matrix of observation- (row-)wise posterior probabilities of belonging to the components (columns).
- **method**: one of "bhat", "ridge.uni", "ridge.ratio", "demp", "dipuni", "diptantrum", "predictive". See details.
- **cutoff**: numeric between 0 and 1. Tuning constant, see details and Hennig (2010). If not specified, the default values given in (9) in Hennig (2010) are used.
- **by**: real between 0 and 1. Interval width for density computation along the ridgeline, used for methods "ridge.uni" and "ridge.ratio". Methods "dipuni" and "dipitrantrum" require ridgeline computations and use it as well.
- **numberstop**: integer. If specified, cutoff is ignored and components are merged until the number of clusters specified here is reached.
- **renumber**: logical. If TRUE merged clusters are renumbered from 1 to their number. If not, numbers of the original clustering are used (numbers of components that were merged into others then will not appear).
- **M**: integer. Number of times the dataset is divided into two halves. Used if method="predictive".
- **...**: additional optional parameters to pass on to `ridgeline.diagnosis` or `mixpredictive` (in mergenormals).
- **object**: object of class `mergenorm`, output of `mergenormals`.
- **x**: object of class `summary.mergenorm`, output of `summary.mergenorm`.

Details

Mixture components are merged in a hierarchical fashion. The merging criterion is computed for all pairs of current clusters and the two clusters with the highest criterion value (lowest, respectively, for method="predictive") are merged. Then criterion values are recomputed for the merged cluster. Merging is continued until the criterion value to merge is below (or above, for method="predictive") the cutoff value. Details are given in Hennig (2010). The following criteria are offered, specified by the method-argument.

- **"ridge.uni"**: components are only merged if their mixture is unimodal according to Ray and Lindsay's (2005) ridgeline theory, see `ridgeline.diagnosis`. This ignores argument cutoff.
"ridge.ratio" ratio between density minimum between components and minimum of density maxima according to Ray and Lindsay’s (2005) ridgeline theory, see ridgeline.diagnosis.

"bhat" Bhattacharyya upper bound on misclassification probability between two components, see bhattacharyya.matrix.

"demp" direct estimation of misclassification probability between components, see Hennig (2010).

"dipuni" this uses method="ridge.ratio" to decide which clusters to merge but stops merging according to the p-value of the dip test computed as in Hartigan and Hartigan (1985), see dip.test.

"diptantrum" as "dipuni", but p-value of dip test computed as in Tantrum, Murua and Stuetzle (2003), see dipp.tantrum.

"predictive" this uses method="demp" to decide which clusters to merge but stops merging according to the value of prediction strength (Tibshirani and Walther, 2005) as computed in mixpredictive.

Value
mergenormals gives out an object of class mergenorm, which is a List with components

clustering integer vector. Final clustering.

clusternumbers vector of numbers of remaining clusters. These are given in terms of the original clusters even of renumber=TRUE, in which case they may be needed to understand the numbering of some further components, see below.

defunct.components vector of numbers of components that were "merged away".

valuemerged vector of values of the merging criterion (see details) at which components were merged.

mergedtonumbers vector of numbers of clusters to which the original components were merged.

parameters a list, if mclustsummary was provided. Entry no. i refers to number i in clusternumbers. The list entry i contains the parameters of the original mixture components that make up cluster i, as extracted by extract.mixturepars.

predvalues vector of prediction strength values for clusternumbers from 1 to the number of components in the original mixture, if method="predictive". See mixpredictive.

orig.decisionmatrix square matrix with entries giving the original values of the merging criterion (see details) for every pair of original mixture components.

new.decisionmatrix square matrix as orig.decisionmatrix, but with final entries; numbering of rows and columns corresponds to clusternumbers; all entries corresponding to other rows and columns can be ignored.

probs final cluster values of probs (see arguments) for merged components, generated by (potentially repeated) execution of mergeparameters out of the original ones. Numbered according to clusternumbers.

muarray final cluster means, analogous to probs.

Sigmaarray final cluster covariance matrices, analogous to probs.
mergenormals

- **z** final matrix of posterior probabilities of observations belonging to the clusters, analogous to probs.
- **noise** logical. If TRUE, there was a noise component fitted in the initial mclust clustering (see help for initialization in **mclustBIC**). In this case, a cluster number 0 indicates noise. noise is ignored by the merging methods and kept as it was originally.
- **method** as above.
- **cutoff** as above.

**summary.mergenorm** gives out a list with components clustering, clusternumbers, defunct.components, valuemerged, mergedtonumbers, predvalues, probs, muarray, Sigmaarray, z, noise, method, cutoff as above, plus onc (original number of components) and mnc (number of clusters after merging).

**Author(s)**

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**References**


**Examples**

```r
require(mclust)
require(MASS)
options(digits=3)
data(crabs)
dc <- crabs[,4:8]
cm <- mclustBIC(crabs[,4:8],G=9,modelNames="EEE")
scm <- summary(cm,crabs[,4:8])
cmnbhat <- mergenormals(crabs[,4:8],scm,method="bhat")
summary(cmnbhat)
cmndemp <- mergenormals(crabs[,4:8],scm,method="demp")
summary(cmndemp)
# Other methods take a bit longer, but try them!
# The values of by and M below are still chosen for reasonably fast execution.
```
# cmnrr <- mergenormals(crabs[,4:8],scm,method="ridge.ratio",by=0.05)
# cmd <- mergenormals(crabs[,4:8],scm,method="dip.tantrum",by=0.05)
# cmp <- mergenormals(crabs[,4:8],scm,method="predictive",M=3)

mergeparameters

New parameters from merging two Gaussian mixture components

Description

Re-computes pointwise posterior probabilities, mean and covariance matrix for a mixture component obtained by merging two mixture components in a Gaussian mixture.

Usage

mergeparameters(xdata, j1, j2, probs, muarray, Sigmaarray, z)

Arguments

xdata data (something that can be coerced into a matrix).

j1 integer. Number of first mixture component to be merged.

j2 integer. Number of second mixture component to be merged.

probs vector of component proportions (for all components; should sum up to one).

muarray matrix of component means (rows).

Sigmaarray array of component covariance matrices (third dimension refers to component number).

z matrix of observation- (row-)wise posterior probabilities of belonging to the components (columns).

Value

List with components

probs see above; sum of probabilities for original components j1 and j2 is now probs[j1]. Note that generally, also for the further components, values for the merged component are in place j1 and values in place j2 are not changed. This means that in order to have only the information for the new mixture after merging, the entries in places j2 need to be suppressed.

muarray see above; weighted mean of means of component j1 and j2 is now in place j1.

Sigmaarray see above; weighted covariance matrix handled as above.

z see above; original entries for columns j1 and j2 are summed up and now in column j1.

Author(s)

Christian Hennig <christian.hennig@unibo.it> https://www.unibo.it/sitoweb/christian.hennig/en/
References


Examples

```r
options(digits=3)
set.seed(98765)
require(mclust)
iriss <- iris[sample(150,20),-5]
irisBIC <- mclustBIC(iriss)
siris <- summary(irisBIC,iriss)
probs <- siris$parameters$pro
muarray <- siris$parameters$mean
Sigmaarray <- siris$parameters$variance$sigma
z <- siris$z
mpi <- mergeparameters(iriss,1,2,probs,muarray,Sigmaarray,z)
mpi$probs
mpi$muarray
```

---

**minsize**  
*Minimum size of regression fixed point cluster*

**Description**

Computes the minimum size of a fixed point cluster (FPC) which is found at least mtf times with approximated probability prob by ir fixed point iterations of fixreg.

Thought for use within fixreg.

**Usage**

```r
minsize(n, p, ir, mtf, prob = 0.5)
```

**Arguments**

- `n`: positive integer. Total number of points.
- `p`: positive integer. Number of independent variables.
- `ir`: positive integer. Number of fixed point iterations.
- `mtf`: positive integer.
- `prob`: numerical between 0 and 1.

**Details**

The computation is based on the binomial distribution with probability given by clusexpect with ir=1.
mixdens

Value
An integer.

Author(s)
Christian Hennig <christian.hennig@unibo.it> https://www.unibo.it/sitoweb/christian.hennig/en/

References

See Also
fixreg, clusexpect, itnumber

Examples

```r
minsize(500,4,7000,2)
```

---

mixdens  
Density of multivariate Gaussian mixture, `mclust` parameterisation

Description
Computes density values for data from a mixture of multivariate Gaussian distributions with parameters based on the way models are specified and parameters are stored in package `mclust`.

Usage

```r
mixdens(modelName, data, parameters)
```

Arguments

```r
modelName  
an mclust model name. See `mclustModelNames`

data  
data matrix; density values are computed for every observation (row).

parameters  
parameters of Gaussian mixture in the format used in the output of `summary.mclustBIC`.
```

Value
Vector of density values for the observations.

Author(s)
Christian Hennig <christian.hennig@unibo.it> https://www.unibo.it/sitoweb/christian.hennig/en/>
Examples

```r
set.seed(98765)
require(mclust)
iriss <- iris[sample(150,20),-5]
irisBIC <- mclustBIC(iriss)
siris <- summary(irisBIC,iriss)
round(mixdens(siris$modelName,iriss,siris$parameters),digits=2)
```

---

mixpredictive  

Prediction strength of merged Gaussian mixture

Description

Computes the prediction strength of clustering by merging Gaussian mixture components, see `mergenormals`. The predictive strength is defined according to Tibshirani and Walther (2005), carried out as described in Hennig (2010), see details.

Usage

```r
mixpredictive(xdata, Gcomp, Gmix, M=50, ...)
```

Arguments

- **xdata**: data (something that can be coerced into a matrix).
- **Gcomp**: integer. Number of components of the underlying Gaussian mixture.
- **Gmix**: integer. Number of clusters after merging Gaussian components.
- **M**: integer. Number of times the dataset is divided into two halves.
- **...**: further arguments that can potentially arrive in calls but are currently not used.

Details

The prediction strength for a certain number of clusters `Gmix` under a random partition of the dataset in halves A and B is defined as follows. Both halves are clustered with `Gmix` clusters. Then the points of A are classified to the clusters of B. This is done by use of the maximum a posteriori rule for mixtures as in Hennig (2010), differently from Tibshirani and Walther (2005). A pair of points A in the same A-cluster is defined to be correctly predicted if both points are classified into the same cluster on B. The same is done with the points of B relative to the clustering on A. The prediction strength for each of the clusterings is the minimum (taken over all clusters) relative frequency of correctly predicted pairs of points of that cluster. The final mean prediction strength statistic is the mean over all 2M clusterings.

Value

List with components

- **predcorr**: vector of length M with relative frequencies of correct predictions (clusterwise minimum).
- **mean.pred**: mean of `predcorr`. 
Author(s)

Christian Hennig <christian.hennig@unibo.it> https://www.unibo.it/sitoweb/christian.hennig/en/

References


See Also

prediction.strength for Tibshirani and Walther’s original method. mergenormals for the clustering method applied here.

Examples

set.seed(98765)
iriss <- iris[sample(150,20),-5]
mp <- mixpredictive(iriss,2,2,M=2)

mvdcoord

Mean/variance differences discriminant coordinates

Description

Discriminant projections as defined in Young, Marco and Odell (1987). The principle is to maximize the projection of a matrix consisting of the differences between the means of all classes and the first mean and the differences between the covariance matrices of all classes and the first covariance matrix.

Usage

mvdcoord(xd, clvecd, cnum=1, sphere="mcd", ...)

Arguments

xd the data matrix; a numerical object which can be coerced to a matrix.
clvecd integer vector of class numbers; length must equal nrow(xd).
cnum integer. Number of the class to which all differences are computed.
sphere a covariance matrix or one of "mve", "mcd", "classical", "none". The matrix used for sphering the data. "mcd" and "mve" are robust covariance matrices as implemented in cov.rob. "classical" refers to the classical covariance matrix. "none" means no sphering and use of the raw data.

... no effect
Value

List with the following components:

- **ev**: eigenvalues in descending order.
- **units**: columns are coordinates of projection basis vectors. New points \( x \) can be projected onto the projection basis vectors by \( x \%*% units \).
- **proj**: projections of \( x_d \) onto \( units \).

Author(s)

Christian Hennig <christian.hennig@unibo.it> https://www.unibo.it/sitoweb/christian.hennig/en/

References


See Also

- `plotcluster` for straightforward discriminant plots. `discrproj` for alternatives. `rFace` for generation of the example data used below.

Examples

```r
set.seed(4634)
faced <- rFace(300,dMoNo=2,dNoEy=0,p=3)
grface <- as.integer(attr(faced,"grouping"))
mcf <- mvcoord(faced,grface)
plot(mcf$proj,col=grface)
# ...done in one step by function plotcluster.
```

Description

Neighborhood based discriminant coordinates as defined in Hastie and Tibshirani (1996) and a robustified version as defined in Hennig (2003). The principle is to maximize the projection of a between classes covariance matrix, which is defined by averaging the between classes covariance matrices in the neighborhoods of all points.

Usage

```r
ncoord(xd, clvecd, nn=50, weighted=FALSE,
       sphere="mcd", orderall=TRUE, countmode=1000, ...)
```
**Arguments**

- **xd**: the data matrix; a numerical object which can be coerced to a matrix.
- **clvecd**: integer vector of class numbers; length must equal `nrow(xd)`.
- **nn**: integer. Number of points which belong to the neighborhood of each point (including the point itself).
- **weighted**: logical. `FALSE` corresponds to the original method of Hastie and Tibshirani (1996). If `TRUE`, the between classes covariance matrices B are weighted by `w/trace B`, where `w` is some weight depending on the sizes of the classes in the neighborhood. Division by `trace B` reduces the effect of outliers. `TRUE` cooresponds to WNC as defined in Hennig (2003).
- **sphere**: a covariance matrix or one of "mve", "mcd", "classical", "none". The matrix used for sphering the data. "mcd" and "mve" are robust covariance matrices as implemented in `cov.rob`. "classical" refers to the classical covariance matrix. "none" means no sphering and use of the raw data.
- **orderall**: logical. By default, the neighborhoods are computed by ordering all points each time. If `FALSE`, the neighborhoods are computed by selecting `nn` times the nearest point from the remaining points, which may be faster sometimes.
- **countmode**: optional positive integer. Every `countmode` algorithm runs `ncoord` shows a mesage.
- **...** no effect

**Value**

List with the following components

- **ev**: eigenvalues in descending order.
- **units**: columns are coordinates of projection basis vectors. New points `x` can be projected onto the projection basis vectors by `x %*% units`
- **proj**: projections of `xd` onto `units`.

**Author(s)**

Christian Hennig <christian.hennig@unibo.it> [https://www.unibo.it/sitoweb/christian.hennig/en/](https://www.unibo.it/sitoweb/christian.hennig/en/)

**References**


neginc

See Also

plotcluster for straightforward discriminant plots. discrproj for alternatives. rFace for generation of the example data used below.

Examples

```r
set.seed(4634)
face <- rFace(600,dMoNo=2,dNoEy=0)
grface <- as.integer(attr(face,"grouping"))
cmp <- ncoord(face,grface)
plot(nmp$proj,col=grface)
ncmp2 <- ncoord(face,grface,weighted=TRUE)
plot(nmp2$proj,col=grface)
# ...done in one step by function plotcluster.
```

neginc

Neg-entropy normality index for cluster validation

Description

Cluster validity index based on the neg-entropy distances of within-cluster distributions to normal distribution, see Lago-Fernandez and Corbacho (2010).

Usage

```r
neginc(x,clustering)
```

Arguments

- `x`: something that can be coerced into a numerical matrix. Euclidean dataset.
- `clustering`: vector of integers with length = nrow(x); indicating the cluster for each observation.

Value

Index value, see Lago-Fernandez and Corbacho (2010). The lower (i.e., the more negative) the better.

Author(s)

Christian Hennig <christian.hennig@unibo.it> https://www.unibo.it/sitoweb/christian.hennig/en/

References

Examples

options(digits=3)
iriss <- as.matrix(iris[c(1:10,51:55,101:105),-5])
irisc <- as.numeric(iris[c(1:10,51:55,101:105),5])
neginc(iriss,irisc)

nselectboot

Selection of the number of clusters via bootstrap

Description

Selection of the number of clusters via bootstrap as explained in Fang and Wang (2012). Several times 2 bootstrap samples are drawn from the data and the number of clusters is chosen by optimising an instability estimation from these pairs.

In principle all clustering methods can be used that have a CBI-wrapper, see clusterboot, kmeansCBI. However, the currently implemented classification methods are not necessarily suitable for all of them, see argument classification.

Usage

nselectboot(data,B=50,distances=inherits(data,"dist"),
            clustermethod=NULL,
            classification="averagedist",centroidname = NULL,
            krange=2:10, count=FALSE,nnk=1,
            largeisgood=FALSE,...)

Arguments

data something that can be coerced into a matrix. The data matrix - either an n*p-data matrix (or data frame) or an n*n-dissimilarity matrix (or dist-object).

B integer. Number of resampling runs.

distances logical. If TRUE, the data is interpreted as dissimilarity matrix. If data is a dist-object, distances=TRUE automatically, otherwise distances=FALSE by default. This means that you have to set it to TRUE manually if data is a dissimilarity matrix.

clustermethod an interface function (the function name, not a string containing the name, has to be provided!). This defines the clustering method. See the "Details"-section of clusterboot and kmeansCBI for the format. Clustering methods for nselectboot must have a k-argument for the number of clusters and must otherwise follow the specifications in clusterboot. Note that nselectboot won’t work with CBI-functions that implicitly already estimate the number of clusters such as pamkCBI; use claraCBI if you want to run it for pam/clara clustering.

classification string. This determines how non-clustered points are classified to given clusters. Options are explained in classifdist (if distances=TRUE) and classifnp (otherwise). Certain classification methods are connected to certain clustering methods. classification="averagedist" is recommended for average
nselectboot

linkage, classification="centroid" is recommended for k-means, clara and pam (with distances it will work with claraCBI only), classification="knn" with nnk=1 is recommended for single linkage and classification="qda" is recommended for Gaussian mixtures with flexible covariance matrices.

centroidname string. Indicates the name of the component of CBIoutput$result that contains the cluster centroids in case of classification="centroid", where CBIoutput is the output object of clustermethod. If clustermethod is kmeansCBI or claraCBI, centroids are recognised automatically if centroidname=NULL. If centroidname=NULL and distances=FALSE, cluster means are computed as the cluster centroids.

krange integer vector; numbers of clusters to be tried.

count logical. If TRUE, numbers of clusters and bootstrap runs are printed.

nnk number of nearest neighbours if classification="knn", see classifdist (if distances=TRUE) and classifnp (otherwise).

largeisgood logical. If TRUE, output component stabk is taken as one minus the original instability value so that larger values of stabk are better.

... arguments to be passed on to the clustering method.

Value

nselectboot returns a list with components kopt, stabk, stab.

kopt optimal number of clusters.

stabk mean instability values for numbers of clusters (or one minus this if largeisgood=TRUE).

stab matrix of instability values for all bootstrap runs and numbers of clusters.

Author(s)

Christian Hennig <christian.hennig@unibo.it> https://www.unibo.it/sitoweb/christian.hennig/en/

References


See Also

classifdist, classifnp, clusterboot, kmeansCBI

Examples

set.seed(20000)
face <- rFace(50,dMoNo=2,dNoEy=0,p=2)
nselectboot(dist(face),B=2,clustermethod=disthclustCBI,
method="average",krange=5:7)

nselectboot(dist(face),B=2,clustermethod=claraCBI,
pamk

**Partitioning around medoids with estimation of number of clusters**

**Description**

This calls the function `pam` or `clara` to perform a partitioning around medoids clustering with the number of clusters estimated by optimum average silhouette width (see `pam.object`) or Calinski-Harabasz index (`calinhara`). The Duda-Hart test (`dudahart2`) is applied to decide whether there should be more than one cluster (unless 1 is excluded as number of clusters or data are dissimilarities).

**Usage**

```r
pamk(data, krange=2:10, criterion="asw", usepam=TRUE, 
     scaling=FALSE, alpha=0.001, diss=inherits(data, "dist"), 
     critout=FALSE, ns=10, seed=NULL, ...)
```

**Arguments**

- `data`: a data matrix or data frame or something that can be coerced into a matrix, or dissimilarity matrix or object. See `pam` for more information.
- `krange`: integer vector. Numbers of clusters which are to be compared by the average silhouette width criterion. Note: average silhouette width and Calinski-Harabasz can't estimate number of clusters `nc=1`. If 1 is included, a Duda-Hart test is applied and 1 is estimated if this is not significant.
- `criterion`: one of "asw", "multiasw" or "ch". Determines whether average silhouette width (as given out by `pam/clara`, or as computed by `distcritmulti` if "multiasw" is specified; recommended for large data sets with `usepam=FALSE`) or Calinski-Harabasz is applied. Note that the original Calinski-Harabasz index is not defined for dissimilarities; if dissimilarity data is run with criterion="ch", the dissimilarity-based generalisation in Hennig and Liao (2013) is used.
- `usepam`: logical. If TRUE, `pam` is used, otherwise `clara` (recommended for large datasets with 2,000 or more observations; dissimilarity matrices can not be used with `clara`).
- `scaling`: either a logical value or a numeric vector of length equal to the number of variables. If scaling is a numeric vector with length equal to the number of variables, then each variable is divided by the corresponding value from scaling. If scaling is TRUE then scaling is done by dividing the (centered) variables by their root-mean-square, and if scaling is FALSE, no scaling is done.
- `alpha`: numeric between 0 and 1, tuning constant for `dudahart2` (only used for 1-cluster test).
**diss**

Logical flag: if TRUE (default for dist or dissimilarity-objects), then data will be considered as a dissimilarity matrix (and the potential number of clusters 1 will be ignored). If FALSE, then data will be considered as a matrix of observations by variables.

**critout**

Logical. If TRUE, the criterion value is printed out for every number of clusters.

**ns**

Passed on to `distcritmulti` if criterion="multiasw".

**seed**

Passed on to `distcritmulti` if criterion="multiasw".

... Further arguments to be transferred to `pam` or `clara`.

### Value

A list with components

- **pamobject**
  - The output of the optimal run of the `pam`-function.
- **nc**
  - The optimal number of clusters.
- **crit**
  - Vector of criterion values for numbers of clusters. `crit[1]` is the p-value of the Duda-Hart test if 1 is in `krange` and `diss=FALSE`.

### Note

`clara` and `pam` can handle NA-entries (see their documentation) but `dudahart2` cannot. Therefore NA should not occur if 1 is in `krange`.

### Author(s)

Christian Hennig &lt;christian.hennig@unibo.it&gt; https://www.unibo.it/sitoweb/christian.hennig/en/

### References


### See Also

`pam`, `clara`, `distcritmulti`
piridge

Examples

```r
options(digits=3)
set.seed(20000)
face <- rFace(50,dMoNo=2,dNoEy=0,p=2)
pk1 <- pamk(face,krange=1:5,criterion="asw",critout=TRUE)
pk2 <- pamk(face,krange=1:5,criterion="multiasw",ns=2,critout=TRUE)
# "multiasw" is better for larger data sets, use larger ns then.
pk3 <- pamk(face,krange=1:5,criterion="ch",critout=TRUE)
```

---

piridge

*Ridgeline Pi-function*

Description

The Pi-function is given in (6) in Ray and Lindsay, 2005. Equating it to the mixture proportion yields locations of two-component Gaussian mixture density extrema.

Usage

```r
piridge(alpha, mu1, mu2, Sigma1, Sigma2, showplot=FALSE)
```

Arguments

- **alpha**: sequence of values between 0 and 1 for which the Pi-function is computed.
- **mu1**: mean vector of component 1.
- **mu2**: mean vector of component 2.
- **Sigma1**: covariance matrix of component 1.
- **Sigma2**: covariance matrix of component 2.
- **showplot**: logical. If TRUE, the Pi-function is plotted against alpha.

Value

Vector of values of the Pi-function for values of alpha.

Author(s)

Christian Hennig <christian.hennig@unibo.it> [https://www.unibo.it/sitoweb/christian.hennig/en/](https://www.unibo.it/sitoweb/christian.hennig/en/)

References


Examples

```r
q <- piridge(seq(0,1,.1),c(1,1),c(2,5),diag(2),diag(2))
```
piridge.zeroes

Extrema of two-component Gaussian mixture

Description
By use of the Pi-function in Ray and Lindsay, 2005, locations of two-component Gaussian mixture
density extrema or saddlepoints are computed.

Usage
piridge.zeroes(prop, mu1, mu2, Sigma1, Sigma2, alphamin=0,
                 alphamax=1, by=0.001)

Arguments
prop proportion of mixture component 1.
mu1 mean vector of component 1.
mu2 mean vector of component 2.
Sigma1 covariance matrix of component 1.
Sigma2 covariance matrix of component 2.
alphamin minimum alpha value.
alphamax maximum alpha value.
by interval between alpha-values where to look for extrema.

Value
list with components
number.zeroes number of zeroes of Pi-function, i.e., extrema or saddlepoints of density.
estimated.roots estimated alpha-values at which extrema or saddlepoints occur.

Author(s)
Christian Hennig <christian.hennig@unibo.it> https://www.unibo.it/sitoweb/christian.
hennig/en/

References
Statistics, 33, 2042-2065.

Examples
q <- piridge.zeroes(0.2, c(1,1), c(2,5), diag(2), diag(2), by=0.1)
plot.valstat

Simulation-standardised plot and print of cluster validation statistics

Description

Visualisation and print function for cluster validation output compared to results on simulated random clusterings. The print method can also be used to compute and print an aggregated cluster validation index.

Unlike for many other plot methods, the additional arguments of plot.valstat are essential. print.valstat should make good sense with the defaults, but for computing the aggregate index need to be set.

Usage

```r
## S3 method for class 'valstat'
plot(x,simobject=NULL,statistic="sindex",
     xlim=NULL,ylim=c(0,1),
     nmethods=length(x)-5,
     col=1:nmethods,cex=1,pch=c("c","f","a","n"),
     simcol=rep(grey(0.7),4),
     shift=c(-0.1,-1/3,1/3,0.1),include.othernc=NULL,...)

## S3 method for class 'valstat'
print(x,statistics=x$statistics,
      nmethods=length(x)-5,aggregate=FALSE,
      weights=NULL,digits=2,
      include.othernc=NULL,...)
```

Arguments

- `x` object of class "valstat", such as sublists stat, qstat, sstat of clusterbenchstats-output.
- `simobject` list of simulation results as produced by randomclustersim and documented there; typically sublist sim of clusterbenchstats-output.
- `statistic` one of "avewithin","mnn","variation","diameter", "gap","sindex","minsep","asw","dindex","highdgap","pg","withinss","entropy","pamc","kdnorm","kdunif","dmode": validation statistic to be plotted.
- `xlim` passed on to plot. Default is the range of all involved numbers of clusters, minimum minus 0.5 to maximum plus 0.5.
- `ylim` passed on to plot.
- `nmethods` integer. Number of clustering methods to involve (these are those from number 1 to nmethods specified in x$name).
col colours used for the different clustering methods.
cex passed on to plot.
pch vector of symbols for random clustering results from `stupidkcentroids, stupidkfn, stupidkaven, stupidknn`. To be passed on to plot.
simcol vector of colours used for random clustering results in order `stupidkcentroids, stupidkfn, stupidkaven, stupidknn`.
shift numeric vector. Indicates the amount to which the results from `stupidkcentroids, stupidkfn, stupidkaven, stupidknn` are plotted to the right of their respective number of clusters (negative numbers plot to the left).
include.othernc this indicates whether methods should be included that estimated their number of clusters themselves and gave a result outside the standard range as given by x$minG and x$maxG. If not NULL, this is a list of integer vectors of length 2. The first number is the number of the clustering method (the order is determined by argument x$name), the second number is the number of clusters for those methods that estimate the number of clusters themselves and estimated a number outside the standard range. Normally what will be used here, if not NULL, is the output parameter cm$othernc of `clusterbenchstats`, see also `cluster.magazine`.
statistics vector of character strings specifying the validation statistics that will be included in the output (unless you want to restrict the output for some reason, the default should be fine.
aggregate logical. If TRUE, an aggregate validation statistic will be computed as the weighted mean of the involved statistic. This requires weights to be set. In order for this to make sense, values of the validation statistics should be comparable, which is achieved by standardisation in `clusterbenchstats`. Accordingly, x should be the qstat or sstat-component of the `clusterbenchstats`-output rather than the stat-component.
weights vector of numericals. Weights for computation of the aggregate statistic in case that aggregate=TRUE. The order of clustering methods corresponding to the weight vector is given by x$name.
digits minimal number of significant digits, passed on to `print.table`.
... no effect.

Details

Whereas `print.valstat`, at least with aggregate=TRUE makes more sense for the qstat or sstat-component of the `clusterbenchstats`-output rather than the stat-component, `plot.valstat` should be run with the stat-component if simobject is specified, because the simulated cluster validity statistics are unstandardised and need to be compared with unstandardised values on the dataset of interest.

`print.valstat` will print all values for all validation indexes and the aggregated index (in case of aggregate=TRUE and set weights will be printed last.

Value

`print.valstats` returns the results table as invisible object.
Author(s)

Christian Hennig <christian.hennig@unibo.it> https://www.unibo.it/sitoweb/christian.hennig/en/

References


See Also

cornerbenchstats.valstat.object, cluster.magazine

Examples

```r
set.seed(20000)
options(digits=3)
face <- rFace(10,dMoNo=2,dNoEy=0,p=2)
clustermethod=c("kmeansCI","hclustCBI","hclustCBI")
clustermethodpars <- list()
clustermethodpars[[2]]$method <- "ward.D2"
clustermethodpars[[3]]$method <- "single"
methodname <- c("kmeans","ward","single")
cbs <- clusterbenchstats(face,G=2:3,clustermethod=clustermethod,
methodname=methodname,distmethod=rep(FALSE,3),
clustermethodpars=clustermethodpars,nnruns=2,kmruns=2,fnruns=2,avenruns=2)
plot(cbs$stat,cbs$sim)
plot(cbs$stat,cbs$sim,statistic="dindex")
plot(cbs$stat,cbs$sim,statistic="avewithin")
pcbs <- print(cbs$sstat,aggregate=TRUE,weights=c(1,0,0,0,1,0,0,0,0,1,0,0,0))
# Some of the values are "NaN" because due to the low number of runs of
# the stupid clustering methods there is no variation. If this happens
# in a real application, nnruns etc. should be chosen higher than 2.
# Also useallg=TRUE in clusterbenchstats may help.
#
# Finding the best aggregated value:
mpcbs <- as.matrix(pcbs[[17]][,-1])
which(mpcbs=max(mpcbs),arr.ind=TRUE)
# row=1 refers to the first clustering method kmeansCI,
# col=2 refers to the second number of clusters, which is 3 in g=2:3.
```
Description

Plots to distinguish given classes by ten available projection methods. Includes classical discriminant coordinates, methods to project differences in mean and covariance structure, asymmetric methods (separation of a homogeneous class from a heterogeneous one), local neighborhood-based methods and methods based on robust covariance matrices. One-dimensional data is plotted against the cluster number.

Usage

plotcluster(x, clvecd, clnum=NULL,
    method=ifelse(is.null(clnum),"dc","awc"),
    bw=FALSE,
    ignorepoints=FALSE, ignoreenum=0, pointsbyclvecd=TRUE,
    xlab=NULL, ylab=NULL,
    pch=NULL, col=NULL, ...)

Arguments

x the data matrix; a numerical object which can be coerced to a matrix.
clvecd vector of class numbers which can be coerced into integers; length must equal nrow(xd).
method one of
    "dc" usual discriminant coordinates, see discrcoord,
    "bc" Bhattacharyya coordinates, first coordinate showing mean differences,
    second showing covariance matrix differences, see batcoord,
    "vbc" variance dominated Bhattacharyya coordinates, see batcoord,
    "mvdc" added mean and variance differences optimizing coordinates, see mvdcoord,
    "adc" asymmetric discriminant coordinates, see adcoord,
    "awc" asymmetric discriminant coordinates with weighted observations, see awcoord,
    "arc" asymmetric discriminant coordinates with weighted observations and robust MCD-covariance matrix, see awcoord,
    "nc" neighborhood based coordinates, see ncoord,
    "wnc" neighborhood based coordinates with weighted neighborhoods, see ncoord,
    "anc" asymmetric neighborhood based coordinates, see ancoord.

Note that "bc", "vbc", "adc", "awc", "arc" and "anc" assume that there are only two classes.

clnum integer. Number of the class which is attempted to plot homogeneously by
    "asymmetric methods", which are the methods assuming that there are only two classes, as indicated above. clnum is ignored for methods "dc" and "nc".
plotcluster

The `plotcluster` function provides a way to visualize the results of a cluster analysis. It allows for the distinction of classes by symbols or colors, and it offers options for handling points with specific labels and for specifying additional plot parameters.

- **bw**: logical. If TRUE, the classes are distinguished by symbols, and the default color is black/white. If FALSE, the classes are distinguished by colors, and the default symbol is pch=1.
- **ignorepoints**: logical. If TRUE, points with label ignorenum in clvecd are ignored in the computation for method and are only projected afterwards onto the resulting units. If pch=NULL, the plot symbol for these points is "N".
- **ignorenum**: one of the potential values of the components of clvecd. Only has effect if ignorepoints=TRUE, see above.
- **pointsbyclvecd**: logical. If TRUE and pch=NULL and/or col=NULL, some hopefully suitable plot symbols (numbers and letters) and colors are chosen to distinguish the values of clvecd, starting with "1"/"black" for the cluster with the smallest clvecd-code (note that colors for clusters with numbers larger than minimum number +3 are drawn at random from all available colors). FALSE produces potentially less reasonable (but nonrandom) standard colors and symbols if method is "dc" or "nc", and will only distinguish whether clvecd=clnum or not for the other methods.
- **xlab**: label for x-axis. If NULL, a default text is used.
- **ylab**: label for y-axis. If NULL, a default text is used.
- **pch**: plotting symbol, see `par`. If NULL, the default is used.
- **col**: plotting color, see `par`. If NULL, the default is used.
- **...**: additional parameters passed to `plot` or the projection methods.

**Note**
For some of the asymmetric methods, the area in the plot occupied by the "homogeneous class" (see clnum above) may be very small, and it may make sense to run plotcluster a second time specifying plot parameters xlim and ylim in a suitable way. It often makes sense to magnify the plot region containing the homogeneous class in this way so that its separation from the rest can be seen more clearly.

**Author(s)**

Christian Hennig <christian.hennig@unibo.it> [https://www.unibo.it/sitoweb/christian.hennig/en/]

**References**


See Also

discrcoord, batcoord, mvdcoord, adcoord, awcoord, ncoord, ancoord.
discrproj is an interface to all these projection methods.
rFace for generation of the example data used below.

Examples

set.seed(4634)
face <- rFace(300, dMoNo=2, dNoEy=0)
grface <- as.integer(attr(face,"grouping"))
plotcluster(face,grface)
plotcluster(face,grface==1)
plotcluster(face,grface, clnum=1, method="vbc")

prediction.strength

Prediction strength for estimating number of clusters

Description

Computes the prediction strength of a clustering of a dataset into different numbers of components. The prediction strength is defined according to Tibshirani and Walther (2005), who recommend to choose as optimal number of cluster the largest number of clusters that leads to a prediction strength above 0.8 or 0.9. See details.

Various clustering methods can be used, see argument clustermethod. In Tibshirani and Walther (2005), only classification to the nearest centroid is discussed, but more methods are offered here, see argument classification.

Usage

prediction.strength(xdata, Gmin=2, Gmax=10, M=50,
clustermethod=kmeansCBI,
classification="centroid", centroidname = NULL,
cutoff=0.8,nnk=1,
distances=inherits(xdata,"dist"),count=FALSE,...)

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

Arguments

xdata data (something that can be coerced into a matrix).
Gmin integer. Minimum number of clusters. Note that the prediction strength for 1 cluster is trivially 1, which is automatically included if GMin>1. Therefore GMin<2 is useless.
Gmax integer. Maximum number of clusters.
M integer. Number of times the dataset is divided into two halves.
clustermethod an interface function (the function name, not a string containing the name, has to be provided!). This defines the clustering method. See the "Details"-section of clusterboot and kmeansCBI for the format. Clustering methods for prediction.strength must have a k-argument for the number of clusters, must operate on n times p data matrices and must otherwise follow the specifications in clusterboot Note that prediction.strength won't work with CBI-functions that implicitly already estimate the number of clusters such as pamkCBI; use claraCBI if you want to run it for pam/clara clustering.

classification string. This determines how non-clustered points are classified to given clusters. Options are explained in classifnp and classifdist, the latter for dissimilarity data. Certain classification methods are connected to certain clustering methods. classification="averagedist" is recommended for average linkage, classification="centroid" is recommended for k-means, clara and pam (with distances it will work with claraCBI only), classification="knn" with nnk=1 is recommended for single linkage and classification="qda" is recommended for Gaussian mixtures with flexible covariance matrices.

centroidname string. Indicates the name of the component of CBIoutput$result that contains the cluster centroids in case of classification="centroid", where CBIoutput is the output object of clustermethod. If clustermethod is kmeansCBI or claraCBI, centroids are recognised automatically if centroidname=NULL. If centroidname=NULL and distances=FALSE, cluster means are computed as the cluster centroids.

cutoff numeric between 0 and 1. The optimal number of clusters is the maximum one with prediction strength above cutoff.

nnk number of nearest neighbours if classification="knn", see classifnp.

distances logical. If TRUE, data will be interpreted as dissimilarity matrix, passed on to clustering methods as "dist"-object, and classifdist will be used for classification.

count logical. TRUE will print current number of clusters and simulation run number on the screen.

x object of class predstr.

... arguments to be passed on to the clustering method.

details

The prediction strength for a certain number of clusters k under a random partition of the dataset in halves A and B is defined as follows. Both halves are clustered with k clusters. Then the points of A are classified to the clusters of B. In the original paper this is done by assigning every observation in A to the closest cluster centroid in B (corresponding to classification="centroid"), but other methods are possible, see classifnp. A pair of points A in the same A-cluster is defined to be correctly predicted if both points are classified into the same cluster on B. The same is done with the points of B relative to the clustering on A. The prediction strength for each of the clusterings is the minimum (taken over all clusters) relative frequency of correctly predicted pairs of points of that cluster. The final mean prediction strength statistic is the mean over all 2M clusterings.
**Value**

`prediction.strength` gives out an object of class `predstr`, which is a list with components

- **`predcorr`**: list of vectors of length `M` with relative frequencies of correct predictions (clusterwise minimum). Every list entry refers to a certain number of clusters.
- **`mean.pred`**: means of `predcorr` for all numbers of clusters.
- **`optimalk`**: optimal number of clusters.
- **`cutoff`**: see above.
- **`method`**: a string identifying the clustering method.
- **`Gmax`**: see above.
- **`M`**: see above.

**Author(s)**

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**References**


**See Also**

- `kmeansCBI`, `classifnp`

**Examples**

```r
options(digits=3)
set.seed(98765)
iriss <- iris[sample(150,20),-5]
prediction.strength(iriss,2,3,M=3)
prediction.strength(iriss,2,3,M=3,clustermethod=claraCBI)
```

# The examples are fast, but of course M should really be larger.

---

**randcmatrix**

**Random partition matrix**

**Description**

For use within `regmix`. Generates a random 0-1-matrix with `n` rows and `cln` columns so that every row contains exactly one one and every columns contains at least `p+3` ones.

**Usage**

`randcmatrix(n,cln,p)`
Arguments

- **n**: positive integer. Number of rows.
- **cln**: positive integer. Number of columns.
- **p**: positive integer. See above.

Value

An n*cln-matrix.

Author(s)

Christian Hennig <christian.hennig@unibo.it> https://www.unibo.it/sitoweb/christian.hennig/en/

See Also

regmix

Examples

```r
set.seed(111)
randcmatrix(10,2,1)
```

---

**randconf**

*Generate a sample indicator vector*

Description

Generates a logical vector of length n with p TRUEs.

Usage

```r
randconf(n, p)
```

Arguments

- **n**: positive integer.
- **p**: positive integer.

Value

A logical vector.

Author(s)

Christian Hennig <christian.hennig@unibo.it> https://www.unibo.it/sitoweb/christian.hennig/en/
randomclustersim

See Also
	sample

Examples

randconf(10,3)

randomclustersim  Simulation of validity indexes based on random clusterings

Description

For a given dataset this simulates random clusterings using stupidkcentroids, stupidknn, stupidkfn, and stupidkaven. It then computes and stores a set of cluster validity indexes for every clustering.

Usage

randomclustersim(datadist, datanp=NULL, npstats=FALSE, useboot=FALSE,
bootmethod="nselectboot",
bootruns=25,
G, nnruns=100, kmruns=100, fnruns=100, avenruns=100,
nnk=4, dnnk=2,
pamcrit=TRUE,
multicore=FALSE, cores=detectCores()-1, monitor=TRUE)

Arguments

datadist distances on which validation-measures are based, dist object or distance matrix.
datanp optional observations times variables data matrix, see npstats.
npstats logical. If TRUE, distsimilarly is called and the two statistics computed there are added to the output. These are based on datanp and require datanp to be specified.
useboot logical. If TRUE, a stability index (either nselectboot or prediction.strength) will be involved.
bootmethod either "nselectboot" or "prediction.strength"; stability index to be used if useboot=TRUE.
bootruns integer. Number of resampling runs. If useboot=TRUE, passed on as B to nselectboot or M to prediction.strength.
G vector of integers. Numbers of clusters to consider.
nnrns integer. Number of runs of stupidknn.
kmruns integer. Number of runs of stupidkcentroids.
fnruns integer. Number of runs of stupidkfn.
avenruns integer. Number of runs of stupidkaven.
randomclusternsim

\texttt{nnk} \hspace{1cm} \texttt{nnk}-argument to be passed on to \texttt{cqcluster.stats}.

\texttt{dnnk} \hspace{1cm} \texttt{nnk}-argument to be passed on to \texttt{distrsimilarity}.

\texttt{pamcrit} \hspace{1cm} \texttt{pamcrit}-argument to be passed on to \texttt{cqcluster.stats}.

\texttt{multicore} \hspace{1cm} logical. If TRUE, parallel computing is used through the function \texttt{mclapply} from package parallel; read warnings there if you intend to use this; it won’t work on Windows.

\texttt{cores} \hspace{1cm} integer. Number of cores for parallelisation.

\texttt{monitor} \hspace{1cm} logical. If TRUE, it will print some runtime information.

\begin{description}
\item[Value] List with components
\item[\texttt{nn}] list, indexed by number of clusters. Every entry is a data frame with \texttt{nnruns} observations for every simulation run of \texttt{stupidknn}. The variables of the data frame are \texttt{avewithin}, \texttt{mnd}, \texttt{cvnnd}, \texttt{maxdiameter}, \texttt{widestgap}, \texttt{sindex}, \texttt{minsep}, \texttt{asw}, \texttt{dindex}, \texttt{denscut}, \texttt{highdgap}, \texttt{pearsongamma}, \texttt{withinss}, \texttt{entropy}. If \texttt{pamcrit}=TRUE also \texttt{pamc}, if \texttt{npstats}=TRUE also \texttt{kdnorm}, \texttt{kdunif}. All these are cluster validation indexes; documented as values of \texttt{clustatsum}.
\item[\texttt{fn}] list, indexed by number of clusters. Every entry is a data frame with \texttt{fnruns} observations for every simulation run of \texttt{stupidkfn}. The variables of the data frame are \texttt{avewithin}, \texttt{mnd}, \texttt{cvnnd}, \texttt{maxdiameter}, \texttt{widestgap}, \texttt{sindex}, \texttt{minsep}, \texttt{asw}, \texttt{dindex}, \texttt{denscut}, \texttt{highdgap}, \texttt{pearsongamma}, \texttt{withinss}, \texttt{entropy}. If \texttt{pamcrit}=TRUE also \texttt{pamc}, if \texttt{npstats}=TRUE also \texttt{kdnorm}, \texttt{kdunif}. All these are cluster validation indexes; documented as values of \texttt{clustatsum}.
\item[\texttt{aven}] list, indexed by number of clusters. Every entry is a data frame with \texttt{avenruns} observations for every simulation run of \texttt{stupidkaven}. The variables of the data frame are \texttt{avewithin}, \texttt{mnd}, \texttt{cvnnd}, \texttt{maxdiameter}, \texttt{widestgap}, \texttt{sindex}, \texttt{minsep}, \texttt{asw}, \texttt{dindex}, \texttt{denscut}, \texttt{highdgap}, \texttt{pearsongamma}, \texttt{withinss}, \texttt{entropy}. If \texttt{pamcrit}=TRUE also \texttt{pamc}, if \texttt{npstats}=TRUE also \texttt{kdnorm}, \texttt{kdunif}. All these are cluster validation indexes; documented as values of \texttt{clustatsum}.
\item[\texttt{km}] list, indexed by number of clusters. Every entry is a data frame with \texttt{kmruns} observations for every simulation run of \texttt{stupidkcentroids}. The variables of the data frame are \texttt{avewithin}, \texttt{mnd}, \texttt{cvnnd}, \texttt{maxdiameter}, \texttt{widestgap}, \texttt{sindex}, \texttt{minsep}, \texttt{asw}, \texttt{dindex}, \texttt{denscut}, \texttt{highdgap}, \texttt{pearsongamma}, \texttt{withinss}, \texttt{entropy}. If \texttt{pamcrit}=TRUE also \texttt{pamc}, if \texttt{npstats}=TRUE also \texttt{kdnorm}, \texttt{kdunif}. All these are cluster validation indexes; documented as values of \texttt{clustatsum}.
\item[\texttt{nnruns}] number of involved runs of \texttt{stupidknn},
\item[\texttt{fnruns}] number of involved runs of \texttt{stupidkfn},
\item[\texttt{avenruns}] number of involved runs of \texttt{stupidkaven},
\item[\texttt{kmruns}] number of involved runs of \texttt{stupidkcentroids},
\item[\texttt{boot}] if \texttt{useboot}=TRUE, stability value; \texttt{stabk} for method \texttt{nselectboot}; \texttt{mean.pred} for method \texttt{prediction.strength}.
\end{description}
**regmix**

**Mixture Model ML for Clusterwise Linear Regression**

**Description**

Computes an ML-estimator for clusterwise linear regression under a regression mixture model with Normal errors. Parameters are proportions, regression coefficients and error variances, all independent of the values of the independent variable, and all may differ for different clusters. Computation is by the EM-algorithm. The number of clusters is estimated via the Bayesian Information Criterion (BIC). Note that package `flexmix` has more sophisticated tools to do the same thing and is recommended. The functions are kept in here only for compatibility reasons.
Usage

regmix(indep, dep, ir=1, nclust=1:7, icrit=1.e-5, minsig=1.e-6, warnings=FALSE)
regem(indep, dep, m, cln, icrit=1.e-5, minsig=1.e-6, warnings=FALSE)

Arguments

indep numerical matrix or vector. Independent variables.
dep numerical vector. Dependent variable.
ir positive integer. Number of iteration runs for every number of clusters.
nclust vector of positive integers. Numbers of clusters.
icrit positive numerical. Stopping criterion for the iterations (difference of loglikelihoods).
minsig positive numerical. Minimum value for the variance parameters (likelihood is unbounded if variances are allowed to converge to 0).
warnings logical. If TRUE, warnings are given during the EM iteration in case of collinear regressors, too small mixture components and error variances smaller than minimum. In the former two cases, the algorithm is terminated without a result, but an optimal solution is still computed from other algorithm runs (if there are others). In the latter case, the corresponding variance is set to the minimum.
cln positive integer. (Single) number of clusters.
m matrix of positive numericals. Number of columns must be cln. Number of rows must be number of data points. Columns must add up to 1. Initial configuration for the EM iteration in terms of a probabilty vector for every point which gives its degree of membership to every cluster. As generated by randcmatrix.

Details

The result of the EM iteration depends on the initial configuration, which is generated randomly by randcmatrix for regmix. regmix calls regem. To provide the initial configuration manually, use parameter m of regem directly. Take a look at the example about how to generate m if you want to specify initial parameters.

The original paper DeSarbo and Cron (1988) suggests the AIC for estimating the number of clusters. The use of the BIC is advocated by Wedel and DeSarbo (1995). The BIC is defined here as $2 \log \text{lik} - \log(n) \times ((p+3) \times \text{cln} - 1)$, $p$ being the number of independent variables, i.e., the larger the better.

See the entry for the input parameter warnings for the treatment of several numerical problems.

Value

regmix returns a list containing the components clnopt, loglik, bic, coef, var, eps, z, g.
regem returns a list containing the components loglik, coef, var, z, g, warn.
clnopt optimal number of clusters according to the BIC.
loglik: loglikelihood for the optimal model.
bic: vector of BIC values for all numbers of clusters in nclust.
var: vector of error variance estimators for the clusters.
eps: vector of cluster proportion estimators.
z: matrix of estimated a posteriori probabilities of the points (rows) to be generated by the clusters (columns). Compare input argument m.
g: integer vector of estimated cluster numbers for the points (via argmax over z).
warn: logical. TRUE if one of the estimated clusters has too few points and/or collinear regressors.

Author(s)
Christian Hennig <christian.hennig@unibo.it> https://www.unibo.it/sitoweb/christian.hennig/en/

References

See Also
Regression mixtures can also (and probably better) be computed with the flexmix package, see *flexmix*. (When I first write the *regmix*-function, *flexmix* didn’t exist.)
fixreg for fixed point clusters for clusterwise linear regression.
EMclust for Normal mixture model fitting (non-regression).

Examples
```r
## Not run:
# This apparently gives slightly different
# but data-analytically fine results
# on some versions of R.
set.seed(12234)
data(tonedata)
attach(tonedata)
rmt1 <- regmix(stretchratio,tuned,nclust=1:2)
# nclust=1:2 makes the example fast;
# a more serious application would rather use the default.
rmt1$g
round(rmt1$bic,digits=2)
# start with initial parameter values
```
rFace <- 3
n <- 150
initeps <- cbind(c(2,0),c(0,1),c(0,2.5))
initvar <- c(0.001,0.0001,0.5)
#
initcoef <- c(0.4,0.3,0.3)
# computation of m from initial parameters
m <- matrix(nrow=n, ncol=cln)
stm <- numeric(0)
for (i in 1:cln)
  for (j in 1:n){
    m[j,i] <- initeps[i]*dnorm(tuned[j],mean=initcoef[1,i]+initcoef[2,i]*stretchratio[j], sd=sqrt(initvar[i]))
  }
for (j in 1:n){
  stm[j] <- sum(m[j,])
  for (i in 1:cln)
    m[j,i] <- m[j,i]/stm[j]
}
rmt2 <- regem(stretchratio, tuned, m, cln)

---

rFace  
"Face-shaped" clustered benchmark datasets

Description

Generates "face-shaped" clustered benchmark datasets. This is based on a collaboration with Martin Maechler.

Usage

rFace(n, p = 6, nrep.top = 2, smile.coef = 0.6, dMoNo = 1.2, dNoEy = 1)

Arguments

n integer greater or equal to 10. Number of points.
p integer greater or equal to 2. Dimension.
nrep.top integer. Number of repetitions of the hair-top point.
smile.coef numeric. Coefficient for quadratic term used for generation of mouth-points. Positive values => smile.
dMoNo number. Distance from mouth to nose.
dNoEy number. Minimum vertical distance from mouth to eyes.
Details

The function generates a nice benchmark example for cluster analysis. There are six "clusters" in this data, of which the first five are clearly homogeneous patterns, but with different distributional shapes and different qualities of separation. The clusters are distinguished only in the first two dimensions. The attribute grouping is a factor giving the cluster numbers, see below. The sixth group of points corresponds to some hairs, and is rather a collection of outliers than a cluster in itself. This group contains \( n_{\text{rep.top}}+2 \) points. Of the remaining points, 20% belong to cluster 1, the chin (quadratic function plus noise). 10% belong to cluster 2, the right eye (Gaussian). 30% belong to cluster 3, the mouth (Gaussian/squared Gaussian). 20% belong to cluster 4, the nose (Gaussian/gamma), and 20% belong to cluster 5, the left eye (uniform).

The distributions of the further variables are homogeneous over all points. The third dimension is exponentially distributed, the fourth dimension is Cauchy distributed, all further distributions are Gaussian.

Please consider the source code for exact generation of the clusters.

Value

An \( n \times p \) numeric matrix with attributes

- grouping: a factor giving the cluster memberships of the points.
- indexlist: a list of six vectors containing the indices of points belonging to the six groups.

Author(s)

Christian Hennig <christian.hennig@unibo.it> https://www.unibo.it/sitoweb/christian.hennig/en/

Examples

```r
set.seed(4634)
face <- rFace(600,dMoNo=2,dNoEy=0)
grface <- as.integer(attr(face,"grouping"))
plot(face, col = grface)
# pairs(face, col = grface, main ="rFace(600,dMoNo=2,dNoEy=0)"
```

Ridgeline computation

Description

Computes \( \alpha \ast \Sigma_{1}^{-1} + (1 - \alpha) * \Sigma_{2}^{-1} \ast \mu_{1} + (1 - \alpha) * (\Sigma_{2}^{-1} * \mu_{2}) \) as required for the computation of the ridgeline (Ray and Lindsay, 2005) to find all density extrema of a two-component Gaussian mixture with mean vectors \( \mu_{1} \) and \( \mu_{2} \) and covariance matrices \( \Sigma_{1} \), \( \Sigma_{2} \).

Usage

```r
ridgeline(alpha, mu1, mu2, Sigma1, Sigma2)
```
Arguments

- **alpha**: numeric between 0 and 1.
- **mu1**: mean vector of component 1.
- **mu2**: mean vector of component 2.
- **Sigma1**: covariance matrix of component 1.
- **Sigma2**: covariance matrix of component 2.

Value

A vector. See above.

Author(s)

Christian Hennig <christian.hennig@unibo.it> https://www.unibo.it/sitoweb/christian.hennig/en/

References


Examples

```r
ridgeline(0.5, c(1,1), c(2,5), diag(2), diag(2))
```

ridgeline.diagnosis  
*Ridgeline plots, ratios and unimodality*

Description

Computes ridgeline ratios and unimodality checks for pairs of components given the parameters of a Gaussian mixture. Produces ridgeline plots.

Usage

```r
ridgeline.diagnosis (propvector, muarray, Sigmaarray, 
  k=length(propvector), 
  ipairs="all", compute.ratio=TRUE, by=0.001, 
  ratiocutoff=NULL, ridgelineplot="matrix")
```
Arguments

- **propvector** vector of component proportions. Length must be number of components, and must sum up to 1.
- **muarray** matrix of component means (different components are in different columns).
- **Sigmaarray** three dimensional array with component covariance matrices (the third dimension refers to components).
- **k** integer. Number of components.
- **ipairs** "all" or list of vectors of two integers. If ipairs="all", computations are carried out for all pairs of components. Otherwise, ipairs gives the pairs of components for which computations are carried out.
- **compute.ratio** logical. If TRUE, a matrix of ridgeline ratios is computed, see Hennig (2010a).
- **by** real between 0 and 1. Interval width for density computation along the ridgeline.
- **ratiocutoff** real between 0 and 1. If not NULL, the connection.matrix (see below) is computed by checking whether ridgeline ratios between components are below ratiocutoff.
- **ridgelineplot** one of "none", "matrix", "pairwise". If "matrix", a matrix of pairwise ridgeline plots (see Hennig 2010b) will be plotted. If "pairwise", pairwise ridgeline plots are plotted (you may want to set par(ask=TRUE) to see them all). No plotting if "none".

Value

A list with components

- **merged.clusters** vector of integers, stating for every mixture component the number of the cluster of components that would be merged by merging connectivity components of the graph specified by connection.matrix.
- **connection.matrix** zero-one matrix, in which a one means that the mixture of the corresponding pair of components of the original mixture is either unimodel (if ratiocutoff=NULL) or that their ridgeline ratio is above ratiocutoff. If ipairs!="all", ignored pairs always have 0 in this matrix, same for ratio.matrix.
- **ratio.matrix** matrix with entries between 0 und 1, giving the ridgeline ratio, which is the density minimum of the mixture of the corresponding pair of components along the ridgeline divided by the minimum of the two maxima closest to the beginning and the end of the ridgeline.

Author(s)

Christian Hennig <christian.hennig@unibo.it> https://www.unibo.it/sitoweb/christian.hennig/en/
References


See Also

`ridgeline`, `dridgeline`, `piridge`, `piridge.zeroes`

Examples

```r
muarray <- cbind(c(0,0),c(0,0.1),c(10,10))
sigmaarray <- array(c(diag(2),diag(2),diag(2)),dim=c(2,2,3))
rd <-
  ridgeline.diagnosis(c(0.5,0.3,0.2),muarray,sigmaarray,ridgelineplot="matrix",by=0.1)
# Much slower but more precise with default by=0.01.
```

simmatrix

*Extracting intersections between clusters from fpc-object*

Description

Extracts the information about the size of the intersections between representative Fixed Point Clusters (FPCs) of stable groups from the output of the FPC-functions `fixreg` and `fixmahal`.

Usage

```r
simmatrix(fpcobj)
```

Arguments

- `fpcobj` an object of class `rfpc` or `mfpc`.

Value

A non-negative real-valued vector giving the number of points in the intersections of the representative FPCs of stable groups.

Note

The intersection between representative FPCs no. i and j is at position `sseg(i,j)`. 
solvecov

Inversion of (possibly singular) symmetric matrices

Description

Tries to invert a matrix by solve. If this fails because of singularity, an eigenvector decomposition is computed, and eigenvalues below 1/cmax are replaced by 1/cmax, i.e., cmax will be the corresponding eigenvalue of the inverted matrix.

Usage

solvecov(m, cmax = 1e+10)

Arguments

  m  a numeric symmetric matrix.
  cmax  a positive value, see above.

Value

A list with the following components:

  inv  the inverted matrix
  coll  TRUE if solve failed because of singularity.

Author(s)

Christian Hennig <christian.hennig@unibo.it> https://www.unibo.it/sitoweb/christian.hennig/en/
See Also

solve, eigen

Examples

```r
x <- c(1,0,0,1,0,1,0,0,1)
dim(x) <- c(3,3)
solvecov(x)
```

---

### sseg

**Position in a similarity vector**

#### Description

`sseg(i, j)` gives the position of the similarity of objects `i` and `j` in the similarity vectors produced by `fixreg` and `fixmahal`. `sseg` should only be used as an auxiliary function in `fixreg` and `fixmahal`.

#### Usage

```r
sseg(i, j)
```

#### Arguments

- `i` positive integer.
- `j` positive integer.

#### Value

A positive integer.

#### Author(s)

Christian Hennig <christian.hennig@unibo.it> https://www.unibo.it/sitoweb/christian.hennig/en/

#### Examples

```r
sseg(3,4)
```
stupidkaven  

Stupid average dissimilarity random clustering

Description

Picks k random starting points from given dataset to initialise k clusters. Then, one by one, the point not yet assigned to any cluster with smallest average dissimilarity to the points of any already existing cluster is assigned to that cluster, until all points are assigned. This is a random versione of average linkage clustering, see Akhanli and Hennig (2020).

Usage

stupidkaven(d,k)

Arguments

d - dist-object or dissimilarity matrix.
k - integer. Number of clusters.

Value

The clustering vector (values 1 to k, length number of objects behind d),

Author(s)

Christian Hennig <christian.hennig@unibo.it> https://www.unibo.it/sitoweb/christian.hennig/en/

References


See Also

stupidkcentroids, stupidknn, stupidkfn

Examples

```r
set.seed(20000)
options(digits=3)
face <- rFace(200,dMoNo=2,dNoEy=0,p=2)
stupidkaven(dist(face),3)
```
stupidkcentroids  Stupid k-centroids random clustering

Description

Picks k random centroids from given dataset and assigns every point to closest centroid. This is called stupid k-centroids in Hennig (2019).

Usage

stupidkcentroids(xdata, k, distances = inherits(xdata, "dist"))

Arguments

- xdata: cases*variables data, dist-object or dissimilarity matrix, see distances.
- k: integer. Number of clusters.
- distances: logical. If TRUE, xdata is interpreted as distances.

Value

A list with components

- partition: vector if integers 1 to k, of length equal to number of objects, indicates to which cluster an object belongs.
- centroids: vector of integers of length k, indicating the centroids of the clusters (observation number).
- distances: as argument distances.

Author(s)

Christian Hennig <christian.hennig@unibo.it> https://www.unibo.it/sitoweb/christian.hennig/en/

References


See Also

stupidknn, stupidkfn, stupidkaven
Examples

```r
set.seed(20000)
options(digits=3)
face <- rFace(200,dMoNo=2,dNoEy=0,p=2)
stupidkcentroids(dist(face),3)
```

---

**Examples**

```
stupidkfn

Stupid farthest neighbour random clustering
```

**Description**

Picks k random starting points from given dataset to initialise k clusters. Then, one by one, a point not yet assigned to any cluster is assigned to that cluster, until all points are assigned. The point/cluster pair to be used is picked according to the smallest distance of a point to the farthest point to it in any of the already existing clusters as in complete linkage clustering, see Akhanli and Hennig (2020).

**Usage**

```
stupidkfn(d,k)
```

**Arguments**

- `d` dist-object or dissimilarity matrix.
- `k` integer. Number of clusters.

**Value**

The clustering vector (values 1 to k, length number of objects behind `d`).

**Author(s)**

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**References**


**See Also**

`stupidkcentroids, stupidknn, stupidkaven`
Examples

```r
set.seed(20000)
options(digits=3)
face <- rFace(200,dMoNo=2,dNoEy=0,p=2)
stupidkfn(dist(face),3)
```

**stupidknn**  
Stupid nearest neighbour random clustering

**Description**

Picks k random starting points from given dataset to initialise k clusters. Then, one by one, the point not yet assigned to any cluster that is closest to an already assigned point is assigned to that cluster, until all points are assigned. This is called stupid nearest neighbour clustering in Hennig (2019).

**Usage**

```r
stupidknn(d,k)
```

**Arguments**

- **d**: dist-object or dissimilarity matrix.
- **k**: integer. Number of clusters.

**Value**

The clustering vector (values 1 to k, length number of objects behind d).

**Author(s)**

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**References**


**See Also**

`stupidkcentroids`, `stupidkfn`, `stupidkaven`
Examples

```r
set.seed(20000)
options(digits=3)
face <- rFace(200,dMoNo=2,dNoEy=0,p=2)
stupidknn(dist(face),3)
```

---

**tdecomp**

Root of singularity-corrected eigenvalue decomposition

---

**Description**

Computes transposed eigenvectors of matrix m times diagonal of square root of eigenvalues so that eigenvalues smaller than 1e-6 are set to 1e-6.

**Usage**

```r
tdecomp(m)
```

**Arguments**

- `m` a symmetric matrix of minimum format 2*2.

**Details**

Thought for use in discrcoord only.

**Value**

a matrix.

**Note**

Thought for use within discrcoord only.

**Author(s)**

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**Examples**

```r
x <- rnorm(10)
y <- rnorm(10)
z <- cov(cbind(x,y))
round(tdecomp(z),digits=2)
```
tonedata  

*Description*

The tone perception data stem from an experiment of Cohen (1980) and have been analyzed in de Veaux (1989). A pure fundamental tone was played to a trained musician. Electronically generated overtones were added, determined by a stretching ratio of \( \text{stretchratio} \). \( \text{stretchratio}=2.0 \) corresponds to the harmonic pattern usually heard in traditional definite pitched instruments. The musician was asked to tune an adjustable tone to the octave above the fundamental tone. \( \text{tuned} \) gives the ratio of the adjusted tone to the fundamental, i.e. \( \text{tuned}=2.0 \) would be the correct tuning for all \( \text{stretchratio} \)-values. The data analyzed here belong to 150 trials with the same musician. In the original study, there were four further musicians.

*Usage*

\[ \text{data(tonedata)} \]

*Format*

A data frame with 2 variables \( \text{stretchratio} \) and \( \text{tuned} \) and 150 cases.

*Source*


*References*


**unimodal.ind**  

*Description*

Checks whether a series of fitted density values (such as given out as \( y \)-component of \text{density}) is unimodal.

*Usage*

\[ \text{unimodal.ind}(y) \]
valstat.object

Arguments

y numeric vector of fitted density values in order of increasing x-values such as given out as y-component of density.

Value

Logical. TRUE if unimodal.

Author(s)

Christian Hennig <christian.hennig@unibo.it> https://www.unibo.it/sitoweb/christian.hennig/en/

Examples

unimodal.ind(c(1,3,3,4,2,1,0,0))

valstat.object  

Cluster validation statistics - object

Description

The objects of class "valstat" store cluster validation statistics from various clustering methods run with various numbers of clusters.

Value

A legitimate valstat object is a list. The format of the list relies on the number of involved clustering methods, nmethods, say, i.e., the length of the method-component explained below. The first nmethods elements of the valstat-list are just numbered. These are themselves lists that are numbered between 1 and the maxG-component defined below. Element [[i]][[j]] refers to the clustering from clustering method number i with number of clusters j. Every such element is a list with components avewithin, mnnd, cvnnd, maxdiameter, widestgap, sindex, minsep, asw, dindex, denscut, highdgap, pearsongamma, withinss, entropy. Further optional components are pamc, kdnorm, kdunif, dmode, aggregated. All these are cluster validation indexes, as follows.

avewithin average distance within clusters (reweighted so that every observation, rather than every distance, has the same weight).

mnnd average distance to nnkth nearest neighbour within cluster. (nnk is a parameter of cqcluster.stats, default 2.)

cvnnd coefficient of variation of dissimilarities to nnkth nearest within-cluster neighbour, measuring uniformity of within-cluster densities, weighted over all clusters, see Sec. 3.7 of Hennig (2019). (nnk is a parameter of cqcluster.stats, default 2.)

maxdiameter maximum cluster diameter.
widestgap \[\text{widest within-cluster gap or average of cluster-wise widest within-cluster gap, depending on parameter averagegap of } \texttt{cqcluster.stats}, \text{ default } \text{FALSE}.\]

sindex \[\text{separation index. Defined based on the distances for every point to the closest point not in the same cluster. The separation index is then the mean of the smallest proportion } \text{sepprob} \text{ (parameter of } \texttt{cqcluster.stats}, \text{ default } 0.1) \text{ of these. See Hennig (2019).} \]

minsep \[\text{minimum cluster separation.}\]

asw \[\text{average silhouette width. See } \texttt{silhouette}.\]

dindex \[\text{this index measures to what extent the density decreases from the cluster mode to the outskirts; } I\text{-densdec} \text{ in Sec. 3.6 of Hennig (2019); low values are good.}\]

denscut \[\text{this index measures whether cluster boundaries run through density valleys; } I\text{-densbound} \text{ in Sec. 3.6 of Hennig (2019); low values are good.}\]

highdgap \[\text{this measures whether there is a large within-cluster gap with high density on both sides; } I\text{-highdgap} \text{ in Sec. 3.6 of Hennig (2019); low values are good.}\]

pearsongamma \[\text{correlation between distances and a } 0\text{-}1\text{-vector where } 0 \text{ means same cluster, } 1 \text{ means different clusters. "Normalized gamma" in Halkidi et al. (2001).}\]

withinss \[\text{a generalisation of the within clusters sum of squares (k-means objective function), which is obtained if } d \text{ is a Euclidean distance matrix. For general distance measures, this is half the sum of the within cluster squared dissimilarities divided by the cluster size.}\]

entropy \[\text{entropy of the distribution of cluster memberships, see Meila(2007).}\]

pamc \[\text{average distance to cluster centroid, which is the observation that minimises this average distance.}\]

kdnorm \[\text{Kolmogorov distance between distribution of within-cluster Mahalanobis distances and appropriate chi-squared distribution, aggregated over clusters (I am grateful to Agustin Mayo-Iscar for the idea).}\]

kdunif \[\text{Kolmogorov distance between distribution of distances to } d\text{nnk} \text{th nearest within-cluster neighbor and appropriate Gamma-distribution, see Byers and Raftery (1998), aggregated over clusters. } d\text{nnk} \text{ is parameter } \text{nnk} \text{ of } \texttt{distrsimilarity}, \text{ corresponding to } \text{nnk} \text{ of } \texttt{clusterbenchstats}.\]

dmode \[\text{aggregated density mode index equal to } 0.75 \times \text{dindex} + 0.25 \times \text{highdgap} \text{ after standardisation by } \texttt{cgrestandard}.\]

Furthermore, a valstat object has the following list components:

maxG \[\text{maximum number of clusters.}\]

minG \[\text{minimum number of clusters (list entries below that number are empty lists).}\]

method \[\text{vector of names (character strings) of clustering CBI-functions, see } \texttt{kmeansCBI}.\]

name \[\text{vector of names (character strings) of clustering methods. These can be user-chosen names (see argument } \texttt{methodnames} \text{ in } \texttt{clusterbenchstats} \text{ and may distinguish different methods run by the same CBI-function but with different parameter values such as complete and average linkage for } \texttt{hclustCBI}.\]

statistics \[\text{vector of names (character strings) of cluster validation indexes.}\]
weightplots

**GENERATION**

These objects are generated as part of the `clusterbenchstats`-output.

**METHODS**

The `valstat` class has methods for the following generic functions: `print`, `plot`, see `plot.valstat`.

**Author(s)**

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**References**


**See Also**

`clusterbenchstats`, `plot.valstat`.

---

**weightplots**

*Ordered posterior plots*

**Description**

Ordered posterior plots for Gaussian mixture components, see Hennig (2010).

**Usage**

```r
weightplots(z, clusternumbers="all", clustercol=2,
            allcol=grey(0.2+((1:ncol(z))-1)*
                       0.6/(ncol(z)-1)),
            lty=rep(1,ncol(z)),clusterlwd=3,
            legendposition="none",
            weightcutoff=0.01,ask=TRUE, ...)
```
Arguments

\textbf{z} matrix with rows corresponding to observations and columns corresponding to mixture components. Entries are probabilities that an observation has been generated by a mixture component. These will normally be estimated a posteriori probabilities, as generated as component \texttt{z} of the output object from \texttt{summary.mclustBIC}.

\textbf{clusternumbers} "all" or vector of integers. Numbers of components for which plots are drawn.

\textbf{clustercol} colour used for the main components for which a plot is drawn.

\textbf{allcol} colours used for respective other components in plots in which they are not main components.

\textbf{lty} line types for components.

\textbf{clusterlwd} numeric. Line width for main component.

\textbf{legendposition} "none" or vector with two coordinates in the plot, where a legend should be printed.

\textbf{weightcutoff} numeric between 0 and 1. Observations are only taken into account for which the posterior probability for the main component is larger than this.

\textbf{ask} logical. If \texttt{TRUE}, it sets \texttt{par(ask=TRUE)} in the beginning and \texttt{par(ask=FALSE)} after all plots were showed.

\dots further parameters to be passed on to \texttt{legend}.

Details

Shows posterior probabilities for observations belonging to all mixture components on the y-axis, with points ordered by posterior probability for main component.

Value

Invisible matrix of posterior probabilities \texttt{z} from \texttt{mclustsummary}.

Author(s)

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References


Examples

\begin{verbatim}
require(mclust)
require(MASS)
data(crabs)
dc <- crabs[,4:8]
cm <- mclustBIC(crabs[,4:8],G=9,modelNames="EEE")
scm <- summary(cm,crabs[,4:8])
\end{verbatim}
weightplots(scm$z, clusternumbers=1:3, ask=FALSE)
weightplots(scm$z, clusternumbers=1:3, allcol=1:9, ask=FALSE,
legendposition=c(5,0.7))
# Remove ask=FALSE to have time to watch the plots.


describe()

weightfunction (for Mahalabobis distances)

Description

Function of the elements of md, which is 1 for arguments smaller than ca, 0 for arguments larger
than ca2 and linear (default: continuous) in between.

Thought for use in fixmahal.

Usage

wfu(md, ca, ca2, a1 = 1/(ca - ca2), a0 = -a1 * ca2)

Arguments

md vector of positive numericals.
ca positive numerical.
ca2 positive numerical.
a1 numerical. Slope.
a0 numerical. Intercept.

Value

A vector of numericals between 0 and 1.

Author(s)

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hennig/en/

See Also

fixmahal

Examples

md <- seq(0,10,by=0.1)
round(wfu(md, ca=5, ca2=8), digits=2)
**Description**

This produces a crosstable between two integer vectors (partitions) of the same length with a given maximum vector entry \( k \) so that the size of the table is \( k \times k \) with zeroes for missing entries between 1 and \( k \) (the command `table` does pretty much the same thing but will leave out missing entries).

**Usage**

```r
xtable(c1,c2,k)
```

**Arguments**

- `c1`: vector of integers.
- `c2`: vector of integers of same length as `c1`.
- `k`: integer. Must be larger or equal to maximum entry in `c1` and `c2`.

**Value**

A matrix of dimensions \( c(k,k) \). Entry \([i,j]\) gives the number of places in which \( c1==i \) & \( c2==j \).

**Author(s)**

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**See Also**

- `table`

**Examples**

```r
c1 <- 1:3
C2 <- c(1,1,2)
xtable(c1,C2,3)
```
Matrix of misclassification probabilities between mixture components

Description

Matrix of misclassification probabilities in a mixture distribution between two mixture components from estimated posterior probabilities regardless of component parameters, see Hennig (2010).

Usage

zmisclassification.matrix(z,pro=NULL,clustering=NULL, ipairs="all",symmetric=TRUE, stat="max")

Arguments

z matrix of posterior probabilities for observations (rows) to belong to mixture components (columns), so entries need to sum up to 1 for each row.
pro vector of component proportions, need to sum up to 1. Computed from z as default.
clustering vector of integers giving the estimated mixture components for every observation. Computed from z as default.
ipairs "all" or list of vectors of two integers. If ipairs="all", computations are carried out for all pairs of components. Otherwise, ipairs gives the pairs of components for which computations are carried out.
symmetric logical. If TRUE, the matrix is symmetrised, see parameter stat.
stat "max" or "mean". The statistic by which the two misclassification probabilities are aggregated if symmetric=TRUE.

Value

A matrix with the (symmetrised, if required) misclassification probabilities between each pair of mixture components. If symmetric=FALSE, matrix entry \([i,j]\) is the estimated probability that an observation generated by component \(j\) is classified to component \(i\) by maximum a posteriori rule.

Author(s)

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References

See Also

confusion

Examples

```r
set.seed(12345)
m <- rpois(20,lambda=5)
dim(m) <- c(5,4)
m <- m/apply(m,1,sum)
round(zmisclassification.matrix(m,symmetric=FALSE),digits=2)
```
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