Package 'drclust'

April 22, 2024

Type Package

Title Simultaneous Clustering and (or) Dimensionality Reduction

Version 0.1

Date 2024-04-19

Description Methods for simultaneous clustering and dimensionality reduction such as: Double k-means, Reduced k-means, Factorial k-means, Clustering with Disjoint PCA but also methods for exclusively dimensionality reduction: Disjoint PCA, Disjoint FA. The statistical methods implemented refer to the following articles: de Soete G., Carroll J. (1994) ``K-means clustering in a low-dimensional Euclidean space" <doi:10.1007/978-3-642-51175-
2_24>; Vichi M. (2001) ``Double k-means Clustering for Simultaneous Classification of Objects and Variables" <doi:10.1007/978-3-642-59471-7_6>; Vichi M., Kiers H.A.L. (2001) ``Factorial k-means analysis for two-way data" <doi:10.1016/S0167-9473(00)00064-
5>; Vichi M., Saporta G. (2009) ``Clustering and disjoint principal component analysis" <doi:10.1007/s11634-016-0263-9>.

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Encoding UTF-8

Imports Rcpp, RcppArmadillo, fpc, cluster, factoextra, pheatmap

LinkingTo Rcpp, RcppArmadillo

RoxygenNote 7.3.1

NeedsCompilation yes

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Repository CRAN

Date/Publication 2024-04-22 18:22:47 UTC

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Index

```
apseudoF
```

pseudoF (pF or Calinski-Harabsz) index for choosing k in partitioning models

Description

Calculates and plots the CH index for k = 2, ..., maxK. The function provides an interval wide (2tol*pF) so that the choice of K is less conservative. Instead of just choosing the maximum pF, if it exists, picks the value such that its upper bound is larger than max pF.

Usage

apseudoF(data, maxK, tol, model, Q)

Arguments

data	Units x variables numeric data matrix.
maxK	Maximum number of clusters for the units to be tested.
tol	Approximation value. It is half of the length of the interval put for each pF. 0 \leq tol < 1. Its default value is 0.05.
model	Partitioning Models to run for each value of k. (1 = doublekm; 2 = redkm; 3 = factkm; 4 = dpcakm)
Q	Number of principal components w.r.t. variables selected for the maxK -1 partitions to be tested.

Value

bestK best value of K (scalar).

Author(s)

Ionel Prunila, Maurizio Vichi

centree

References

Calinski T., Harabasz J. (1974) "A dendrite method for cluster analysis" <doi:10.1080/03610927408827101>

Examples

```
# Iris data
# Loading the numeric variables of iris data
iris <- as.matrix(iris[,-5])
apF <- apseudoF(iris, maxK=10, tol = 0.05, model = 3, Q = 2)</pre>
```

centree

Ward-dendrogeam of centroids of partitioning models

Description

Plots the Ward-dendrogram of the centroids of a partitioning model. The plot is useful as a diagnosis tool for the choice o the number of clusters.

Usage

centree(drclust_out)

Arguments

drclust_out Output of either doublekm, redkm, factkm or dpcakm.

Value

centroids-dkm Centroids x centroids distance matrix.

Author(s)

Ionel Prunila, Maurizio Vichi

References

Ward J. H. (1963) "Hierarchical Grouping to Optimize an Objective Function" <doi:10.1080/01621459.1963.10500845>

```
# Iris data
# Loading the numeric variables of iris data
iris <- as.matrix(iris[,-5])
dc_out <- dpcakm(iris, 20, 3)
d <- centree(dc_out)</pre>
```

cluster

Description

Recodes the binary and row-stochastic membership matrix U into the classification variable (similar to the "cluster" output returned by kmeans()).

Usage

cluster(U)

Arguments

U Binary and row-stochastic matrix.

Value

cl vector of length n indicating, for each element, the index of the cluster to which it has been assigned.

Author(s)

Ionel Prunila, Maurizio Vichi

```
# Iris data
# Loading the numeric variables of iris data
iris <- as.matrix(iris[,-5])
# standardizing the data
iris <- scale(iris)
# double k-means with 3 unit-clusters and 2 components for the variables
p1 <- redkm(iris, K = 3, Q = 2)
cl <- cluster(p1$U)</pre>
```

CronbachAlpha

Description

Computes the Cronbach Alpha index on a units x variables data matrix. It measures the internal reliability, i.e., the propensity of J variables of a data matrix (n units x J variables) to be concordantly correlated with a single factor (composite indicator).

Usage

CronbachAlpha(X)

Arguments

Value

as Cronbach's Alpha

Author(s)

Ionel Prunila, Maurizio Vichi

References

Cronbach L. J. (1951) "Coefficient alpha and the internal structure of tests" <doi:10.1007/BF02310555>

```
# Iris data
# Loading the numeric variables of iris data
iris <- as.matrix(iris[,-5])
# standardizing the data
iris <- scale(iris)
# compute Cronbach's Alpha
as <- CronbachAlpha(iris)</pre>
```

Description

Performs disjoint factor analysis, i.e., a Factor Analysis with a simple structure. In fact, each factor is defined by a disjoint subset of variables, resulting thus, in a simplified, easier to interpret loading matrix A and factors. Estimation is carried out via Maximum Likelihood.

Usage

```
disfa(X, Q, Rndstart, verbose, maxiter, tol, constr, prep, print)
```

Arguments

Х	Units x variables numeric data matrix.
Q	Number of factors.
Rndstart	Number of runs to be performed (Defaults is 20).
verbose	Outputs basic summary statistics for each run $(1 = \text{enabled}; 0 = \text{disabled}, \text{default option}).$
maxiter	Maximum number of iterations allowed (if convergence is not yet reached. Default is 100).
tol	Tolerance threshold (maximum difference between the values of the objective function of two consecutive iterations such that convergence is assumed. Default is 1e-6).
constr	is a vector of length $J = nr$. of variables, pre-specifying to which cluster some of the variables must be assigned. Each component of the vector can assume integer values from 1 o Q (See example for more details), or 0 if no constraint on the variable is imposed (i.e., it will be assigned based on the plain algorithm).
prep	Pre-processing of the data. 1 performs the z-score transform (default choice); 2 performs the min-max transform; 0 leaves the data un-pre-processed.
print	Prints summary statistics of the performed method $(1 = \text{enabled}; 0 = \text{disabled}, \text{default option}).$

Value

returns a list of estimates and some descriptive quantities of the final results.

V	Variables x factors membership matrix (binary and row-stochastic). Each row is a dummy variable indicating to which cluster each variable has been assigned.
A	Variables x components loading matrix.
Psi	Specific variance of each observed variable, not accounted for by the common factors (matrix).

disfa

dispca

discrepancy	Value of the objective function, to be minimized. Difference between the observed and estimated covariance matrices (scalar).
RMSEA	Adjusted Root Mean Squared Error (scalar).
AIC	Aikake Information Criterion (scalar).
BIC	Bayesian Information Criterion (scalar).
GFI	Goodness of Fit Index (scalar).

Author(s)

Ionel Prunila, Maurizio Vichi

References

Vichi M. (2017) "Disjoint factor analysis with cross-loadings" <doi:10.1007/s11634-016-0263-9>

Examples

```
# Iris data
# Loading the numeric variables of iris data
iris <- as.matrix(iris[,-5])
# No constraint on variables
out <- disfa(iris, Q = 2)
# Constraint: the first two variables must contribute to the same factor.
outc <- disfa(iris, Q = 2, constr = c(1,1,0,0))</pre>
```

dispca

Disjoint Principal Components Analysis

Description

Performs disjoint PCA, that is, a simplified version of PCA. Computes each one of the Q principal components from a different subset of the J variables (resulting thus, in a simplified, easier to interpret loading matrix A).

Usage

dispca(X, Q, Rndstart, verbose, maxiter, tol, prep, print, constr)

Arguments

Х	Units x variables numeric data matrix.
Q	Number of factors.
Rndstart	Number of runs to be performed (Defaults is 20).
verbose	Outputs basic summary statistics for each run ($1 =$ enabled; $0 =$ disabled, default option).
maxiter	Maximum number of iterations allowed (if convergence is not yet reached. Default is 100).
tol	Tolerance threshold (maximum difference between the values of the objective function of two consecutive iterations such that convergence is assumed). Default is 1e-6.
prep	Pre-processing of the data. 1 performs the z-score transform (default choice); 2 performs the min-max transform; 0 leaves the data un-pre-processed.
print	Prints summary statistics of the results $(1 = \text{enabled}; 0 = \text{disabled}, \text{default option}).$
constr	is a vector of length $J = nr$. of variables, pre-specifying to which cluster some of the variables must be assigned. Each component of the vector can assume integer values from 1 o Q (See example for more details), or 0 if no constraint on the variable is imposed (i.e., it will be assigned based on the plain algorithm).

Value

returns a list of estimates and some descriptive quantities of the final results.

V	Variables x factors membership matrix (binary and row-stochastic). Each row is a dummy variable indicating to which cluster it has been assigned.
А	Variables x components loading matrix.
betweenss	Amount of deviance captured by the model (scalar).
totss	total amount of deviance (scalar).
size	Number of variables assigned to each column-cluster (vector).
loop	The index of the (best) run from which the results have been chosen.
it	the number of iterations performed during the (best) run.

Author(s)

Ionel Prunila, Maurizio Vichi

References

Vichi M., Saporta G. (2009) "Clustering and disjoint principal component analysis" <doi:10.1016/j.csda.2008.05.028>

doublekm

Examples

```
# Iris data
# Loading the numeric variables of iris data
iris <- as.matrix(iris[,-5])
# No constraint on variables
out <- dispca(iris, Q = 2)
# Constraint: the first two variables must contribute to the same factor.
outc <- dispca(iris, Q = 2, constr = c(1,1,0,0))</pre>
```

doublekm

Double k-means Clustering

Description

Performs simultaneous *k*-means partitioning on units and variables (rows and columns of the data matrix).

Usage

```
doublekm(Xs, K, Q, Rndstart, verbose, maxiter, tol, prep, print)
```

Arguments

Xs	Units x variables numeric data matrix.
К	Number of clusters for the units.
Q	Number of clusters for the variables.
Rndstart	Number of runs to be performed (Defaults is 20).
verbose	Outputs basic summary statistics for each run ($1 =$ enabled; $0 =$ disabled, default option).
maxiter	Maximum number of iterations allowed (if convergence is not yet reached. Default is 100).
tol	Tolerance threshold. It is the maximum difference between the values of the objective function of two consecutive iterations such that convergence is assumed (default is 1e-6).
prep	Pre-processing of the data. 1 performs the z-score transform (default choice); 2 performs the min-max transform; 0 leaves the data un-pre-processed.
print	Prints summary statistics of the results $(1 = \text{enabled}; 0 = \text{disabled}, \text{default option}).$

Value

returns a list of estimates and some descriptive quantities of the final results.

U	Units x clusters membership matrix (binary and row-stochastic). Each row is a dummy variable indicating to which unit-cluster each unit has been assigned.					
V	Variables x clusters membership matrix (binary and row-stochastic). Each row is a dummy variable indicating to which variable-cluster each variable has been assigned.					
centers	K x Q matrix of centers containing the row means expressed in terms of column means.					
totss	The total sum of squares (scalar).					
withinss	Vector of within-row-cluster sum of squares, one component per cluster.					
columnwise_withinss						
	Vector of within-column-cluster sum of squares, one component per cluster.					
betweenss	Amount of deviance captured by the model (scalar).					
K-size	Number of units assigned to each row-cluster (vector).					
Q-size	Number of variables assigned to each column-cluster (vector).					
pseudoF	Calinski-Harabasz index of the resulting (row-) partition (scalar).					
loop	The index of the (best) run from which the results have been chosen.					
it	the number of iterations performed during the (best) run.					

Author(s)

Ionel Prunila, Maurizio Vichi

References

Vichi M. (2001) "Double k-means Clustering for Simultaneous Classification of Objects and Variables" <doi:10.1007/978-3-642-59471-7_6>

```
# Iris data
# Loading the numeric variables of iris data
iris <- as.matrix(iris[,-5])
# double k-means with 3 unit-clusters and 2 variable-clusters
out <- doublekm(iris, K = 3, Q = 2)</pre>
```

dpcakm

Description

Performs simultaneously k-means partitioning on units and disjoint PCA on the variables, computing each principal component from a different subset of variables. The result is a simplified, easier to interpret loading matrix A, the principal components and the clustering. The reduced subspace is identified by the centroids.

Usage

```
dpcakm(X, K, Q, Rndstart, verbose, maxiter, tol, constr, print, prep)
```

Arguments

Х	Units x variables numeric data matrix.
К	Number of clusters for the units.
Q	Number of principal components.
Rndstart	Number of runs to be performed (Defaults is 20).
verbose	Outputs basic summary statistics for each run ($1 =$ enabled; $0 =$ disabled, default option).
maxiter	Maximum number of iterations allowed (if convergence is not yet reached. Default is 100).
tol	Tolerance threshold (maximum difference between the values of the objective function of two consecutive iterations such that convergence is assumed. Default is 1e-6).
constr	is a vector of length $J = nr$. of variables, pre-specifying to which cluster some of the variables must be assigned. Each component of the vector can assume integer values from 1 o Q = nr. of variable-cluster / principal components (See examples for more details), or 0 if no constraint on the variable is imposed (i.e., it will be assigned based on the plain algorithm).
print	Prints summary statistics of the results $(1 = \text{enabled}; 0 = \text{disabled}, \text{default option}).$
prep	Pre-processing of the data. 1 performs the z-score transform (default choice); 2 performs the min-max transform; 0 leaves the data un-pre-processed.

Value

returns a list of estimates and some descriptive quantities of the final results.

V	Variables x factors membership matrix (binary and row-stochastic). Each row is a dummy variable indicating to which cluster each variable has been assigned.
U	Units x clusters membership matrix (binary and row-stochastic). Each row is a dummy variable indicating to which cluster each unit has been assigned.

A	Variables x components loading matrix.
centers	K x Q matrix of centers containing the row means expressed in the reduced space of Q principal components.
totss	The total sum of squares (scalar).
withinss	Vector of within-cluster sum of squares, one component per cluster.
betweenss	Amount of deviance captured by the model (scalar).
K-size	Number of units assigned to each row-cluster (vector).
Q-size	Number of variables assigned to each column-cluster (vector).
pseudoF	Calinski-Harabasz index of the resulting partition (scalar).
loop	The index of the (best) run from which the results have been chosen.
it	the number of iterations performed during the (best) run.

Author(s)

Ionel Prunila, Maurizio Vichi

References

Vichi M., Saporta G. (2009) "Clustering and disjoint principal component analysis" <doi:10.1016/j.csda.2008.05.028>

Examples

```
# Iris data
# Loading the numeric variables of iris data
iris <- as.matrix(iris[,-5])
# No constraint on variables
out <- dpcakm(iris, K = 3, Q = 2, Rndstart = 5)
# Constraint: the first two variables must contribute to the same factor.
outc <- dpcakm(iris, K = 3, Q = 2, Rndstart = 5, constr = c(1,1,0,0))</pre>
```

dpseudoF

double pseudoF (Calinski-Harabsz) index

Description

A pseudoF version for double partitioning, for the choice of the number of clusters of the units and variables (rows and columns of the data matrix). It is a diagnostic tool for inspecting simultaneously the optimal number of unit-clusters and variable-clusters.

Usage

dpseudoF(data, maxK, maxQ)

factkm

Arguments

data	Units x variables numeric data matrix.
maxK	Maximum number of clusters for the units to be tested.
maxQ	Maximum number of clusters for the variables to be tested.

Value

dpseudoF matrix containing the pF value for each pair of K and Q within the specified range

Author(s)

Ionel Prunila, Maurizio Vichi

References

R. Rocci, M. Vichi (2008)" Two-mode multi-partitioning" <doi:10.1016/j.csda.2007.06.025>

T. Calinski & J. Harabasz (1974). A dendrite method for cluster analysis. Communications in Statistics, 3:1, 1-27

Examples

```
# Iris data
# Loading the numeric variables of iris data
iris <- as.matrix(iris[,-5])</pre>
```

dpeudoF <- dpseudoF(iris, maxK=10, maxQ = 3)</pre>

factkm

Factorial k-means

Description

Performs simultaneously k-means partitioning on units and principal component analysis on the variables. Identifies the best partition in a Least-Squares sense in the best reduced space of the data. Both the data and the centroids are used to identify the best Least-Squares reduced subspace, where also their distances is measured.

Usage

factkm(X, K, Q, Rndstart, verbose, maxiter, tol, rot, prep, print)

Arguments

Х	Units x variables numeric data matrix.
К	Number of clusters for the units.
Q	Number of principal components w.r.t. variables.
Rndstart	Number of runs to be performed (Defaults is 20).
verbose	Outputs basic summary statistics for each run ($1 = $ enabled; $0 = $ disabled, default option).
maxiter	Maximum number of iterations allowed (if convergence is not yet reached. Default is 100).
tol	Tolerance threshold (maximum difference in the values of the objective function of two consecutive iterations such that convergence is assumed. Default is 1e-6).
rot	performs varimax rotation of axes obtained via PCA. (=1 enabled; =0 disabled, default option)
prep	Pre-processing of the data. 1 performs the z-score transform (default choice); 2 performs the min-max transform; 0 leaves the data un-pre-processed.
print	Prints summary statistics of the results $(1 = \text{enabled}; 0 = \text{disabled}, \text{default option}).$

Value

returns a list of estimates and some descriptive quantities of the final results.

U	Units x clusters membership matrix (binary and row-stochastic). Each row is a dummy variable indicating to which cluster each unit has been assigned.
A	Variables x components loading matrix (orthonormal).
centers	K x Q matrix of centers containing the row means expressed in the reduced space of Q principal components.
totss	The total sum of squares.
withinss	Vector of within-cluster sum of squares, one component per cluster.
betweenss	amount of deviance captured by the model.
size	Number of units assigned to each cluster.
pseudoF	Calinski-Harabasz index of the resulting partition.
loop	The index of the (best) run from which the results have been chosen.
it	the number of iterations performed during the (best) run.

Author(s)

Ionel Prunila, Maurizio Vichi

References

Vichi M., Kiers H.A.L. (2001) "Factorial k-means analysis for two-way data" <doi:10.1016/S0167-9473(00)00064-5>

Kaiser H.F. (1958) "The varimax criterion for analytic rotation in factor analysis" <doi:10.1007/BF02289233>

heatm

Examples

```
# Iris data
# Loading the numeric variables of iris data
iris <- as.matrix(iris[,-5])
# factorial k-means with 3 unit-clusters and 2 components for the variables
out <- factkm(iris, K = 3, Q = 2, Rndstart = 15, verbose = 0, maxiter = 100, tol = 1e-7, rot = 1)</pre>
```

heatm

Heatmap of a partition in a reduced subspace

Description

Plots the heatmap of a partition on a reduced subspace obtained via either: doublekm, redkm, factkm or dpcakm.

Usage

```
heatm(data, drclust_out)
```

Arguments

data	Units x variables data matrix.
drclust_out	Out of either doublekm, redkm, factkm or dpcakm.

Value

No return value, called for side effects

Author(s)

Ionel Prunila, Maurizio Vichi

References

Kolde R. (2019) "pheatmap: Pretty Heatmaps" < https://cran.r-project.org/web/packages/pheatmap/index.html>

```
# Iris data
# Loading the numeric variables of iris data
iris <- as.matrix(iris[,-5])
# standardizing the data
iris <- scale(iris)</pre>
```

```
drclust_out <- dpcakm(iris, 20, 3)
# obtain a heatmap based on the output of the clustering algorithm and the data
h <- heatm(iris, drclust_out)</pre>
```

kaiserCrit	Selecting the number of principal components to be extracted from a
	dataset

Description

Selects the optimal number of principal components to be extracted from a dataset based on Kaiser's criterion

Usage

kaiserCrit(data)

Arguments

data Units x variables data matrix.

Value

bestQ Number of components to be extracted (scalar).

Author(s)

Ionel Prunila, Maurizio Vichi

References

Kaiser H. F. (1960) "The Application of Electronic Computers to Factor Analysis" <doi:10.1177/001316446002000>

Examples

```
# Iris data
# Loading the numeric variables of iris data
iris <- scale(as.matrix(iris[,-5]))
# Apply the Kaiser rule
h <- kaiserCrit(iris)</pre>
```

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mrand

Description

Performs the Adjusted Rand Index on a confusion matrix (row-by-column product of two partitionmatrices). ARI is a measure of the similarity between two data clusterings.

Usage

mrand(N)

Arguments

Value

mri Adjusted Rand Index of a confusion matrix (scalar).

Author(s)

Ionel Prunila, Maurizio Vichi

References

Rand W. M. (1971) "Objective criteria for the evaluation of clustering methods" <doi:10.2307/2284239>

```
# Iris data
# Loading the numeric variables of iris data
iris <- as.matrix(iris[,-5])
# standardizing the data
iris <- scale(iris)
# double k-means with 3 unit-clusters and 2 components for the variables
p1 <- redkm(iris, K = 3, Q = 2, Rndstart = 10)
p2 <- doublekm(iris, K=3, Q=2, Rndstart = 10)
mri <- mrand(t(p1$U)%*%p2$U)</pre>
```

Description

Performs simultaneously k-means partitioning on units and principal component analysis on the variables.

Usage

redkm(X, K, Q, Rndstart, verbose, maxiter, tol, rot, prep, print)

Arguments

Х	Units x variables numeric data matrix.
К	Number of clusters for the units.
Q	Number of principal components w.r.t. variables.
Rndstart	Number of runs to be performed (Defaults is 20).
verbose	Outputs basic summary statistics for each run $(1 = \text{enabled}; 0 = \text{disabled}, \text{default option})$.
maxiter	Maximum number of iterations allowed (if convergence is not yet reached. Default is 100).
tol	Tolerance threshold (maximum difference between the values of the objective function of two consecutive iterations such that convergence is assumed. Default is 1e-6).
rot	performs varimax rotation of axes obtained via PCA. (=1 enabled; =0 disabled, default option)
prep	Pre-processing of the data. 1 performs the z-score transform (default choice); 2 performs the min-max transform; 0 leaves the data un-pre-processed.
print	Tolerancestats summary statistics of the performed method ($1 =$ enabled; $0 =$ disabled, default option).

Value

returns a list of estimates and some descriptive quantities of the final results.

U	Units x clusters membership matrix (binary and row-stochastic). Each row is a dummy variable indicating to which cluster each unit has been assigned.
A	Variables x components loading matrix (orthonormal).
centers	K x Q matrix of centers containing the row means expressed in the reduced space of Q principal components.
totss	The total sum of squares (scalar).
withinss	Vector of within-cluster sum of squares, one component per cluster.

silhouette

betweenss	Amount of deviance captured by the model (scalar).
size	Number of units assigned to each cluster (vector).
pseudoF	Calinski-Harabasz index of the resulting partition (scalar).
loop	The index of the (best) run from which the results have been chosen.
it	the number of iterations performed during the (best) run.

Author(s)

Ionel Prunila, Maurizio Vichi

References

de Soete G., Carroll J. (1994) "K-means clustering in a low-dimensional Euclidean space" <doi:10.1007/978-3-642-51175-2_24>

Kaiser H.F. (1958) "The varimax criterion for analytic rotation in factor analysis" <doi:10.1007/BF02289233>

Examples

```
# Iris data
# Loading the numeric variables of iris data
iris <- as.matrix(iris[,-5])</pre>
```

```
# reduced k-means with 3 unit-clusters and 2 components for the variables
out <- redkm(iris, K = 3, Q = 2, Rndstart = 15, verbose = 0, maxiter = 100, tol = 1e-7, rot = 1)</pre>
```

silhouette Silhouette

Description

Computes and plots the silhouette of a partition

Usage

```
silhouette(data, drclust_out)
```

Arguments

data	Units x variables data matrix.
drclust_out	Out of either doublekm, redkm, factkm or dpcakm.

Value

cl.silhouette	Silhouette index for the given partition, for each object (matrix).
fe.silhouette	Factoextra silhouette graphical object

Author(s)

Ionel Prunila, Maurizio Vichi

References

Rousseeuw P. J. (1987) "Silhouettes: a Graphical Aid to the Interpretation and Validation of Cluster Analysis" <doi:10.1016/0377-0427(87)90125-7>

Maechler M. et al. (2023) "cluster: Cluster Analysis Basics and Extensions" https://CRAN.R-project.org/package=cluster>

Kassambara A. (2022) "factoextra: Extract and Visualize the Results of Multivariate Data Analyses" https://cran.r-project.org/web/packages/factoextra/index.html

Examples

```
# Iris data
# Loading the numeric variables of iris data
iris <- as.matrix(iris[,-5])</pre>
```

```
#standardizing the data
iris <- scale(iris)</pre>
```

#applying a clustering algorithm
drclust_out <- dpcakm(iris, 20, 3)</pre>

#silhouette based on the data and the output of the clustering algorithm
d <- silhouette(iris, drclust_out)</pre>

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