Package ‘kmed’

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Type  Package
Title  Distance-Based k-Medoids
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Description  Algorithms of distance-based k-medoids clustering: simple and fast
  k-medoids, ranked k-medoids, and increasing number of clusters in k-medoids.
  Calculate distances for mixed variable data such as Gower, Podani, Wishart,
  Huang, Harikumar-PV, and Ahmad-Dey. Cluster validation applies internal and
  relative criteria. The internal criteria includes silhouette index and shadow
  values. The relative criterium applies bootstrap procedure producing a heatmap
  with a flexible reordering matrix algorithm such as complete, ward, or average
  linkages. The cluster result can be plotted in a marked barplot or pca biplot.
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R topics documented:

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Description

This function creates a barplot from a cluster result. A barplot indicates the location and dispersion of each cluster. The x-axis of the barplot is variable’s mean, while the y-axis is the variable’s name.

Usage

barplotnum(dataori, clust, nc = 1, alpha = 0.05)

Arguments

dataori    An original data set.
clust   A vector of cluster membership (see Details).
nc   A number of columns for the plot of all cluster (see Details).
alpha   A numeric number to set the significant level (between 0 and 0.2).

Details

This is a marked barplot because some markers are added, i.e. a significant test, a population mean for each (numerical) variable. The significance test applies t-test between the population’s mean and cluster’s mean in every variable. The alpha is set in between 0 to 20%. If the population mean differs to the cluster’s mean, the bar shade in the barplot also differs.

clust is a vector with the length equal to the number of objects (n), or the function will be an error otherwise. nc controls the layout (grid) of the plot. If nc = 1, the plot of each cluster is placed in a column. When the number of clusters is 6 and nc = 2, for example, the plot has a layout of 3-row and 2-column grids.
Value

Function returns a barplot.

Author(s)

Weksi Budiaji
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References


Examples

dat <- iris[,1:4]
memb <- cutree(hclust(dist(dat)),3)
barplotnum(dat, memb)
barplotnum(dat, memb, 2)

---

clust4 4-clustered data set

Description

A dataset containing two variables of 300 objects and their class memberships generated by the clusterGeneration package.

Usage

clust4

Format

A data frame with 300 rows and 3 variables:

x1  X1.
x2  X2.
class  Class membership.
Source

Data is generated via the genRandomClust function in the clusterGeneration package. The code to generate this data set is

```r
set.seed(2016)
randclust <- clusterGeneration::genRandomClust(4, sepVal = 0.001, numNonNoisy = 2, numRepli-
cate = 1, clustszind = 3, clustSizes = as.numeric(table(sample(1:4, 300, replace = TRUE))), output-
DatFlag=FALSE, outputLogFlag=FALSE, outputEmpirical=FALSE, outputInfo=FALSE)
clust4 <- as.data.frame(randclust$datList$test_1)
clust4$class <- randclust$memList$test_1
```

References


---

clust5 5-clustered data set

Description

A dataset containing two variables of 800 objects and their class memberships generated by the clusterGeneration package.

Usage

clust5

Format

A data frame with 800 rows and 3 variables:

- `x1` X1.
- `x2` X2.
- `class` Class membership.
Source
Data is generated via the genRandomClust function in the clusterGeneration package. The code to generate this data set is

```r
set.seed(2016)
randclust <- clusterGeneration::genRandomClust(5, sepVal = 0.2, numNonNoisy = 2, numReplicate = 1, clustszind = 3, clustSizes = as.numeric(table(sample(1:5, 800, replace = TRUE))), outputDatFlag=FALSE, outputLogFlag=FALSE, outputEmpirical=FALSE, outputInfo=FALSE)
clust5 <- as.data.frame(randclust$datList$test_1)
clust5$class <- randclust$memList$test_1
```

References

---

**clustboot**

**Bootstrap replications for clustering algorithm**

**Description**
This function does bootstrap replications for a clustering algorithm. Any hard clustering algorithm is valid.

**Usage**

```r
clustboot(distdata, nclust = 2, algorithm = fastclust, nboot = 25, diss = TRUE)
```

**Arguments**

- **distdata** A distance matrix (n x n)/dist object or a data frame.
- **nclust** A number of clusters.
- **algorithm** A clustering algorithm function (see Details).
- **nboot** A number of bootstrap replicates.
- **diss** A logical if distdata is a distance matrix/ object or a data frame.
Details

This is a function to obtain bootstrap evaluation for cluster results. The algorithm argument is a function where this function has two input arguments. The two input arguments are a distance matrix/object or a data frame, and number of clusters. Then the output is only a vector of cluster memberships.

The default algorithm is fastclust applying the fastkmed function. The code of the fastclust is

\[
\text{fastclust} \leftarrow \text{function}(x, \text{nclust}) \{
\text{res} \leftarrow \text{fastkmed}(x, \text{nclust}, \text{iterate} = 50)
\text{return}(\text{res}$\text{cluster})
\}
\]

For other examples, see Examples. It applies ward and kmeans algorithms. When kmeans is applied, for example, diss is set to be FALSE because the input of the kmclust and clustboot is a data frame instead of a distance.

Value

Function returns a matrix of bootstrap replicates with a dimension of \( n \times b \), where \( n \) is the number of objects and \( b \) is the number of bootstrap replicates.

Author(s)

Weksi Budiaji
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References


Examples

\[
\text{num} \leftarrow \text{as.matrix(iris[,1:4])}
\text{mrwdist} \leftarrow \text{distNumeric(num, num, method = "mrw")}
\text{ward.D2} \leftarrow \text{function}(x, \text{nclust}) \{
\text{res} \leftarrow \text{hclust}(\text{as.dist}(x), \text{method} = "\text{ward.D2"})
\text{member} \leftarrow \text{cutree}(\text{res}, \text{nclust})
\text{return}(\text{member})
\}
\text{kmclust} \leftarrow \text{function}(x, \text{nclust}) \{
\text{res} \leftarrow \text{kmeans}(x, \text{nclust})
\text{return}(\text{res}$\text{cluster})
\}
\text{irisfast} \leftarrow \text{clustboot(mrwdist, nclust=3, nboot=7)}
\text{head(irisfast)}
\text{irisward} \leftarrow \text{clustboot(mrwdist, nclust=3, algorithm = ward.D2, nboot=7)}
\text{head(irisward)}
\text{irkmeans} \leftarrow \text{clustboot(num, nclust=3, algorithm = kmclust, nboot=7, diss = FALSE)}
\]
clustheatmap

head(iriskmeans)

---

clustheatmap  

*Consensus matrix heatmap from A consensus matrix*

**Description**

This function creates a consensus matrix heatmap from a consensus/agreement matrix. The values of the consensus/agreement matrix are transformed in order to plot the heatmap.

**Usage**

```r
clustheatmap(consmat, title = "")
```

**Arguments**

- `consmat`: A matrix of consensus/agreement matrix *(see Details)*.
- `title`: A title of the plot.

**Details**

This is a function to produce a consensus matrix heatmap from a consensus/agreement matrix. A matrix produced by the `consensumat` function can be directly provided in the `consmat` argument. The values of the consensus matrix, A, are then transformed via a non-linear transformation by applying

\[
a_{ij}^{trf} = \frac{a_{ij} - \min(a_\cdot)}{\max(a_\cdot) - \min(a_\cdot)}
\]

where \(a_{ij}\) is the value of the consensus matrix in row \(i\) and column \(j\), and \(a_\cdot\) is the all values of the matrix \((\forall A)\).

**Value**

Function returns a heatmap plot.

**Author(s)**

Weksi Budiaji  
Contact: <budiaji@untirta.ac.id>

**References**


Examples

num <- as.matrix(iris[,1:4])
mrwdist <- distNumeric(num, num, method = "mrw")
irisfast <- clustboot(mrwdist, nclust=3, nboot=7)
complete <- function(x, nclust) {
  res <- hclust(as.dist(x), method = "complete")
  member <- cutree(res, nclust)
  return(member)
}
consensuscomplete <- consensusmatrix(irisfast, nclust = 3, reorder = complete)
clustheatmap(consensuscomplete)

consensusmatrix | Consensus matrix from A matrix of bootstrap replicates

Description

This function creates a consensus matrix from a matrix of bootstrap replicates. It transforms an \( n \times b \) matrix into an \( n \times n \) matrix, where \( n \) is the number of objects and \( b \) is the number of bootstrap replicates.

Usage

consensusmatrix(bootdata, nclust, reorder = fastclust)

Arguments

- **bootdata**: A matrix of bootstrap replicate \((n \times b)\) (see Details).
- **nclust**: A number of clusters.
- **reorder**: Any distance-based clustering algorithm function (see Details).

Details

This is a function to obtain a consensus matrix from a matrix of bootstrap replicates to evaluate the clustering result. The bootdata argument can be supplied directly from a matrix produced by the clustboot function. The values of the consensus matrix, \( A \), are calculated by

\[
a_{ij} = a_{ji} = \frac{\text{# of objects } i \text{ and } j \text{ in the same cluster}}{\text{# of objects } i \text{ and } j \text{ sampled at the same time}}
\]

where \( a_{ij} \) is the agreement index between objects \( i \) and \( j \). Note that due to the agreement between objects \( i \) and \( j \) equal to the agreement between objects \( j \) and \( i \), the consensus matrix is a symmetric matrix.

Meanwhile, the reorder argument is a function to reorder the objects in both the row and column of the consensus matrix such that similar objects are close to each other. This task can be solved by applying a clustering algorithm in the consensus matrix. The reorder has to consist of two
input arguments. The two input arguments are a distance matrix/ object and number of clusters. The output is only a vector of cluster memberships. Thus, the algorithm that can be applied in the reorder argument is the distance-based algorithm with a distance as the input.

The default reorder is `fastclust` applying the `fastkmed` function. The code of the `fastclust` is:

```r
fastclust <- function(x, nclust) {
  res <- fastkmed(x, nclust, iterate = 50)
  return(res$cluster)
}
```

For other examples, see Examples. It applies centroid and complete linkage algorithms.

Value

Function returns a consensus/ agreement matrix of \( n \times n \) dimension.

Author(s)

Weksi Budiaji

Contact: <budiaji@untirta.ac.id>

References


Examples

```r
num <- as.matrix(iris[,1:4])
mrwdist <- distNumeric(num, num, method = "mrw")
irisfast <- clustboot(mrwdist, nclust=3, n.boot=7)
consensusfast <- consensusmatrix(irisfast, nclust = 3)
centroid <- function(x, nclust) {
  res <- hclust(as.dist(x), method = "centroid")
  member <- cutree(res, nclust)
  return(member)
}
consensuscentroid <- consensusmatrix(irisfast, nclust = 3, reorder = centroid)
complete <- function(x, nclust) {
  res <- hclust(as.dist(x), method = "complete")
  member <- cutree(res, nclust)
  return(member)
}
consensuscomplete <- consensusmatrix(irisfast, nclust = 3, reorder = complete)
consensusfast[,c(1:5,51:55,101:105),c(1:5,51:55,101:105)]
consensuscentroid[,c(1:5,51:55,101:105),c(1:5,51:55,101:105)]
consensuscomplete[,c(1:5,51:55,101:105),c(1:5,51:55,101:105)]
```
Description

This function calculates the co-occurrence distance proposed by Ahmad and Dey (2007).

Usage

```
cooccur(data)
```

Arguments

data

A matrix or data frame of binary/categorical variables (see Details).

Details

This function computes co-occurrence distance, which is a binary/categorical distance, that based on the other variable’s distribution (see Examples). In the Examples, we have a data set:

<table>
<thead>
<tr>
<th>object</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>3</td>
<td>2</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>4</td>
<td>2</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>5</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>6</td>
<td>2</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>7</td>
<td>2</td>
<td>1</td>
<td>2</td>
</tr>
</tbody>
</table>

The co-occurrence distance transforms each category of binary/categorical in a variable based on the distribution of other variables, for example, the distance between categories 1 and 2 in the x variable can be different to the distance between categories 1 and 2 in the z variable. As an example, the transformed distance between categories 1 and 2 in the z variable is presented.

A cross tabulation between the z and x variables with corresponding (column) proportion is

<table>
<thead>
<tr>
<th></th>
<th>1</th>
<th>2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.0</td>
<td>0.2</td>
</tr>
<tr>
<td>2</td>
<td>0.0</td>
<td>0.8</td>
</tr>
</tbody>
</table>

A cross tabulation between the z and y variables with corresponding (column) proportion is

<table>
<thead>
<tr>
<th></th>
<th>1</th>
<th>2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.5</td>
<td>0.6</td>
</tr>
<tr>
<td>2</td>
<td>0.5</td>
<td>0.4</td>
</tr>
</tbody>
</table>

Then, the maximum values of the proportion in each row are taken such that they are 1.0, 0.8, 0.6,
and 0.5. The new distance between categories 1 and 2 in the \( z \) variable is

\[
\delta_{1,2}^z = \frac{(1.0 + 0.8 + 0.6 + 0.5) - 2}{2} = 0.45
\]

The constant 2 in the formula applies because the \( z \) variable depends on the 2 other variable distributions, i.e the \( x \) and \( y \) variables. The new distances of each category in the for the \( x \) and \( y \) variables can be calculated in a similar way.

Thus, the distance between objects 1 and 2 is 0.45. It is only the \( z \) variable counted to calculate the distance between objects 1 and 2 because objects 1 and 2 have similar values in both the \( x \) and \( y \) variables.

The data argument can be supplied with either a matrix or data frame, in which the class of the element has to be an integer. If it is not an integer, it will be converted to an integer class. If the data of a variable only, a simple matching is calculated. The co-occurrence is absent due to its dependency to the distribution of other variables and a warning message appears.

Value

Function returns a distance matrix \((n \times n)\).

Author(s)

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References


Examples

```r
set.seed(1)
a <- matrix(sample(1:2, 7*3, replace = TRUE), 7, 3)
cooccur(a)
```

---

**csv**

**Centroid shadow value (CSV) index and plot**

**Description**

This function computes centroid shadow values and shadow value plots of each cluster. The plot presents the mean of the shadow values as well.
Usage

```r
csv(distdata, idmedoid, idcluster, title = "")
```

Arguments

- `distdata`: A distance matrix \((n \times n)\) or `dist` object.
- `idmedoid`: A vector of id medoids (see Details).
- `idcluster`: A vector of cluster membership (see Details).
- `title`: A title of the plot.

Details

The origin of the centroid shadow value is calculated in the `shadow` function of the `flexclust` package, in which it is based on the first and second closest centroid. The `csv` function in this package modifies the centroid into medoid such that the formula to compute shadow value of object \(i\) is

\[
csv(i) = \frac{2d(i, m(i))}{d(i, m(i)) + d(i, m'(i))}
\]

where \(d(i, m(i))\) is the distance between object \(i\) to the first closest medoid and \(d(i, m'(i))\) is the distance between object \(i\) to the second closest medoid.

The `idmedoid` argument corresponds to the `idcluster` argument. If the length of `idmedoid` is 3, for example, the `idcluster` has to have 3 unique cluster memberships, or it returns Error otherwise. The length of the `idcluster` has also to be equal to \(n\) (the number of objects). In contrast to the silhouette value, the centroid shadow value is interpreted that lower value is the better cluster separation.

Value

Function returns a list with following components:

- `result`: is a data frame of the shadow values for all objects
- `plot`: is the shadow value plots of each cluster.

Author(s)

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References


Examples

distiris <- as.matrix(dist(iris[,1:4]))
res <- fastkmed(distiris, 3)
sha <- csv(distiris, res$medoid, res$cluster)
sha$result[c(1:3,70:75,101:103),]
sha$plot

distmix

Distances for mixed variables data set

Description
This function computes a distance matrix for a mixed variable data set applying various methods.

Usage
distmix(data, method = "gower", idnum = NULL, idbin = NULL, idcat = NULL)

Arguments

data A data frame or matrix object.
method A method to calculate the mixed variables distance (see Details).
idnum A vector of column index of the numerical variables.
idbin A vector of column index of the binary variables.
idcat A vector of column index of the categorical variables.

Details
There are six methods available to calculate the mixed variable distance. They are gower, wishart, podani, huang, harikumar, ahmad.

gower
The Gower (1971) distance is the most common distance for a mixed variable data set. Although the Gower distance accommodates missing values, a missing value is not allowed in this function. If there is a missing value, the Gower distance from the daisy function in the cluster package can be applied. The Gower distance between objects \( i \) and \( j \) is computed by

\[
d_{ij} = 1 - s_{ij},
\]

where

\[
s_{ij} = \frac{\sum_{l=1}^{p} \omega_{ijl}s_{ijl}}{\sum_{l=1}^{p} \omega_{ijl}}
\]

\( \omega_{ijl} \) is a weight in variable \( l \) that is usually 1 or 0 (for a missing value). If the variable \( l \) is a numerical variable,

\[
s_{ijl} = 1 - \frac{|x_{il} - x_{jl}|}{R_l}
\]

\( s_{ijl} \in \{0, 1\} \), if the variable \( l \) is a binary/categorical variable.
Wishart (2003) has proposed a different measure compared to Gower (1971) in the numerical variable part. Instead of a range, it applies a variance of the numerical variable in the $s_{ijl}$ such that the distance becomes

$$d_{ij} = \sqrt{\sum_{l=1}^{p} \omega_{ijl} \left( \frac{x_{il} - x_{jl}}{\delta_{ijl}} \right)^2}$$

where $\delta_{ijl} = s_l$ when $l$ is a numerical variable and $\delta_{ijl} \in \{0, 1\}$ when $l$ is a binary/ categorical variable.

Podani (1999) has suggested a different method to compute a distance for a mixed variable data set. The Podani distance is calculated by

$$d_{ij} = \sqrt{\sum_{l=1}^{p} \omega_{ijl} \left( \frac{x_{il} - x_{jl}}{R_l} \right)^2}$$

where $\delta_{ijl} = R_l$ when $l$ is a numerical variable and $\delta_{ijl} \in \{0, 1\}$ when $l$ is a binary/ categorical variable.

Huang (1997) distance between objects $i$ and $j$ is computed by

$$d_{ij} = \sum_{r=1}^{P_n} (x_{ir} - x_{jr})^2 + \gamma \sum_{s=1}^{P_c} \delta_c(x_{is} - x_{js})$$

where $P_n$ and $P_c$ are the number of numerical and categorical variables, respectively,

$$\gamma = \frac{\sum_{r=1}^{P_n} s_r^2}{P_n}$$

and $\delta_c(x_{is} - x_{js})$ is the mismatch/ simple matching distance (see matching) between object $i$ and object $j$ in the variable $s$.

Harikumar-PV (2015) has proposed a distance for a mixed variable data set:

$$d_{ij} = \sum_{r=1}^{P_n} |x_{ir} - x_{jr}| + \sum_{s=1}^{P_c} \delta_c(x_{is} - x_{js}) + \sum_{t=1}^{P_b} \delta_b(x_{it}, x_{jt})$$

where $P_b$ is the number of binary variables, $\delta_c(x_{is}, x_{js})$ is the co-occurrence distance (see cooccur), and $\delta_b(x_{it}, x_{jt})$ is the Hamming distance.

Ahmad and Dey (2007) has computed a distance of a mixed variable set via

$$d_{ij} = \sum_{r=1}^{P_n} (x_{ir} - x_{jr})^2 + \sum_{s=1}^{P_c} \delta_c(x_{is} - x_{js})$$
where \( \delta_c(x_{it}, x_{jt}) \) are the co-occurrence distance (see \texttt{cooccur}). In the Ahmad and Dey distance, the binary and categorical variables are not separable such that the co-occurrence distance is based on the combined these two classes, i.e. binary and categorical variables.

At least two arguments of the \texttt{idnum}, \texttt{idbin}, and \texttt{idcat} have to be provided because this function calculates the mixed distance. If the method is harikumar, the categorical variables have to be at least two variables such that the co-occurrence distance can be computed. It also applies when \texttt{method = "ahmad"}. The \texttt{idbin} + \texttt{idcat} has to be more than 1 column. It returns to an \texttt{Error} message otherwise.

**Value**

Function returns a distance matrix \((n \times n)\).

**Author(s)**

Weksi Budiaji
Contact: <budiaji@untirta.ac.id>

**References**


Huang, Z., 1997. Clustering large data sets with mixed numeric and categorical values, in: The First Pacific-Asia Conference on Knowledge Discovery and Data Mining, pp. 21-34.


**Examples**

```r
set.seed(1)
a <- matrix(sample(1:2, 7*3, replace = TRUE), 7, 3)
a1 <- matrix(sample(1:3, 7*3, replace = TRUE), 7, 3)
mixdata <- cbind(iris[1:7,1:3], a, a1)
colnames(mixdata) <- c(paste(c("num"), 1:3, sep = ""),
paste(c("bin"), 1:3, sep = ""),
paste(c("cat"), 1:3, sep = ""))
distmix(mixdata, method = "gower", idnum = 1:3, idbin = 4:6, idcat = 7:9)
```
**distNumeric**

*A pair distance for numerical variables*

**Description**

This function computes a pairwise numerical distance between two numerical data sets.

**Usage**

```r
distNumeric(x, y, method = "mrw", xyequal = TRUE)
```

**Arguments**

- **x**: A first data matrix (see Details).
- **y**: A second data matrix (see Details).
- **method**: A method to calculate the pairwise numerical distance (see Details).
- **xyequal**: A logical if x is equal to y (see Details).

**Details**

The `x` and `y` arguments have to be matrices with the same number of columns where the row indicates the object and the column is the variable. This function calculates all pairwise distances between rows in the `x` and `y` matrices. Although it calculates a pairwise distance between two data sets, the default function computes all distances in the `x` matrix. If the `x` matrix is not equal to the `y` matrix, the `xyequal` has to be set FALSE.

The method available are `mrw` (Manhattan weighted by range), `sev` (squared Euclidean weighted by variance), `ser` (squared Euclidean weighted by range), `ser.2` (squared Euclidean weighted by squared range) and `se` (squared Euclidean). Their formulas are:

\[
\begin{align*}
mrw_{ij} &= \frac{p_n}{n} \sum_{r=1}^{p} \frac{|x_{ir} - x_{jr}|}{R_r} \\
sev_{ij} &= \frac{p_n}{n} \sum_{r=1}^{p} \frac{(x_{ir} - x_{jr})^2}{s_r^2} \\
ser_{ij} &= \frac{p_n}{n} \sum_{r=1}^{p} \frac{(x_{ir} - x_{jr})^2}{R_r} \\
ser.2_{ij} &= \frac{p_n}{n} \sum_{r=1}^{p} \frac{(x_{ir} - x_{jr})^2}{R_r^2} \\
se_{ij} &= \sum_{r=1}^{p} (x_{ir} - x_{jr})^2
\end{align*}
\]

where `p_n` is the number of numerical variables, `R_r` is the range of the `r`-th variables, `s_r^2` is the variance of the `r`-th variables.
Value

Function returns a distance matrix with the number of rows equal to the number of objects in the x matrix \((n_x)\) and the number of columns equals to the number of objects in the y matrix \((n_y)\).

Author(s)

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Examples

```r
num <- as.matrix(iris[,1:4])
mrwdist <- distNumeric(num, num, method = "m rw")
mrwdist[1:6,1:6]
```

---

**fastkmed**  
*Simple and fast k-medoid algorithm*

Description

This function runs the simple and fast k-medoid algorithm proposed by Park and Jun (2009).

Usage

```r
fastkmed(distdata, ncluster, iterate = 10, init = NULL)
```

Arguments

- `distdata`: A distance matrix \((n x n)\) or `dist` object.
- `ncluster`: A number of clusters.
- `iterate`: A number of iterations for the clustering algorithm.
- `init`: A vector of initial objects as the cluster medoids (see Details).

Details

The simple and fast k-medoids, which sets a set of medoids as the cluster centers, adapts the k-means algorithm for medoid up-dating. The new medoids of each iteration are calculated in the within cluster only such that it gains speed.

`init = NULL` is required because the Park and Jun (2009) has a particular method to select the initial medoids. The initial medoids are selected by

\[
v_j = \frac{\sum_{i=1}^{n} d_{ij}}{\sum_{i=1}^{n} d_{ij}}, \quad j = 1, 2, 3, \ldots, n
\]

where the first \(k\) of the \(v_j\) is selected if the number of clusters is \(k\).
init can be provided with a vector of id objects. The length of the vector has to be equal to the number of clusters. However, assigning a vector in the init argument, the algorithm is no longer the simple and fast k-medoids algorithm. The inckmed function, for example, defines a different method to select the initial medoid though it applies the fastkmed function.

Value

Function returns a list of components:

- cluster is the clustering memberships result.
- medoid is the id medoids.
- minimum_distance is the distance of all objects to their cluster medoid.

Author(s)

Weksi Budiaji
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References


Examples

```r
num <- as.matrix(iris[,1:4])
mrwdist <- distNumeric(num, num, method = "mrw")
result <- fastkmed(mrwdist, ncluster = 3, iterate = 50)
table(result$cluster, iris[,5])
```

---

**globalfood**

*Global food security index*

Description

A dataset containing four variables of 113 countries for their food security index based on panelists evaluation in 2017.

Usage

globalfood
Format

A data frame with 113 rows and 4 variables:

affordability  Index of food affordability.
availability    Index of food availability.
safety          Index of food quality and safety.
resilience      Index of natural resources and resilience.

Source

The original indicator variables consist of 27 variables. Then, they are summarized into four pillars of food security; they are affordability, availability, quality and safety, and natural resources and resilience. Food-security expertise panelists evaluate the score of each country from 0 to 100, where 0 is the least favorable towards food security.

http://foodsecurityindex.eiu.com

Description

A mixed variable dataset containing 14 variables of 297 patients for their heart disease diagnosis.

Usage

heart

Format

A data frame with 297 rows and 14 variables:

age  Age in years (numerical).
sex  Sex: 1 = male, 0 = female (logical).

sex  Four chest pain types: (1) typical angina, (2) atypical angina (3)non-anginal pain, (4) asymptomatic (categorical).

trestbps  Resting blood pressure (in mm Hg on admission to the hospital) (numerical).
chol  Serum cholesterol in mg/dl (numerical).
fbs  Fasting blood sugar more than 120 mg/dl (logical).

restecg  Resting electrocardiographic results: (0) normal, (1) having ST-T wave abnormality, (2) showing probable or definite left ventricular hypertrophy by Estes’ criteria (categorical).
thalach  Maximum heart rate achieved (numerical).
exang  Exercise induced angina (logical).
oldpeak  ST depression induced by exercise relative to rest (numerical).
The slope of the peak exercise ST segment: (1) upsloping, (2) flat, (3) downsloping (categorical).

ca  Number of major vessels (0-3) colored by flourosopy (numerical).

thal (3) normal, (6) fixed defect, (7) reversible defect (categorical).

class Diagnosis of heart disease (4 classes). It can be 2 classes by setting 0 for 0 values and 1 for non-0 values.

Source

The data set is taken from machine learning repository of UCI. The original data set consists of 303 patients with 6 NA’s. Then, the missing values are omitted such that it reduces into 297 patients.

https://archive.ics.uci.edu/ml/datasets/Heart+Disease

References


inckmed

*Increasing number of clusters in k-medoids algorithm*

Description

This function runs the increasing number of clusters in the k-medoids algorithm proposed by Yu et. al. (2018).

Usage

inckmed(distdata, ncluster, iterate = 10, alpha = 1)

Arguments

distdata A distance matrix (n x n) or dist object.
ncluster A number of clusters.
iterate A number of iterations for the clustering algorithm.
alpha A stretch factor to determine the range of initial medoid selection (see Details).

Details

This algorithm is claimed to manage with the weakness of the simple and fast-kmedoids (fastkmed).
The origin of the algorithm is a centroid-based algorithm by applying the Euclidean distance. Then, because the function is a medoid-based algorithm, the object mean (centroid) and variance are redefined into medoid and deviation, respectively.

The alpha argument is a stretch factor, i.e. a constant defined by the user. It is applied to determine a set of medoid candidates. The medoid candidates are calculated by $O = \{X_i | \sigma_i \leq \alpha \sigma, i = \}$
matching 1, 2, …, n \}, where \( \sigma_i \) is the average deviation of object \( i \), and \( \sigma \) is the average deviation of the data set. They are computed by

\[
\sigma = \sqrt{\frac{1}{n-1} \sum_{i=1}^{n} d(O_i, v_1)}
\]

\[
\sigma_i = \sqrt{\frac{1}{n-1} \sum_{i=1}^{n} d(O_i, O_j)}
\]

where \( n \) is the number of objects, \( O_i \) is the object \( i \), and \( v_1 \) is the most centrally located object.

**Value**

Function returns a list of components:
- cluster is the clustering memberships result.
- medoid is the id medoids.
- minimum_distance is the distance of all objects to their cluster medoid.

**Author(s)**

Weksi Budiaji
Contact: <budiaji@untirta.ac.id>

**References**


**Examples**

num <- as.matrix(iris[,1:4])
mrwdist <- distNumeric(num, num, method = "mrw")
result <- inckmed(mrwdist, ncluster = 3, iterate = 50, alpha = 1.5)
table(result$cluster, iris[,5])

**Description**

This function computes the simple matching distance from two data frames/matrices.

**Usage**

matching(x, y)
**Arguments**

- **x** A first data frame or matrix (see Details).
- **y** A second data frame or matrix (see Details).

**Details**

The `x` and `y` arguments have to be data frames/ matrices with the same number of columns where the row indicates the object and the column is the variable. This function calculates all pairwise distance between rows in the `x` and `y` data frames/ matrices. If the `x` data frame/ matrix is equal to the `y` data frame/ matrix, it explicitly calculates all distances in the `x` data frame/ matrix.

The simple matching distance between objects `i` and `j` is calculated by

\[ d_{ij} = \frac{\sum_{s=1}^{P} (x_{is} - x_{js})}{P} \]

where `P` is the number of variables, and `x_{is} - x_{js} \in \{0, 1\}`. `x_{is} - x_{js} = 0`, if `x_{is} = x_{js}` and `x_{is} - x_{js} = 1`, when `x_{is} \neq x_{js}`.

As an example, the distance between objects 1 and 2 is presented.

<table>
<thead>
<tr>
<th>object</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>2</td>
<td>1</td>
</tr>
</tbody>
</table>

The distance between objects 1 and 2 is

\[ d_{12} = \frac{\sum_{s=1}^{3} (x_{is} - x_{js})}{3} = \frac{0 + 0 + 1}{3} = \frac{1}{3} = 0.33 \]

**Value**

Function returns a distance matrix with the number of rows equal to the number of objects in the `x` data frame/ matrix (`n_x`) and the number of columns equals to the number of objects in the `y` data frame/ matrix (`n_y`).

**Author(s)**

Weksi Budiaji
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**Examples**

```r
c <- set.seed(1)
a <- matrix(sample(1:2, 7*3, replace = TRUE), 7, 3)
mapping(a, a)
```
Description

This function computes medoid shadow values and shadow value plots of each cluster. The plot presents the mean of the shadow values as well.

Usage

```r
msv(distdata, idmedoid, idcluster, title = "")
```

Arguments

- `distdata`: A distance matrix (n x n) or `dist` object.
- `idmedoid`: A vector of id medoids (see Details).
- `idcluster`: A vector of cluster membership (see Details).
- `title`: A title of the plot.

Details

The origin of the shadow value is calculated in the `shadow` function of the `flexclust` package, in which it is based on the first and second closest centroid. The `msv` function in this package modifies the centroid into medoid such that the formula to compute shadow value of object \( i \) is

\[
msv(i) = \frac{d(i, m'(i)) - d(i, m(i))}{d(i, m'(i))}
\]

where \( d(i, m(i)) \) is the distance between object \( i \) to the first closest medoid and \( d(i, m'(i)) \) is the distance between object \( i \) to the second closest medoid.

The `idmedoid` argument corresponds to the `idcluster` argument. If the length of `idmedoid` is 3, for example, the `idcluster` has to have 3 unique cluster memberships, or it returns Error otherwise. The length of the `idcluster` has also to be equal to \( n \) (the number of objects). In contrast to the centroid shadow value, the medoid shadow value is interpreted likewise a silhouette value, the higher value the better separation.

Value

Function returns a list with following components:

- `result` is a data frame of the shadow values for all objects
- `plot` is the shadow value plots of each cluster.

Author(s)

Weksi Budiaji
Contact: <budiaji@untirta.ac.id>
References


Examples

distiris <- as.matrix(dist(iris[,1:4]))
res <- fastkmed(distiris, 3)
sha <- msv(distiris, res$medoid, res$cluster)
sha$result[1:3,70:75,101:103],]
sha$plot

pcabiplot

Biplot of a PCA object

Description

This function creates a biplot from a pca object, which is generated by the prcomp function from the stats package.

Usage

pcabiplot(PC, x = "PC1", y = "PC2", var.line = TRUE, colobj = rep(1, nrow(PC$x)), o.size = 1)

Arguments

PC A pca object generated by prcomp function.
x X axis (see Details).
y Y axis (see Details).
var.line A logical input, if variable lines are plotted.
colobj A vector to provide color in the objects (see Details).
o.size A numeric number to set the object size.

Details

This is a function to plot a pca biplot from a pca object. The x and y axes can be supplied with any principle component. The length of the colobj vector has to be equal to the number of objects. This argument controls the color of the objects and is very convenient to explore the clustering result. The default value is that all object have the same color.

Value

Function returns a plot of pca.
Rank k-medoid algorithm

This function runs the rank k-medoids algorithm proposed by Zadegan et. al. (2013).

Usage

rankkmed(distdata, ncluster, m = 3, iterate = 10, init = NULL)

Arguments

distdata A distance matrix (n x n) or dist object.
ncluster A number of clusters.
m A number of objects to compute hostility (see Details).
iterate A number of iterations for the clustering algorithm.
init A vector of initial objects as the cluster medoids (see Details).

Details

This algorithm is claimed to cope with the local optima problem of the simple and fast-kmedoids algorithm (fastkmed). The m argument is defined by the user and has to be 1 < m ≤ n. The m is a hostility measure computed by

\[ m_i = \sum_{X_j \in Y} r_{ij} \]

where \( x_j \) is the object \( j \), \( Y \) is the set of objects as many as \( m \), and \( r_{ij} \) is the rank distance, i.e. sorted distance, between object \( i \) and \( j \).

init can be provided with a vector of id objects. The length of the vector has to be equal to the number of clusters. However, assigning a vector in the init argument, the algorithm is no longer the rank k-medoids algorithm.
Value

Function returns a list of components:
cluster is the clustering memberships result.
medoid is the id medoids.
minimum_distance is the distance of all objects to their cluster medoid.

Author(s)

Weksi Budiaji
Contact: <budiaji@untirta.ac.id>

References


Examples

num <- as.matrix(iris[,1:4])
mrwdist <- distNumeric(num, num, method = "mrw")
result <- rankkmed(mrwdist, ncluster = 3, iterate = 50)
table(result$cluster, iris[,5])

sil

Silhouette index and plot

Description

This function creates silhouette indices and silhouette plots of each cluster. The plot presents also the mean of the silhouette indices per cluster.

Usage

sil(distdata, idmedoid, idcluster, title = "")

Arguments

distdata A distance matrix (n x n) or dist object.
idmedoid A vector of id medoids (see Details).
idcluster A vector of cluster membership (see Details).
title A title of the plot.
**Details**

The silhouette index of object \(i\) is calculated by

\[
si(i) = \frac{b_i - a_i}{\max(a_i, b_i)}
\]

where \(a_i\) is the average distance of object \(i\) to all objects within the cluster, and \(b_i\) is the average distance of object \(i\) to all objects within the nearest cluster.

The \textit{idmedoid} argument corresponds to the \textit{idcluster} argument. If the length of \textit{idmedoid} is 3, for example, the \textit{idcluster} has to have 3 unique memberships, or it returns \texttt{Error} otherwise. The length of the \textit{idcluster} has also to be equal to \(n\) (the number of objects).

**Value**

Function returns a list with following components:

- \texttt{result} is a data frame of the silhouette indices for all objects
- \texttt{plot} is the silhouette plots of each cluster.

**Author(s)**

Weksi Budiaji  
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**References**


**Examples**

```r
distiris <- as.matrix(dist(iris[,1:4]))
res <- fastkmed(distiris, 3)
silhouette <- sil(distiris, res$medoid, res$cluster)
silhouette$result[c(1:3,70:75,101:103),]
silhouette$plot
```

**Description**

This function runs the simple k-medoid algorithm proposed by Budiaji and Leisch (2019).

**Usage**

```r
skm(distdata, ncluster, seeding = 20, iterate = 10)
```
Arguments

distdata  A distance matrix ($n \times n$) or dist object.
ncluster  A number of clusters.
seeding   A number of seedings to run the algorithm (see Details).
iterate   A number of iterations for each seeding (see Details).

Details

The simple k-medoids, which sets a set of medoids as the cluster centers, adapts the simple and fast k-medoid algorithm. The best practice to run the simple and fast k-medoid is by running the algorithm several times with different random seeding options.

Value

Function returns a list of components:

cluster is the clustering memberships result.
medoid is the id medoids.
minimum_distance is the distance of all objects to their cluster medoid.

Author(s)

Weksi Budiaji
Contact: <budiaji@untirta.ac.id>

References


Examples

num <- as.matrix(iris[,1:4])
mrwdist <- distNumeric(num, num, method = "mrw")
result <- skm(mrwdist, ncluster = 3, seeding = 50)
table(result$cluster, iris[,5])
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