Package 'clusterHD'

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Type Package

Title Tools for Clustering High-Dimensional Data

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Author Jakob Raymaekers [aut, cre],
Ruben Zamar [aut]

Maintainer Jakob Raymaekers <j.raymaekers@maastrichtuniversity.nl>

Description Tools for clustering high-dimensional data.
In particular, it contains the methods described in
<doi:10.1093/bioinformatics/btaa243>,
<arXiv:2010.00950>.

URL https://arxiv.org/abs/2010.00950

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R topics documented:

diagPlot *diagnostic plots for HTK-Means Clustering*

Description

Make diagnostic plots for HTK-means clustering.

Usage

```
diagPlot(HTKmeans.out, type = 1)
```

Arguments

HTKmeans.out	the output of a call to HTKmeans.
type	if type = 1, plots the regularization path. If type = 2, plots the differences in WCSS and ARI against the number of active variables.

Details

This visualization plots the regularization path or the differences in WCSS and ARI against the number of active variables.

Value

No return value, makes the plot directly.

Author(s)

J. Raymaekers and R.H. Zamar

References

Raymaekers, Jakob, and Ruben H. Zamar. "Regularized K-means through hard-thresholding." arXiv preprint arXiv:2010.00950 (2020).

See Also

HTKmeans

Examples

```
X <- iris[, -5]
lambdas <- seq(0, 1, by = 0.01)
HTKmeans.out <- HTKmeans(X, 3, lambdas)

diagPlot(HTKmeans.out, 1)
diagPlot(HTKmeans.out, 2)
```

getLambda *select lambda based on AIC or BIC*

Description

Select the regularization parameter for HTK-means clustering based on information criteria.

Usage

```
getLambda(HTKmeans.out, type  = "AIC")
```

Arguments

HTKmeans.out	the output of a call to HTKmeans.
type	either "AIC" (default) or "BIC".

Details

This function selects the best lambda (based on information criteria AIC or BIC) out of the HTKmeans.out$inputargs$lambd sequence of values.

Value

The selected value for lambda

Author(s)

J. Raymaekers and R.H. Zamar

References

Raymaekers, Jakob, and Ruben H. Zamar. "Regularized K-means through hard-thresholding." arXiv preprint arXiv:2010.00950 (2020).

See Also

HTKmeans

Examples

```
X <- mclust::banknote
y <- as.numeric(as.factor(X[, 1]))
lambdas <- seq(0, 1, by = 0.01)
X <- X[, -1]
HTKmeans.out <- HTKmeans(X, 2, lambdas)

# Both AIC and BIC suggest a lambda of 0.02 here:
```

```
getLambda(HTKmeans.out, "AIC")
getLambda(HTKmeans.out, "BIC")
```

`HTKmeans` *HTK-Means Clustering*

Description

Perform HTK-means clustering (Raymaekers and Zamar, 2022) on a data matrix.

Usage

```
HTKmeans(X, k, lambdas = NULL,
         standardize = TRUE,
         iter.max = 100, nstart = 100,
         nlambdas = 50,
         lambda_max = 1,
         verbose = FALSE)
```

Arguments

`X`	a matrix containing the data.
`k`	the number of clusters.
`lambdas`	a vector of values for the regularization parameter `lambda`. Defaults to `NULL`, which generates a sequence of values automatically.
`standardize`	logical flag for standardization to mean 0 and variance 1 of the data in `X`. This is recommended, unless the variance of the variables is known to quantify relevant information.
`iter.max`	the maximum number of iterations allowed.
`nstart`	number of starts used when k-means is applied to generate the starting values for HTK-means. See below for more info.
`nlambdas`	Number of lambda values to generate automatically.
`lambda_max`	Maximum value for the regularization paramater $lambda$. If `standardize = TRUE`, the default of 1 works well.
`verbose`	Whether or not to print progress. Defaults to `FALSE`.

Details

The algorithm starts by generating a number of sparse starting values. This is done using k-means on subsets of variables. See Raymaekers and Zamar (2022) for details.

Value

A list with components:

- `HTKmeans.out`
  A list with length equal to the number of lambda values supplied in `lambdas`. Each element of this list is in turn a list containing centers A matrix of cluster centres. cluster A vector of integers (from 1:k) indicating the cluster to which each point is allocated. itnb The number of iterations executed until convergence converged Whether the algorithm stopped by converging or through reaching the maximum number of itertions.
- `inputargs`
  the input arguments to the function.

Author(s)

J. Raymaekers and R.H. Zamar

References

Raymaekers, Jakob, and Ruben H. Zamar. "Regularized K-means through hard-thresholding." arXiv preprint arXiv:2010.00950 (2020).

See Also

`kmeans`

Examples

```
X <- iris[, 1:4]
HTKmeans.out <- HTKmeans(X, k = 3, lambdas = 0.8)
HTKmeans.out[[1]]$centers
pairs(X, col = HTKmeans.out[[1]]$cluster)
```

PVS *Pooled variable scaling for cluster analysis*

Description

The function computes a scale for each variable in the data. The result can then be used to standardize a dataset before applying a clustering algorithm (such as k-means). The scale estimation is based on pooled scale estimators, which result from clustering the individual variables in the data. The method is proposed in Raymaekers, and Zamar (2020) <doi:10.1093/bioinformatics/btaa243>.

Usage

```
PVS(X, kmax = 3, dist = "euclidean",
    method = "gap", B = 1000,
    gapMethod = "firstSEmax",
    minSize = 0.05, rDist = runif,
    SE.factor = 1, refDist = NULL)
```

Arguments

X	an n by p data matrix.
kmax	maximum number of clusters in one variable. Default is 3.
dist	"euclidean" for pooled standard deviation and "manhattan" for pooled mean absolute deviation. Default is "euclidean".
method	either "gap" or "jump" to determine the number of clusters. Default is "gap".
B	number of bootstrap samples for the reference distribution of the gap statistic. Default is 1000.
gapMethod	method to define number of clusters in the gap statistic. See cluster::maxSE for more info. Defaults to "firstSEmax".
minSize	minimum cluster size as a percentage of the total number of observations. Defaults to 0.05.
rDist	Optional. Reference distribution (as a function) for the gap statistic. Defaults to runif, the uniform distribution.
SE.factor	factor for determining number of clusters when using the gap statistic. See cluster::maxSE for more details. Defaults to 1
refDist	Optional. A k by 2 matrix with the mean and standard error of the reference distribution of the gap statistic in its columns. Can be used to avoid bootstrapping when repeatedly applying the function to same size data.

Value

A vector of length p containing the estimated scales for the variables.

Author(s)

Jakob Raymaekers

References

Raymaekers, J, Zamar, R.H. (2020). Pooled variable scaling for cluster analysis. *Bioinformatics*, **36**(12), 3849-3855. doi: 10.1093/bioinformatics/btaa243

Examples

```
X <- iris[, -5]
y <- unclass(iris[, 5])
```

```
# Compute scales using different scale estimators.
# the pooled standard deviation is considerably smaller for variable 3 and 4:
sds     <- apply(X, 2, sd); round(sds, 2)
ranges  <- apply(X, 2, function(y) diff(range(y))); round(ranges, 2)
psds    <- PVS(X); round(psds, 2)

# Now cluster using k-means after scaling the data

nbclus <- 3
kmeans.std <- kmeans(X, nbclus, nstart = 100) # no scaling
kmeans.sd  <- kmeans(scale(X), nbclus, nstart = 100)
kmeans.rg  <- kmeans(scale(X, scale = ranges), nbclus, nstart = 100)
kmeans.psd <- kmeans(scale(X, scale = psds), nbclus, nstart = 100)

# Calculate the Adjusted Rand Index for each of the clustering outcomes
round(mclust::adjustedRandIndex(y, kmeans.std$cluster), 2)
round(mclust::adjustedRandIndex(y, kmeans.sd$cluster), 2)
round(mclust::adjustedRandIndex(y, kmeans.rg$cluster), 2)
round(mclust::adjustedRandIndex(y, kmeans.psd$cluster), 2)
```

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