Package 'clustMixType'

December 14, 2022

Version 0.3-9

Date 2022-12-13			
Title k-Prototypes Clustering for Mixed Variable-Type Data			
Author Gero Szepannek [aut, cre], Rabea Aschenbruck [aut]			
Maintainer Gero Szepannek <gero.szepannek@web.de></gero.szepannek@web.de>			
Imports RColorBrewer, tibble			
Suggests testthat			
Description Functions to perform k-prototypes partitioning clustering for mixed variable-type data according to Z.Huang (1998): Extensions to the k-Means Algorithm for Clustering Large Data Sets with Categorical Variables, Data Mining and Knowledge Discovery 2, 283-304.			
License GPL (>= 2)			
RoxygenNote 7.2.0			
NeedsCompilation no			
Encoding UTF-8			
Repository CRAN			
Date/Publication 2022-12-14 19:50:02 UTC			
R topics documented:			
clprofiles			
kproto			
kproto_gower			
lambdaest			
predict.kproto			
summary.kproto			
validation_kproto			
Index 18			

2 clprofiles

_				_	
റി	n	rn	fi	1	es

Profiling k-Prototypes Clustering

Description

Visualization of a k-prototypes clustering result for cluster interpretation.

Usage

```
clprofiles(object, x, vars = NULL, col = NULL)
```

Arguments

object	Object resulting from a call of resulting kproto. Also other kmeans like objects with object\$cluster and object\$size are possible.
x	Original data.
vars	Optional vector of either column indices or variable names.
col	Palette of cluster colours to be used for the plots. As a default RColorBrewer's brewer.pal($max(unique(object\$cluster))$, "Set3") is used for $k > 2$ clusters and lightblue and orange else.

Details

For numerical variables boxplots and for factor variables barplots of each cluster are generated.

Author(s)

```
<gero.szepannek@web.de>
```

```
# generate toy data with factors and numerics

n <- 100
prb <- 0.9
muk <- 1.5
clusid <- rep(1:4, each = n)

x1 <- sample(c("A","B"), 2*n, replace = TRUE, prob = c(prb, 1-prb))
x1 <- c(x1, sample(c("A","B"), 2*n, replace = TRUE, prob = c(1-prb, prb)))
x1 <- as.factor(x1)

x2 <- sample(c("A","B"), 2*n, replace = TRUE, prob = c(prb, 1-prb))
x2 <- c(x2, sample(c("A","B"), 2*n, replace = TRUE, prob = c(1-prb, prb)))
x2 <- as.factor(x2)

x3 <- c(rnorm(n, mean = -muk), rnorm(n, mean = muk), rnorm(n, mean = muk), rnorm(n, mean = muk))
x4 <- c(rnorm(n, mean = -muk), rnorm(n, mean = muk), rnorm(n, mean = muk), rnorm(n, mean = muk))</pre>
```

kproto 3

```
x <- data.frame(x1,x2,x3,x4)

# apply k-prototyps
kpres <- kproto(x, 4)
clprofiles(kpres, x)

# in real world clusters are often not as clear cut
# by variation of lambda the emphasize is shifted towards factor / numeric variables
kpres <- kproto(x, 2)
clprofiles(kpres, x)

kpres <- kproto(x, 2, lambda = 0.1)
clprofiles(kpres, x)</pre>
kpres <- kproto(x, 2, lambda = 25)
clprofiles(kpres, x)
```

kproto

k-Prototypes Clustering

Description

Computes k-prototypes clustering for mixed-type data.

Usage

```
kproto(x, ...)
## Default S3 method:
kproto(
    x,
    k,
    lambda = NULL,
    type = "standard",
    iter.max = 100,
    nstart = 1,
    na.rm = "yes",
    keep.data = TRUE,
    verbose = TRUE,
    ...
)
```

Arguments

x Data frame with both numerics and factors.

... Currently not used.

4 kproto

k Either the number of clusters, a vector specifying indices of initial prototypes,

or a data frame of prototypes of the same columns as x.

lambda Parameter > 0 to trade off between Euclidean distance of numeric variables and

simple matching coefficient between categorical variables. Also a vector of variable specific factors is possible where the order must correspond to the order of the variables in the data. In this case all variables' distances will be multiplied

by their corresponding lambda value.

type Character, to specify the distance for clustering. Either "standard" (cf. details

below) or "gower". The latter calls kproto_gower.

iter.max Maximum number of iterations if no convergence before.

nstart If > 1 repetitive computations with random initializations are computed and the

result with minimum tot.dist is returned.

na.rm Character; Either "yes" to strip NA values for complete case analysis, "no" to

keep and ignore NA values, "imp.internal" to impute the NAs within the algorithm or "imp.onestep" to apply the algorithm ignoring the NAs and impute them

after the partition is determined.

keep.data Logical whether original should be included in the returned object.

verbose Logical whether additional information about process should be printed. Cau-

tion: For verbose=FALSE, if the number of clusters is reduced during the itera-

tions it will not mentioned.

Details

The algorithm like k-means iteratively recomputes cluster prototypes and reassigns clusters. For type = "standard" clusters are assigned using $d(x,y) = d_{euclid}(x,y) + \lambda d_{simple\ matching}(x,y)$. Cluster prototypes are computed as cluster means for numeric variables and modes for factors (cf. Huang, 1998). Ordered factors variables are treated as categorical variables. In case of na.rm = FALSE: for each observation variables with missings are ignored (i.e. only the remaining variables are considered for distance computation). In consequence for observations with missings this might result in a change of variable's weighting compared to the one specified by lambda. For these observations distances to the prototypes will typically be smaller as they are based on fewer variables. For type = "gower" cf. kproto_gower.

Value

kmeans like object of class kproto:

cluster Vector of cluster memberships.
centers Data frame of cluster prototypes.
lambda Distance parameter lambda.

type Type argument of the function call.

size Vector of cluster sizes.

withinss Vector of within cluster distances for each cluster, i.e. summed distances of all

observations belonging to a cluster to their respective prototype.

tot.withinss Target function: sum of all observations' distances to their corresponding cluster

prototype.

kproto 5

dists	Matrix with distances of observations to all cluster prototypes.
iter	Prespecified maximum number of iterations.
stdization	Only returned for type = "gower": List of standardized ranks for ordinal variables and an additional element num_ranges with ranges of all numeric variables. Used by predict.kproto.
trace	List with two elements (vectors) tracing the iteration process: tot.dists and moved number of observations over all iterations.

Author(s)

```
<gero.szepannek@web.de>
```

References

- Szepannek, G. (2018): clustMixType: User-Friendly Clustering of Mixed-Type Data in R, *The R Journal 10/2*, 200-208, doi:10.32614/RJ2018048.
- Aschenbruck, R., Szepannek, G., Wilhelm, A. (2022): Imputation Strategies for Clustering Mixed-Type Data with Missing Values, *Journal of Classification*, doi:10.1007/s00357022-09422y.
- Z.Huang (1998): Extensions to the k-Means Algorithm for Clustering Large Data Sets with Categorical Variables, Data Mining and Knowledge Discovery 2, 283-304.

```
# generate toy data with factors and numerics
n <- 100
prb <- 0.9
muk <- 1.5
clusid \leftarrow rep(1:4, each = n)
x1 \leftarrow sample(c("A", "B"), 2*n, replace = TRUE, prob = c(prb, 1-prb))
x1 \leftarrow c(x1, sample(c("A", "B"), 2*n, replace = TRUE, prob = c(1-prb, prb)))
x1 <- as.factor(x1)</pre>
x2 \leftarrow sample(c("A","B"), 2*n, replace = TRUE, prob = c(prb, 1-prb))
x^2 < c(x^2, sample(c("A","B"), 2*n, replace = TRUE, prob = c(1-prb, prb)))
x2 <- as.factor(x2)
x3 <- c(rnorm(n, mean = -muk), rnorm(n, mean = muk), rnorm(n, mean = -muk), rnorm(n, mean = muk))
x4 <- c(rnorm(n, mean = -muk), rnorm(n, mean = muk), rnorm(n, mean = -muk), rnorm(n, mean = muk))
x \leftarrow data.frame(x1,x2,x3,x4)
# apply k-prototypes
kpres <- kproto(x, 4)
clprofiles(kpres, x)
# in real world clusters are often not as clear cut
# by variation of lambda the emphasize is shifted towards factor / numeric variables
```

kproto_gower

```
kpres <- kproto(x, 2)
clprofiles(kpres, x)

kpres <- kproto(x, 2, lambda = 0.1)
clprofiles(kpres, x)

kpres <- kproto(x, 2, lambda = 25)
clprofiles(kpres, x)</pre>
```

kproto_gower

k-Prototypes Clustering using Gower Dissimilarity

Description

Internal function. Computes k-prototypes clustering for mixed-type data using Gower dissimilarity.

Usage

```
kproto_gower(
    x,
    k,
    lambda = NULL,
    iter.max = 100,
    na.rm = "yes",
    keep.data = TRUE,
    verbose = TRUE
)
```

tioned.

Arguments

x	Data frame with both numerics and factors (also ordered factors are possible).
k	Either the number of clusters, a vector specifying indices of initial prototypes, or a data frame of prototypes of the same columns as x.
lambda	Parameter > 0 to trade off between Euclidean distance of numeric variables and simple matching coefficient between categorical variables. Also a vector of variable specific factors is possible where the order must correspond to the order of the variables in the data. In this case all variables' distances will be multiplied by their corresponding lambda value.
iter.max	Maximum number of iterations if no convergence before.
na.rm	Character; passed from kproto. For "no" observations where all variables are missinf are assigned cluster membershim NA.
keep.data	Logical whether original should be included in the returned object.
verbose	Logical whether information about the cluster procedure should be given. Caution: If verbose=FALSE, the reduction of the number of clusters is not men-

kproto_gower 7

Details

Internal function called by kproto. Note that there is no nstart argument. Higher values than nstart = 1 can be specified within kproto which will call kproto_gower several times. For Gower dissimilarity range-normalized absolute distances from the cluster median are computed for the numeric variables (and for the ranks of the ordered factors respectively). For factors simple matching distance is used as in the original k prototypes algorithm. The prototypes are given by the median for numeric variables, the mode for factors and the level with the closest rank to the median rank of the corresponding cluster. In case of na.rm = "no": for each observation variables with missings are ignored (i.e. only the remaining variables are considered for distance computation). In consequence for observations with missings this might result in a change of variable's weighting compared to the one specified by lambda. Further note: For these observations distances to the prototypes will typically be smaller as they are based on fewer variables.

Value

kmeans like object of class kproto:

cluster	Vector of cluster memberships.
centers	Data frame of cluster prototypes.
lambda	Distance parameter lambda. For codetype = "gower" only a vector of variable specific weights is possible.
size	Vector of cluster sizes.
withinss	Vector of within cluster distances for each cluster, i.e. summed distances of all observations belonging to a cluster to their respective prototype.
tot.withinss	Target function: sum of all observations' distances to their corresponding cluster prototype.
dists	Matrix with distances of observations to all cluster prototypes.
iter	Prespecified maximum number of iterations.
stdization	List of standardized ranks for ordinal variables and an additional element num_ranges with ranges of all numeric variables. Used by predict.kproto.
trace	List with two elements (vectors) tracing the iteration process: tot.dists and moved number of observations over all iterations.

Author(s)

<gero.szepannek@web.de>

References

- Gower, J. C. (1971): A General Coefficient of Similarity and Some of Its Properties. *Biometrics*, 27(4), 857–871. doi:10.2307/2528823.
- Podani, J. (1999): Extending Gower's general coefficient of similarity to ordinal characters. *TAXON*, 48, 331-340. doi:10.2307/1224438.

8 lambdaest

Examples

```
datasim \leftarrow function(n = 100, k.ord = 2, muk = 1.5){
 clusid \leftarrow rep(1:4, each = n)
 # numeric
 mus <- c(rep(-muk, n),
           rep(-muk, n),
           rep(muk, n),
           rep(muk, n))
           x1 <- rnorm(4*n) + mus
 # ordered factor
 mus <- c(rep(-muk, n),</pre>
           rep(muk, n),
           rep(-muk, n),
           rep(muk, n))
 x2 <- rnorm(4*n) + mus
 # ordered factor
 quants <- quantile(x2, seq(0, 1, length.out = (k.ord+1)))
quants[1] <- -Inf
quants[length(quants)] <- Inf</pre>
x2 <- as.ordered(cut(x2, quants))</pre>
x < - data.frame(x1, x2)
return(x)
}
       <- 100
n
       <- datasim(n = n, k.ord = 10, muk = 2)
 truth \leftarrow rep(1:4, each = n)
 # calling the internal kproto_gower() directly
 kgres <- kproto_gower(x, 4, verbose = FALSE)</pre>
 # calling kproto gower via kproto:
 kgres2 <- kproto(x, 4, verbose = FALSE, type = "gower", nstart = 10)
 table(kgres$cluster, truth)
 clprofiles(kgres, x)
```

lambdaest

Compares Variability of Variables

Description

Investigation of the variables' variances/concentrations to support specification of lambda for k-prototypes clustering.

Usage

```
lambdaest(x, num.method = 1, fac.method = 1, outtype = "numeric")
```

lambdaest 9

Arguments

X	Original data.
num.method	Integer 1 or 2. Specifies the heuristic used for numeric variables.
fac.method	Integer 1 or 2. Specifies the heuristic used for factor variables.
outtype	Specifies the desired output: either 'numeric', 'vector' or 'variation'.

Details

Variance (num.method = 1) or standard deviation (num.method = 2) of numeric variables and $1 - \sum_i p_i^2$ (fac.method = 1) or $1 - \max_i p_i$ (fac.method = 2) for factors is computed.

Value

lambda

Ratio of averages over all numeric/factor variables is returned. In case of outtype = "vector" the separate lambda for all variables is returned as the inverse of the single variables' variation as specified by the num.method and fac.method argument. outtype = "variation" directly returns these quantities and is not ment to be passed directly to kproto().

Author(s)

```
<gero.szepannek@web.de>
```

```
# generate toy data with factors and numerics
n <- 100
prb <- 0.9
muk <- 1.5
clusid \leftarrow rep(1:4, each = n)
x1 \leftarrow sample(c("A", "B"), 2*n, replace = TRUE, prob = c(prb, 1-prb))
x1 \leftarrow c(x1, sample(c("A", "B"), 2*n, replace = TRUE, prob = c(1-prb, prb)))
x1 <- as.factor(x1)</pre>
x2 \leftarrow sample(c("A","B"), 2*n, replace = TRUE, prob = c(prb, 1-prb))
x2 \leftarrow c(x2, sample(c("A","B"), 2*n, replace = TRUE, prob = c(1-prb, prb)))
x2 <- as.factor(x2)</pre>
x3 <- c(rnorm(n, mean = -muk), rnorm(n, mean = muk), rnorm(n, mean = -muk), rnorm(n, mean = muk))
x4 <- c(rnorm(n, mean = -muk), rnorm(n, mean = muk), rnorm(n, mean = -muk), rnorm(n, mean = muk))
x \leftarrow data.frame(x1,x2,x3,x4)
lambdaest(x)
res <- kproto(x, 4, lambda = lambdaest(x))
```

10 plot.kproto

plot.kproto

Assign k-Prototypes Clusters

Description

Plot distributions of the clusters across the variables.

Usage

```
## S3 method for class 'kproto'
plot(x, ...)
```

Arguments

x Object resulting from a call of kproto.

... Additional arguments to be passet to clprofiles such as e.g. vars.

Details

Wrapper around clprofiles. Only works for kproto object created with keep.data = TRUE.

Author(s)

```
<gero.szepannek@web.de>
```

```
# generate toy data with factors and numerics
n <- 100
prb <- 0.9
muk <- 1.5
clusid <- rep(1:4, each = n)
x1 \leftarrow sample(c("A","B"), 2*n, replace = TRUE, prob = c(prb, 1-prb))
x1 \leftarrow c(x1, sample(c("A", "B"), 2*n, replace = TRUE, prob = c(1-prb, prb)))
x1 <- as.factor(x1)</pre>
x2 \leftarrow sample(c("A","B"), 2*n, replace = TRUE, prob = c(prb, 1-prb))
x2 \leftarrow c(x2, sample(c("A","B"), 2*n, replace = TRUE, prob = c(1-prb, prb)))
x2 <- as.factor(x2)</pre>
x3 <- c(rnorm(n, mean = -muk), rnorm(n, mean = muk), rnorm(n, mean = -muk), rnorm(n, mean = muk))
x4 <- c(rnorm(n, mean = -muk), rnorm(n, mean = muk), rnorm(n, mean = -muk), rnorm(n, mean = muk))
x \leftarrow data.frame(x1,x2,x3,x4)
# apply k-prototyps
kpres <- kproto(x, 4)
```

predict.kproto 11

```
plot(kpres, vars = c("x1", "x3"))
```

predict.kproto

Assign k-Prototypes Clusters

Description

Predicts k-prototypes cluster memberships and distances for new data.

Usage

```
## S3 method for class 'kproto'
predict(object, newdata, ...)
```

Arguments

object Object resulting from a call of kproto.

dicted.

... Currently not used.

Value

kmeans like object of class kproto:

cluster Vector of cluster memberships.

dists Matrix with distances of observations to all cluster prototypes.

Author(s)

```
<gero.szepannek@web.de>
```

```
# generate toy data with factors and numerics

n <- 100
prb <- 0.9
muk <- 1.5
clusid <- rep(1:4, each = n)

x1 <- sample(c("A","B"), 2*n, replace = TRUE, prob = c(prb, 1-prb))
x1 <- c(x1, sample(c("A","B"), 2*n, replace = TRUE, prob = c(1-prb, prb)))
x1 <- as.factor(x1)

x2 <- sample(c("A","B"), 2*n, replace = TRUE, prob = c(prb, 1-prb))</pre>
```

12 summary.kproto

```
x2 <- c(x2, sample(c("A","B"), 2*n, replace = TRUE, prob = c(1-prb, prb)))
x2 <- as.factor(x2)

x3 <- c(rnorm(n, mean = -muk), rnorm(n, mean = muk), rnorm(n, mean = -muk), rnorm(n, mean = muk))
x4 <- c(rnorm(n, mean = -muk), rnorm(n, mean = muk), rnorm(n, mean = -muk), rnorm(n, mean = muk))
x <- data.frame(x1,x2,x3,x4)

# apply k-prototyps
kpres <- kproto(x, 4)
predicted.clusters <- predict(kpres, x)</pre>
```

summary.kproto

Summary Method for kproto Cluster Result

Description

Investigation of variances to specify lambda for k-prototypes clustering.

Usage

```
## S3 method for class 'kproto'
summary(object, data = NULL, pct.dig = 3, ...)
```

Arguments

object	Object of class kproto.
data	Optional data set to be analyzed. If !(is.null(data)) clusters for data are assigned by predict(object, data). If not specified the clusters of the original data are analyzed which is only possible if kproto has been called using keep.data = TRUE.
pct.dig	Number of digits for rounding percentages of factor variables.
	Further arguments to be passed to internal call of summary() for numeric variables.

Details

For numeric variables statistics are computed for each clusters using summary(). For categorical variables distribution percentages are computed.

Value

List where each element corresponds to one variable. Each row of any element corresponds to one cluster.

Author(s)

```
<gero.szepannek@web.de>
```

Examples

```
# generate toy data with factors and numerics
   <- 100
prb <- 0.9
muk <- 1.5
clusid \leftarrow rep(1:4, each = n)
x1 \leftarrow sample(c("A","B"), 2*n, replace = TRUE, prob = c(prb, 1-prb))
x1 \leftarrow c(x1, sample(c("A","B"), 2*n, replace = TRUE, prob = c(1-prb, prb)))
x1 <- as.factor(x1)</pre>
x2 \leftarrow sample(c("A","B"), 2*n, replace = TRUE, prob = c(prb, 1-prb))
x2 \leftarrow c(x2, sample(c("A","B"), 2*n, replace = TRUE, prob = c(1-prb, prb)))
x2 <- as.factor(x2)</pre>
x3 <- c(rnorm(n, mean = -muk), rnorm(n, mean = muk), rnorm(n, mean = -muk), rnorm(n, mean = muk))
x4 <- c(rnorm(n, mean = -muk), rnorm(n, mean = muk), rnorm(n, mean = -muk), rnorm(n, mean = muk))
x \leftarrow data.frame(x1,x2,x3,x4)
res \leftarrow kproto(x, 4)
summary(res)
```

validation_kproto

Validating k Prototypes Clustering

Description

Calculating the prefered validation index for a k-Prototypes clustering with k clusters or computing the optimal number of clusters based on the choosen index for k-Prototype clustering. Possible validation indices are: cindex, dunn, gamma, gplus, mcclain, ptbiserial, silhouette and tau.

Usage

```
validation_kproto(
  method = NULL,
  object = NULL,
  data = NULL,
  k = NULL,
  lambda = NULL,
  kp_obj = "optimal",
  ...
)
```

Arguments

character specifying the validation index: cindex, dunn, gamma, gplus, mcclain, method ptbiserial, silhouette or tau. object Object of class kproto resulting from a call with kproto(..., keep.data=TRUE) Original data; only required if object == NULL and neglected if object != NULL. data Vector specifying the search range for optimum number of clusters; if NULL the k range will set as 2:sqrt(n). Only required if object == NULL and neglected if object != NULL. lambda Factor to trade off between Euclidean distance of numeric variables and simple matching coefficient between categorical variables. character either "optimal" or "all": Output of the index-optimal clustering (kp_obj kp_obj == "optimal") or all computed clusterpartitions (kp_obj == "all"); only required if object != NULL.

Further arguments passed to kproto, like:

- nstart: If > 1 repetetive computations of kproto with random initializations are computed.
- verbose: Logical whether information about the cluster procedure should be given. Caution: If verbose=FALSE, the reduction of the number of clusters is not mentioned.

Details

More information about the implemented validation indices:

• cindex

$$Cindex = \frac{S_w - S_{min}}{S_{max} - S_{min}}$$

For S_{min} and S_{max} it is nessesary to calculate the distances between all pairs of points in the entire data set $(\frac{n(n-1)}{2})$. S_{min} is the sum of the "total number of pairs of objects belonging to the same cluster" smallest distances and S_{max} is the sum of the "total number of pairs of objects belonging to the same cluster" largest distances. S_w is the sum of the within-cluster distances.

The minimum value of the index is used to indicate the optimal number of clusters.

• dunn

$$Dunn = \frac{\min_{1 \le i < j \le q} d(C_i, C_j)}{\max_{1 \le k \le q} diam(C_k)}$$

The following applies: The dissimilarity between the two clusters C_i and C_j is defined as $d(C_i, C_j) = \min_{x \in C_i, y \in C_j} d(x, y)$ and the diameter of a cluster is defined as $diam(C_k) = \max_{x,y \in C} d(x,y)$.

The maximum value of the index is used to indicate the optimal number of clusters.

• gamma

$$Gamma = \frac{s(+) - s(-)}{s(+) + s(-)}$$

Comparisons are made between all within-cluster dissimilarities and all between-cluster dissimilarities. s(+) is the number of concordant comparisons and s(-) is the number of discordant comparisons. A comparison is named concordant (resp. discordant) if a within-cluster dissimilarity is strictly less (resp. strictly greater) than a between-cluster dissimilarity.

The maximum value of the index is used to indicate the optimal number of clusters.

• gplus

$$Gplus = \frac{2 \cdot s(-)}{\frac{n(n-1)}{2} \cdot (\frac{n(n-1)}{2} - 1)}$$

Comparisons are made between all within-cluster dissimilarities and all between-cluster dissimilarities. s(-) is the number of discordant comparisons and a comparison is named discordant if a within-cluster dissimilarity is strictly greater than a between-cluster dissimilarity. The minimum value of the index is used to indicate the optimal number of clusters.

• mcclain

$$McClain = \frac{\bar{S}_w}{\bar{S}_b}$$

 \bar{S}_w is the sum of within-cluster distances divided by the number of within-cluster distances and \bar{S}_b is the sum of between-cluster distances divided by the number of between-cluster distances.

The minimum value of the index is used to indicate the optimal number of clusters.

• ptbiserial

$$Ptbiserial = \frac{(\bar{S}_b - \bar{S}_w) \cdot (\frac{N_w \cdot N_b}{N_t^2})^{0.5}}{s_d}$$

 \bar{S}_w is the sum of within-cluster distances divided by the number of within-cluster distances and \bar{S}_b is the sum of between-cluster distances divided by the number of between-cluster distances.

 N_t is the total number of pairs of objects in the data, N_w is the total number of pairs of objects belonging to the same cluster and N_b is the total number of pairs of objects belonging to different clusters. s_d is the standard deviation of all distances.

The maximum value of the index is used to indicate the optimal number of clusters.

• silhouette

$$Silhouette = \frac{1}{n} \sum_{i=1}^{n} \frac{b(i) - a(i)}{max(a(i), b(i))}$$

a(i) is the average dissimilarity of the ith object to all other objects of the same/own cluster. b(i) = min(d(i, C)), where d(i, C) is the average dissimilarity of the ith object to all the other clusters except the own/same cluster.

The maximum value of the index is used to indicate the optimal number of clusters.

• tau

$$Tau = \frac{s(+) - s(-)}{\left(\left(\frac{N_t(N_t - 1)}{2} - t\right)\frac{N_t(N_t - 1)}{2}\right)^{0.5}}$$

Comparisons are made between all within-cluster dissimilarities and all between-cluster dissimilarities. s(+) is the number of concordant comparisons and s(-) is the number of discordant comparisons. A comparison is named concordant (resp. discordant) if a within-cluster

dissimilarity is strictly less (resp. strictly greater) than a between-cluster dissimilarity. N_t is the total number of distances $\frac{n(n-1)}{2}$ and t is the number of comparisons of two pairs of objects where both pairs represent within-cluster comparisons or both pairs are between-cluster comparisons.

The maximum value of the index is used to indicate the optimal number of clusters.

Value

For computing the optimal number of clusters based on the choosen validation index for k-Prototype clustering the output contains:

```
k_opt optimal number of clusters (sampled in case of ambiguity) index_opt index value of the index optimal clustering indices calculated indices for k=2,...,k_{max} kp_obj if(kp_obj == "optimal") the kproto object of the index optimal clustering and if(kp_obj == "all") all kproto which were calculated
```

For computing the index-value for a given k-Prototype clustering the output contains:

```
index calculated index-value
```

Author(s)

Rabea Aschenbruck

References

- Aschenbruck, R., Szepannek, G. (2020): Cluster Validation for Mixed-Type Data. Archives of Data Science, Series A, Vol 6, Issue 1. doi:10.5445/KSP/1000098011/02.
- Charrad, M., Ghazzali, N., Boiteau, V., Niknafs, A. (2014): NbClust: An R Package for Determining the Relevant Number of Clusters in a Data Set. *Journal of Statistical Software*, *Vol* 61, *Issue* 6. doi:10.18637/jss.v061.i06.

```
## Not run:
# generate toy data with factors and numerics
n <- 10
prb <- 0.99
muk <- 2.5

x1 <- sample(c("A","B"), 2*n, replace = TRUE, prob = c(prb, 1-prb))
x1 <- c(x1, sample(c("A","B"), 2*n, replace = TRUE, prob = c(1-prb, prb)))
x1 <- as.factor(x1)
x2 <- sample(c("A","B"), 2*n, replace = TRUE, prob = c(prb, 1-prb))
x2 <- c(x2, sample(c("A","B"), 2*n, replace = TRUE, prob = c(1-prb, prb)))
x2 <- as.factor(x2)
x3 <- c(rnorm(n, mean = -muk), rnorm(n, mean = muk), rnorm(n, mean = -muk), rnorm(n, mean = muk))
x4 <- c(rnorm(n, mean = -muk), rnorm(n, mean = muk), rnorm(n, mean = muk))
x <- data.frame(x1,x2,x3,x4)</pre>
```

```
# calculate optimal number of cluster, index values and clusterpartition with Silhouette-index
val <- validation_kproto(method = "silhouette", data = x, k = 3:5, nstart = 5)

# apply k-prototypes
kpres <- kproto(x, 4, keep.data = TRUE)

# calculate cindex-value for the given clusterpartition
cindex_value <- validation_kproto(method = "cindex", object = kpres)

## End(Not run)</pre>
```

Index

```
* classif
    kproto, 3
    kproto_gower, 6
* cluster
    kproto, 3
    kproto_gower, 6
* multivariate
    kproto, 3
    kproto_gower, 6
clprofiles, 2, 10
kmeans, 4, 7, 11
kproto, 3, 6, 7, 14
kproto_gower, 4, 6
lambdaest, 8
plot.kproto, 10
predict.kproto, 5, 7, 11
summary.kproto, 12
validation\_kproto, 13
```