Package ‘tclust’

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tclust-package .......................................................... 2
tclcurves ................................................................. 2
DiscrFact ................................................................. 5
discr_coords ............................................................. 6
geyser2 ................................................................. 7
M5data ................................................................. 8
plot.tclcurves .......................................................... 9
plot.DiscrFact ......................................................... 10
plot.tclust ............................................................ 12
summary.DiscrFact .................................................... 14
swissbank ............................................................. 15
tclust ................................................................. 16
tkmeans ............................................................... 19

Index 23
tclust-package  General Trimmed Cluster Analysis

Description

A package implementing different (robust) clustering algorithms (tclust) based on trimming and including some graphical diagnostic tools (ctlcurves and DiscrFact)

Details

Package:  tclust
Type:      Package
Version:   1.0
Date:      2009-05-13
License:   GPL-3

Author(s)

Agustin Mayo Iscar, Heinrich Fritz, Maintainer: Luis Angel Garcia Escudero <lagarcia@eio.uva.es>

References


ctlcurves  Classification Trimmed Likelihood Curves

Description

The function applies tclust several times on a given dataset while parameters alpha and k are altered. The resulting object gives an idea of the optimal trimming level and number of clusters considering a particular dataset.

Usage

ctlcurves (x, k = 1:4, alpha = seq (0, 0.2, len = 6), restr.fac t = 50, trace = 1, ...)
Arguments

- **x**: A matrix or data frame of dimension n x p, containing the observations (row-wise).
- **k**: A vector of cluster numbers to be checked. By default cluster numbers from 1 to 5 are examined.
- **alpha**: A vector containing the alpha levels to be checked. By default alpha levels from 0 to 0.2 (continuously increased by 0.01), are checked.
- **restr.fact**: The restriction factor passed to `tclust`.
- **...**: Further arguments (as e.g. `restr`), passed to `tclust`.
- **trace**: Defines the tracing level, which is set to 1 by default. Tracing level 2 gives additional information on the current iteration.

Details

These curves show the values of the trimmed classification (log-)likelihoods when altering the trimming proportion alpha and the number of clusters k. The careful examination of these curves provides valuable information for choosing these parameters in a clustering problem. For instance, an appropriate k to be chosen is one that we do not observe a clear increase in the trimmed classification likelihood curve for k with respect to the k+1 curve for almost all the range of alpha values. Moreover, an appropriate choice of parameter alpha may be derived by determining where an initial fast increase of the trimmed classification likelihood curve stops for the final chosen k. A more detailed explanation can be found in García-Escudero et al. (2010).

Value

The function returns an S3 object of type `ctlcurves` with components:

- **par**: A list containing all the parameters passed to this function.
- **obj**: An array containing the objective functions values of each computed cluster-solution.
- **min.weights**: An array containing the minimum cluster weight of each computed cluster-solution.

So far there is no output available for `print.ctlcurves`. Use `plot` on an `ctlcurves` object for a graphical interpretation of it.

Author(s)

Agustin Mayo Iscar, Luis Angel Garcia Escudero, Heinrich Fritz

References

See Also

plot.ctlcurves

Examples

```r
## Not run:
#--- EXAMPLE 1 ---------------------------------------

sig <- diag(2)
cen <- rep(1, 2)
x <- rbind(rmvnorm(108, cen * 0, sig), 
          rmvnorm(162, cen * 5, sig * 6 - 2),
          rmvnorm(30, cen * 2.5, sig * 50))

ctl <-ctlcurves(x, k = 1:4)

## ctl-curves
plot (ctl) ## -- selecting k = 2, alpha = 0.08

## the selected model
plot (tclust (x, k = 2, alpha = 0.08, restr.fact = 7))

#--- EXAMPLE 2 ---------------------------------------

data (geyser)
ctl <- ctlcurves (geyser2, k = 1:5)

## ctl-curves
plot (ctl) ## -- selecting k = 3, alpha = 0.08

## the selected model
plot (tclust (geyser2, k = 3, alpha = 0.08, restr.fact = 5))

#--- EXAMPLE 3 ---------------------------------------

data (swissbank)
ctl <- ctlcurves (swissbank, k = 1:5, alpha = seq (0, 0.3, by = 0.025))

## ctl-curves
plot (ctl) ## -- selecting k = 2, alpha = 0.1

## the selected model
plot (tclust (swissbank, k = 2, alpha = 0.1, restr.fact = 50))

## End(Not run)
```
DiscrFact

Discriminant Factor Analysis for tclust Objects

Description

Analyzes a tclust-object by calculating discriminant factors and comparing the quality of the actual cluster assignments and the second best possible assignment for each observation. Discriminant factors, measuring the strength of the "trimming" decision may also be defined. Cluster assignments of observations with large discriminant factors are considered as "doubtful" decisions. Silhouette plots give a graphical overview of the discriminant factors distribution (see plot.DiscrFact). More details can be found in García-Escudero et al. (2010).

Usage

DiscrFact(x, threshold = 1/10)

Arguments

x A tclust object.
threshold A cluster assignment or a trimming decision for an observation with a discriminant factor larger than log(threshold) is considered as a "doubtful" decision.

Details

This function compares the actual (best) assignment of each observation to its second best possible assignment. This comparison is based on the discriminant factors of each observation, which are calculated here. If the discriminant factor of an observation is larger than a given level (log(threshold)), the observation is considered as "doubtfully" assigned to a cluster. More information is shown when plotting the returned DiscrFact object.

Value

The function returns an S3 object of type DiscrFact containing the following components:

x A tclust object.
ylimmin A minimum y-limit calculated for plotting purposes.
ind The actual cluster assignment.
ind2 The second most likely cluster assignment for each observation.
disc The (weighted) likelihood of the actual cluster assignment of each observation.
disc2 The (weighted) likelihood of the second best cluster assignment of each observation.
assignfact The factor log (disc/disc2).
threshold The threshold used for deciding whether assignfact indicates a "doubtful" assignment.
mean.DiscrFact A vector of length k + 1 containing the mean discriminant factors for each cluster (including the outliers).
Author(s)

Agustin Mayo-Iscar, Luis Angel García-Escudero, Heinrich Fritz

References


See Also

plot.DiscrFact

Examples

```r
sig <- diag(2)
cen <- rep(1, 2)
x <- cbind(mvtnorm::rmvnorm(360, cen * 0, sig),
           mvtnorm::rmvnorm(340, cen * 5, sig * 6 - 2),
           mvtnorm::rmvnorm(100, cen * 5, sig * 50))
clus.1 <- tclust(x, k = 2, alpha = 0.1, restr.fact = 12)
clus.2 <- tclust(x, k = 3, alpha = 0.1, restr.fact = 1)
## restr.fact and k are chosen improperly for pointing out the
difference in the plot of DiscrFact
dsc.1 <- discr_coords(clus.1)
plot(dsc.1)
dsc.2 <- discr_coords(clus.2)
plot(dsc.2)
```

discr_coords

Discriminant coordinates/canonical variates of tclust objects

Description

Computes the two first discriminant coordinates (canonical coordinates) directly from a tclust object to obtain a graphical representations of cluster solutions in higher dimensional (p > 2) cases.

Usage

discr_coords(x, equal.weights)
geyser2

Arguments

x A tclust object.

equal.weights A logical value, controlling whether the clusters should be considered as equal-sized (TRUE) when combining their covariance structures, or if their actual size shall be considered (FALSE). By default value x$par$equal.weights is assumed.

Details

The functionality of discr.coords is directly derived from discrcoord as implemented in the package "fpc" by Christian Hennig. It has been adopted in order to directly use the covariance information contained in the tclust-object. The function fails, if "store.x = FALSE" is specified in tclust, because the original data matrix is required here.

Value

A two-dimensional matrix, containing the canonical coordinates of all observations given by the tclust-object.

Author(s)

Agustin Mayo Iscar, Luis Angel Garcia Escudero, Heinrich Fritz

References


geyser2 Old Faithful Geyser Data

Description

A bivariate data set obtained from the Old Faithful Geyser, containing the eruption length and the length of the previous eruption for 271 eruptions of this geyser in minutes.

Usage

drug

Format

Eruption length The eruption length in minutes.

Previous eruption length The length of the previous eruption in minutes.
**Source**

This particular data structure can be obtained by applying the following code to the "Old Faithful Geyser" (faithful data set (Härdle 1991) in the package datasets):

```r
f1 <- faithful[,1]  
geyser2 <- cbind(f1[-length(f1)], f1[-1])  
colnames(geyser2) <- c("Eruption length",  
"Previous eruption length")
```

**References**


---

**M5data**

*Mixture M5 Data*

**Description**

A bivariate data set obtained from three normal bivariate distributions with different scales and proportions 1:2:2. One of the components is very overlapped with another one. A 10% background noise is added uniformly distributed in a rectangle containing the three normal components and not very overlapped with the three mixture components. A precise description of the M5 data set can be found in García-Escudero et al. (2008).

**Usage**

M5data

**Format**

The first two columns are the two variables. The last column is the true classification vector where symbol "0" stands for the contaminating data points.

**Source**

Description

The plot method for class ctlcurves: This function plots a ctlcurves object, comparing the target functions values with different values of parameter restr.fact.

Usage

```r
## S3 method for class 'ctlcurves'
plot(x, what = c("obj", "min.weights", "doubtful"),
     main, xlab, ylab, xlim, ylim, col, lty = 1, ...)
```

Arguments

- `x` The ctlcurves object to be printed.
- `what` A string indicating which type of plot shall be drawn. See the details section for more information.
- `main` A character-string containing the title of the plot.
- `xlab`, `ylab`, `xlim`, `ylim` Arguments passed to `plot`.
- `col` A single value or vector of line colors passed to `lines`.
- `lty` A single value or vector of line types passed to `lines`.
- `...` Arguments to be passed to or from other methods.

Details

These curves show the values of the trimmed classification (log-)likelihoods when altering the trimming proportion alpha and the number of clusters k. The careful examination of these curves provides valuable information for choosing these parameters in a clustering problem. For instance, an appropriate k to be chosen is one that we do not observe a clear increase in the trimmed classification likelihood curve for k with respect to the k+1 curve for almost all the range of alpha values. Moreover, an appropriate choice of parameter alpha may be derived by determining where an initial fast increase of the trimmed classification likelihood curve stops for the final chosen k. A more detailed explanation can be found in García-Escudero et al. (2010).

This function implements a series of plots, which display characteristic values of the each model, computed with different values for k and alpha. The plot type is selected by setting argument what to one of the following values:

- "obj" Objective function values.
- "min.weights" The minimum cluster weight found for each computed model. This plot is intended to spot spurious clusters, which in general yield quite small weights.
- "doubtful" The number of "doubtful" decisions identified by DiscrFact.
Author(s)

Agustin Mayo Iscar, Luis Angel Garcia Escudero, Heinrich Fritz

References


Examples

```r
sig <- diag(2)
cen <- rep(1, 2)
x <- rbind(mvtnorm::rmvnorm(100, cen * 0, sig),
           mvtnorm::rmvnorm(102, cen * 5, sig * 6 - 2),
           mvtnorm::rmvnorm(30, cen * 2.5, sig * 50))

ctl <- ctlcurves(x, k = 1:4)
plot(ctl)
```

plot.DiscrFact

**plot Method for DiscrFact Objects**

Description

The `plot` method for class `DiscrFact`: Next to a plot of the `tclust` object which has been used for creating the `DiscrFact` object, a silhouette plot indicates the presence of groups with a large amount of doubtfully assigned observations. A third plot similar to the standard `tclust` plot serves to highlight the identified doubtful observations.

Usage

```r
## S3 method for class 'DiscrFact'
plot(x, enum.plots = FALSE, ...)
plot_DiscrFact_p2(x, xlab = "Discriminant Factor",
                 ylab = "Clusters", main, xlim,
                 print.Discr = TRUE, main.pre, ...)

plot_DiscrFact_p3(x, main = "Doubtful Assignments", col, pch,
                  col.nodoubt = grey(0.8), by.cluster = FALSE,
                  ...)```
plot.DiscrFact

Arguments

- **x**: An object of class "DiscrFact" as from `DiscrFact()`.  
- **enum.plots**: A logical value indicating whether the plots shall be enumerated in their title ("(a)","(b)","(c)").  
- **xlab, ylab, xlim**: Arguments passed to function `plot.tclust`.  
- **main**: Argument passed to function `plot`.  
- **print.Discr**: A logical value indicating whether each clusters mean discriminant factor shall be plotted.  
- **main.pre**: An optional string which is appended to the plot's caption.  
- **pch, col**: Arguments passed to function `plot`.  
- **col.nodoubt**: Color of all observations not considered as to be assigned doubtfully.  
- **by.cluster**: Logical value indicating whether parameters `pch` and `col` refer to observations (FALSE) or clusters (TRUE).  
- **...**: Arguments to be passed to or from other methods.

Details

The `plot.DiscrFact` function displays a silhouette plot based on the discriminant factors of the observations. A solution with many large discriminant factors is not reliable. Such clusters can be identified with this silhouette plot. Thus `plot.DiscrFact` displays the dataset, highlighting observations with discriminant factors greater than the given threshold. Function `plot.DiscrFact` combines the standard plot of a `tclust` object, and the two plots introduced here.

Value

No return value is provided.

Author(s)

Agustin Mayo Iscar, Luis Angel García Escudero, Heinrich Fritz

References


Examples

```r
sig <- diag(2)  
cen <- rep(1, 2)  
x <- rbind(mvtnorm::rmvnorm(360, cen * 0, sig),  
           mvtnorm::rmvnorm(360, cen * 5, sig * 6 - 2),  
           mvtnorm::rmvnorm(100, cen * 2.5, sig * 50))
```

plot.tclust

clus.1 <- tclust (x, k = 2, alpha=0.1, restr.fact=12)
clus.2 <- tclust (x, k = 3, alpha=0.1, restr.fact=1)
dsc.1 <- DiscrFact (clus.1)
plot(dsc.1)
dsc.2 <- DiscrFact (clus.2)
plot (dsc.2)
dev.off ()
plot_DiscrFact_p2 (dsc.1)
plot_DiscrFact_p3 (dsc.2)

plot.tclust

plot Method for tclust Objects

Description
The plot method for classes tclust and tkmeans.

Usage
## S3 method for class 'tclust'
plot(x, ...)
## S3 method for class 'tkmeans'
plot(x, ...)

Arguments
x The tclust or tkmeans object to be displayed.
... Further (optional) arguments which specify the details of the resulting plot (see section "Further Arguments").

Details
One and two dimensional structures are treated separately (e.g. tolerance intervals/ellipses are displayed). Higher dimensional structures are displayed by plotting the two first Fisher’s canonical coordinates (evaluated by discr_coords) and derived from the final cluster assignments (trimmed observations are not taken into account). plot.tclust.Nd can be called with one or two-dimensional tclust-objects too. The function fails, if "store.x = FALSE" is specified in tclust, because the original data matrix is required here.

Further Arguments
xlab, ylab, xlim, ylim, pch, col Arguments passed to plot.
main The title of the plot. Use "/p" for displaying the chosen parameters alpha and k or "/r" for plotting the chosen restriction (tclust only).
main.pre An optional string which is added to the plot’s caption.
sub A string specifying the subtitle of the plot. Use "/p" (default) for displaying the chosen parameters alpha and k, "/r" for plotting the chosen restriction (tclust only) and "/pr" for both.

sub1 A secondary (optional) subtitle.

labels A string specifying the type of labels to be drawn. Either "none" (default), "cluster" or "observation" can be specified. If specified, parameter pch is ignored.

text A vector of length n (the number of observations) containing strings which are used as labels for each observation. If specified, the parameters labels and pch are ignored.

by.cluster Logical value indicating whether parameters pch and col refer to observations (FALSE) or clusters (TRUE).

jitter.y Logical value, specifying whether the drawn values shall be jittered in y-direction for better visibility of structures in 1 dimensional data.

tol The tolerance interval. 95% tolerance ellipsoids (assuming normality) are plotted by default (tclust only).

tol.col, tol.lty, tol.lwd Vectors of length k or 1 containing the col, lty and lwd arguments for the tolerance ellipses/lines (tclust only).

Author(s)

Agustin Mayo Iscar, Luis Angel Garcia Escudero, Heinrich Fritz

Examples

```r
#--- EXAMPLE 1-------------------------------
sig <- diag(2)
cen <- rep(1, 2)
x <- rbind(mvtnorm::rmvnorm(360, cen * 0, sig),
            mvtnorm::rmvnorm(540, cen * 5, sig * 6 - 2),
            mvtnorm::rmvnorm(100, cen * 2.5, sig * 50))
# Two groups and 10% trimming level
a <- tclust(x, k = 2, alpha = 0.1, restr.fact = 12)

plot(a)
plot(a, labels = "observation")
plot(a, labels = "cluster")
plot(a, by.cluster = TRUE)

#--- EXAMPLE 2-------------------------------
x <- c(rnorm(72,0, 1),
      rnorm(108, 10, 1),
      rnorm(20, 2.5, 10))

a <- tkmeans(x, k = 2, alpha = 0.1)
plot(a, jitter.y = TRUE)
```
Summary

The summary method for class DiscrFact.

Usage

```r
## S3 method for class 'DiscrFact'
summary(object, hide.empty = TRUE, show.clust, show.alt, ...)
```

Arguments

- `object` An object of class "DiscrFact" as from DiscrFact ().
- `hide.empty` A logical value specifying whether clusters without doubtful assignment shall be hidden.
- `show.clust` A logical value specifying whether the number of doubtful assignments per cluster shall be displayed.
- `show.alt` A logical value specifying whether the alternative cluster assignment shall be displayed.
- `...` Arguments passed to or from other methods.

Value

No return value is provided.

Author(s)

Agustin Mayo Iscar, Luis Angel Garcia Escudero, Heinrich Fritz

References


See Also

- plot.DiscrFact
Examples

```r
sig <- diag(2)
cen <- rep(1, 2)
x <- rbind(mvtnorm::rmvnorm(360, cen * 0, sig), 
            mvtnorm::rmvnorm(540, cen * 5, sig * 6 - 2), 
            mvtnorm::rmvnorm(100, cen * 2.5, sig * 50))
clus.1 <- tclust(x, k = 2, alpha = 0.1, restr.fact = 12)
clus.2 <- tclust(x, k = 3, alpha = 0.1, restr.fact = 1)
## restr.fact and k are chosen improperly for pointing out the
## difference in the plot of DiscrFact
dsc.1 <- DiscrFact(clus.1)
summary(dsc.1)
dsc.2 <- DiscrFact(clus.2)
summary(dsc.2)
```

---

**swissbank**

*SwissBankNotes Data*

**Description**

Six variables measured on 100 genuine and 100 counterfeit old Swiss 1000-franc bank notes (Flury and Riedwyl, 1988).

**Usage**

`swissbank`

**Format**

- `Length` Length of the bank note
- `Ht_Left` Height of the bank note, measured on the left
- `Ht_Right` Height of the bank note, measured on the right
- `IF_Lower` Distance of inner frame to the lower border
- `IF_Upper` Distance of inner frame to the upper border
- `Diagonal` Length of the diagonal

**Details**

Observations 1-100 are the genuine bank notes and the other 100 observations are the counterfeit bank notes.
### tclust

**General Trimming Approach to Robust Cluster Analysis**

**Description**

`tclust` searches for $k$ (or less) clusters with different covariance structures in a data matrix $x$. Relative cluster scatter can be restricted by a constant value `restr.fact`. For robustifying the estimation, a proportion $\alpha$ of observations may be trimmed.

In particular, the trimmed k-means method (`tkmeans`) is represented by the `tclust` method, setting parameters `$\text{restr = "eigen"}$`, `$\text{restr.fact = 1}$`, and `$\text{equal.weights = TRUE}$`.

**Usage**

```r
tclust(x, k = 3, alpha = 0.05, nstart = 50, iter.max = 20,
       restr = c("eigen", "deter", "sigma"), restr.fact = 12,
       equal.weights = FALSE, center, scale, store.x = TRUE,
       drop.empty.clust = TRUE, trace = 0, warnings = 3,
       zero.tol = 1e-16)
```

**Arguments**

- **x**: A matrix or data.frame of dimension $n \times p$, containing the observations (row-wise).
- **k**: The number of clusters initially searched for.
- **alpha**: The proportion of observations to be trimmed.
- **nstart**: The number of random initializations to be performed.
- **iter.max**: The maximum number of concentration steps to be performed. The concentration steps are stopped, whenever two consecutive steps lead to the same data partition.
- **restr**: The type of restriction to be applied on the cluster scatter matrices. Valid values are "eigen" (default), "deter" and "sigma".
  - See the detail section for further explanation.
- **restr.fact**: The constant `$\text{restr.fact } >= 1$` constrains the allowed differences among group scatters. Larger values imply larger differences of group scatters, a value of 1 specifies the strongest restriction. When using `$\text{restr = "sigma"}$` this parameter is not considered, as all cluster variances are averaged, always implying `$\text{restr.fact = 1}$`. 

**Source**

equal.weights  A logical value, specifying whether equal cluster weights (TRUE) or not (FALSE) shall be considered in the concentration and assignment steps.

center, scale  A center and scale vector, each of length p which can optionally be specified for centering and scaling x before calculation.

store.x  A logical value, specifying whether the data matrix x shall be included in the result structure. By default this value is set to TRUE, because functions plot.tclust and DiscrFact depend on this information. However, when big data matrices are handled, the result structure’s size can be decreased noticeably when setting this parameter to FALSE.

drop.empty.clust  Logical value specifying, whether empty clusters shall be omitted in the resulting object. (The result structure does not contain center and covariance estimates of empty clusters anymore. Cluster names are reassigned such that the first l clusters (1 <= k) always have at least one observation.

trace  Defines the tracing level, which is set to 0 by default. Tracing level 2 gives additional information on the iteratively decreasing objective function’s value.

warnings  The warning level (0: no warnings; 1: warnings on unexpected behavior; 2: warnings if restr.fact causes artificially restricted results).

zero.tol  The zero tolerance used. By default set to 1e-16.

Details

This iterative algorithm initializes k clusters randomly and performs "concentration steps" in order to improve the current cluster assignment. The number of maximum concentration steps to be performed is given by iter.max. For approximately obtaining the global optimum, the system is initialized nstart times and concentration steps are performed until convergence or iter.max is reached. When processing more complex data sets higher values of nstart and iter.max have to be specified (obviously implying extra computation time). However, if more then half of the iterations would not converge, a warning message is issued, indicating that nstart has to be increased.

The parameter restr defines the cluster’s shape restrictions, which are applied on all clusters during each iteration. Options “eigen”/”deter” restrict the ratio between the maximum and minimum eigenvalue/determinant of all cluster’s covariance structures to parameter restr.fact. Setting restr.fact to 1, yields the strongest restriction, forcing all eigenvalues/determinants to be equal and so the method looks for similarly scattered (respectively spherical) clusters. Option “sigma” is a simpler restriction, which averages the covariance structures during each iteration (weighted by cluster sizes) in order to get similar (equal) cluster scatters.

Value

The function returns an S3 object of type tclust, containing the following values:

centers  A matrix of size p x k containing the centers (column-wise) of each cluster.
cov  An array of size p x p x k containing the covariance matrices of each cluster.
cluster  A numerical vector of size n containing the cluster assignment for each observation. Cluster names are integer numbers from 1 to k, 0 indicates trimmed observations.
par A list, containing the parameters the algorithm has been called with (x, if not suppressed by store.x = FALSE, k, alpha, restr.fact, nstart, KStep, and equal.weights).

k The (final) resulting number of clusters. Some solutions with a smaller number of clusters might be found when using the option equal.weights = FALSE.

obj The value of the objective function of the best (returned) solution.

size An integer vector of size k, returning the number of observations contained by each cluster.

weights A numerical vector of length k, containing the weights of each cluster.

int A list of values internally used by function related to tclust objects.

Author(s)

Agustin Mayo Iscar, Luis Angel Garcia Escudero, Heinrich Fritz

References


Examples

```r
#--- EXAMPLE 1 -----------------------------------------------
sig <- diag(2)
cen <- rep(1,2)
x <- rbind(mvtnorm::rmvnorm(360, cen * 0, sig),
           mvtnorm::rmvnorm(540, cen * 5, sig * 6 - 2),
           mvtnorm::rmvnorm(100, cen * 2.5, sig * 50))

# Two groups and 10% trimming level
clus <- tclust(x, k = 2, alpha = 0.1, restr.fact = 8)
plot(clus)
plot(clus, labels = "observation")
plot(clus, labels = "cluster")

# Three groups (one of them very scattered) and 0% trimming level
clus <- tclust(x, k = 3, alpha=0.0, restr.fact = 100)
plot(clus)
```
#--- EXAMPLE 3 -----------------------------
data (M5data)
x <- M5data[, 1:2]
clus.a <- tclust (x, k = 3, alpha = 0.1, restr.fact = 1, restr = "eigen", equal.weights = TRUE, warnings = 1)
clus.b <- tclust (x, k = 3, alpha = 0.1, restr.fact = 1, equal.weights = TRUE, warnings = 1)
clus.c <- tclust (x, k = 3, alpha = 0.1, restr.fact = 1, restr = "deter", equal.weights = TRUE, iter.max = 100, warnings = 1)
clus.d <- tclust (x, k = 3, alpha = 0.1, restr.fact = 50, restr = "eigen", equal.weights = FALSE)
pa <- par (mfrow = c (2, 2))
plot (clus.a, main = "(a) tkmeans")
plot (clus.b, main = "(b) Gallegos and Ritter")
plot (clus.c, main = "(c) Gallegos")
plot (clus.d, main = "(d) tclust")
par (pa)

#--- EXAMPLE 4 -----------------------------
data (swissbank)
# Two clusters and 8% trimming level
clus <- tclust (swissbank, k = 2, alpha = 0.08, restr.fact = 50)

# Pairs plot of the clustering solution
pairs (swissbank, col = clus$cluster + 1)
  # Two coordinates
plot (swissbank[, 4], swissbank[, 6], col = clus$cluster + 1, xlab = "Distance of the inner frame to lower border", ylab = "Length of the diagonal")
plot (clus)

# Three clusters and 0% trimming level
clus <- tclust (swissbank, k = 3, alpha = 0.0, restr.fact = 110)

# Pairs plot of the clustering solution
pairs (swissbank, col = clus$cluster + 1)
  # Two coordinates
plot (swissbank[, 4], swissbank[, 6], col = clus$cluster + 1, xlab = "Distance of the inner frame to lower border", ylab = "Length of the diagonal")
plot (clus)
Description

tkmeans searches for \( k \) (or less) spherical clusters in a data matrix \( x \), whereas the ceiling (alpha \( n \)) most outlying observations are trimmed.

Usage

\[
\text{tkmeans} \( (x, k = 3, \alpha = 0.05, nstart = 50, \text{iter.max} = 20, \text{equal.weights} = \text{FALSE}, \text{center} = 0, \text{scale} = 1, \text{store.x} = \text{TRUE}, \text{drop.empty.clust} = \text{TRUE}, \text{trace} = 0, \text{warnings} = 2, \text{zero.tol} = 1e-16) \]

Arguments

- \( x \): A matrix or data.frame of dimension \( n \times p \), containing the observations (row-wise).
- \( k \): The number of clusters initially searched for.
- \( \alpha \): The proportion of observations to be trimmed.
- \( nstart \): The number of random initializations to be performed.
- \( \text{iter.max} \): The maximum number of concentration steps to be performed. The concentration steps are stopped, whenever two consecutive steps lead to the same data partition.
- \( \text{equal.weights} \): A logical value, specifying whether equal cluster weights (TRUE) or not (FALSE) shall be considered in the concentration and assignment steps.
- \( \text{center}, \text{scale} \): A center and scale vector, each of length \( p \) which can optionally be specified for centering and scaling \( x \) before calculation.
- \( \text{store.x} \): A logical value, specifying whether the data matrix \( x \) shall be included in the result structure. By default this value is set to TRUE, because functions \text{plot.tkmeans} depends on this information. However, when big data matrices are handled, the result structure’s size can be decreased noticeably when setting this parameter to FALSE.
- \( \text{drop.empty.clust} \): Logical value specifying, whether empty clusters shall be omitted in the resulting object. (The result structure does not contain center and covariance estimates of empty clusters anymore. Cluster names are reassigned such that the first \( l \) clusters (\( l \leq k \)) always have at least one observation.
- \( \text{trace} \): Defines the tracing level, which is set to 0 by default. Tracing level 2 gives additional information on the iteratively decreasing objective function’s value.
- \( \text{warnings} \): The warning level (0: no warnings; 1: warnings on unexpected behavior.
- \( \text{zero.tol} \): The zero tolerance used. By default set to 1e-16.

Value

The function returns an S3 object of type \text{tkmeans}, containing the following values:

- \( \text{centers} \): A matrix of size \( p \times k \) containing the centers (column-wise) of each cluster.
cluster A numerical vector of size \( n \) containing the cluster assignment for each observation. Cluster names are integer numbers from 1 to \( k \), 0 indicates trimmed observations.

par A list, containing the parameters the algorithm has been called with (\( x \), if not suppressed by \( \text{store.}x = \text{FALSE} \), \( k \), \( \alpha \), \( \text{restr.fact} \), \( \text{nstart} \), \( \text{KStep} \), and \( \text{equal.weights} \)).

\( k \) The (final) resulting number of clusters. Some solutions with a smaller number of clusters might be found when using the option \( \text{equal.weights} = \text{FALSE} \).

obj The value of the objective function of the best (returned) solution.

size An integer vector of size \( k \), returning the number of observations contained by each cluster.

weights A numerical vector of length \( k \), containing the weights of each cluster.

int A list of values internally used by function related to \text{tkmeans} objects.

Author(s)

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References


Examples

```r
#--- EXAMPLE 1 -----------------------------------------------
sig <- diag(2)
cen <- rep(1:2)
x <- rbind(mvtnorm::rmvnorm(360, cen * 0, sig),
           mvtnorm::rmvnorm(540, cen * 5, sig * 6 - 2),
           mvtnorm::rmvnorm(100, cen * 2.5, sig * 50))

# Two groups and 10% trimming level
clus <- tkmeans(x, k = 2, alpha = 0.1)

plot(clus)
plot(clus, labels = "observation")
plot(clus, labels = "cluster")

#--- EXAMPLE 2 -----------------------------------------------
data(geyser2)
clus <- tkmeans(geyser2, k = 3, alpha = 0.03)
plot(clus)

#--- EXAMPLE 3 -----------------------------------------------
data(swissbank)
# Two clusters and 8% trimming level
```
clus <- tkmeans(swissbank, k = 2, alpha = 0.08)

  # Pairs plot of the clustering solution
pairs(swissbank, col = clus$cluster + 1)
  # Two coordinates
plot(swissbank[, 4], swissbank[, 6], col = clus$cluster + 1,
    xlab = "Distance of the inner frame to lower border",
    ylab = "Length of the diagonal")
plot(clus)

# Three clusters and 0% trimming level
clus <- tkmeans(swissbank, k = 3, alpha = 0.0)

  # Pairs plot of the clustering solution
pairs(swissbank, col = clus$cluster + 1)

  # Two coordinates
plot(swissbank[, 4], swissbank[, 6], col = clus$cluster + 1,
    xlab = "Distance of the inner frame to lower border",
    ylab = "Length of the diagonal")
plot(clus)
Index

*Topic **cluster**
  
  ctlcurves, 2  
  discr_coords, 6  
  DiscrFact, 5  
  plot.ctlcurves, 9  
  plot.DiscrFact, 10  
  plot.tclust, 12  
  summary.DiscrFact, 14  
  tclust, 16  
  tkmeans, 20

*Topic **hplot**
  
  ctlcurves, 2  
  discr_coords, 6  
  DiscrFact, 5  
  plot.ctlcurves, 9  
  plot.DiscrFact, 10  
  plot.tclust, 12  
  summary.DiscrFact, 14

*Topic **multivariate**
  
  ctlcurves, 2  
  discr_coords, 6  
  DiscrFact, 5  
  plot.ctlcurves, 9  
  plot.DiscrFact, 10  
  plot.tclust, 12  
  summary.DiscrFact, 14  
  tclust, 16  
  tkmeans, 20

*Topic **package**
  
  tclust-package, 2

*Topic **robust**
  
  ctlcurves, 2  
  discr_coords, 6  
  DiscrFact, 5  
  plot.ctlcurves, 9  
  plot.DiscrFact, 10  
  plot.tclust, 12  
  summary.DiscrFact, 14  
  tclust, 16

  tkmeans, 20
  
  print.tclust (tclust), 16  
  tclust (tclust), 16  
  tkmeans (tkmeans), 20

  ctlcurves, 2, 2  
  discr_coords, 6, 12  
  DiscrFact, 2, 5, 9, 17

  geyser2, 7

  lines, 9

  M5data, 8

  plot, 9–12  
  plot.ctlcurves, 4, 9  
  plot.DiscrFact, 5, 6, 10, 14  
  plot.tclust, 11, 12, 17  
  plot.tkmeans, 20  
  plot.tkmeans (plot.tclust), 12  
  plot_DiscrFact_p2 (plot.DiscrFact), 10  
  plot_DiscrFact_p3 (plot.DiscrFact), 10  
  plotting, 5  
  print.ctlcurves (ctlcurves), 2  
  print.DiscrFact (DiscrFact), 5

  summary, 14  
  summary.DiscrFact, 14  
  swissbank, 15

  tclust, 2, 3, 7, 12, 16
  tclust-package, 2
  tkmeans, 16, 19