

Package: clusterHD (via r-universe)

October 15, 2024

Type Package

Title Tools for Clustering High-Dimensional Data

Version 1.0.2

Date 2022-08-10

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Description Tools for clustering high-dimensional data. In particular, it contains the methods described in <[doi:10.1093/bioinformatics/btaa243](https://doi.org/10.1093/bioinformatics/btaa243)>, <[arXiv:2010.00950](https://arxiv.org/abs/2010.00950)>.

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

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Encoding UTF-8

RoxygenNote 7.1.2

Imports Rcpp (>= 1.0.7), stats, mclust, Ckmeans.1d.dp, cluster

LinkingTo Rcpp, RcppArmadillo

NeedsCompilation yes

Repository CRAN

Date/Publication 2022-08-10 10:50:02 UTC

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`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$inputargs$lambda` 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

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

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 iterations.
- `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)
```

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 <code>cluster::maxSE</code> 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 <code>runif</code> , the uniform distribution.
SE.factor	factor for determining number of clusters when using the gap statistic. See <code>cluster::maxSE</code> 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](https://doi.org/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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