# Package 'RclusTool'

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Type Package

Title Graphical Toolbox for Clustering and Classification of Data

Frames

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**Description** Graphical toolbox for clustering and classification of data frames.

It proposes a graphical interface to process clustering and classification methods on features data-frames, and to view initial data as well as resulted cluster or classes. According to the level of available labels, different approaches are proposed: unsupervised clustering, semi-supervised clustering and supervised classification.

To assess the processed clusters or classes, the toolbox can import and show some supplementary data formats: either profile/time series, or images.

These added information can help the expert to label clusters (clustering), or to constrain data frame rows (semi-supervised clustering), using Constrained spectral embedding algorithm by Wacquet et al. (2013) <doi:10.1016/j.patrec.2013.02.003> and the methodology provided by Wacquet et al. (2013) <doi:10.1007/978-3-642-35638-4\_21>.

License GPL (>= 2) RoxygenNote 7.2.3

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add0p	peration Add operation	

# Description

addOperation create configuration object for the datasample

# Usage

```
addOperation(parameterList, featureOperations)
```

# **Arguments**

# Value

The configuration object created by the list of preprocessing instructions parameterList in featureOperations.

applyPreprocessing 3

### **Examples**

```
featOp <- matrix(ncol=4,nrow=0)</pre>
#Adding two differents variables
featOp <- addOperation(list("+","x","y"), featOp)</pre>
#Select a variable
featOp <- addOperation(list("select", "x"), featOp)</pre>
#Change a profile color
featOp <- addOperation(list("signalColor", "x", "grey"), featOp)</pre>
#Make a PCA projection (with the number of dimensions)
featOp <- addOperation(list("projection","pca","0"), featOp)</pre>
#Make a spectral projection
featOp <- addOperation(list("projection", "spectral"), featOp)</pre>
#Scale the data
featOp <- addOperation(list("scaling","on"), featOp)</pre>
#Sample the data (with a sampling size)
featOp <- addOperation(list("sampling","150"), featOp)</pre>
#Make a log transformation of a variable
featOp <- addOperation(list("log","x"), featOp)</pre>
```

applyPreprocessing

Preprocessing application

# Description

Apply a new preprocess to a data.sample object.

# Usage

```
applyPreprocessing(
  data.sample,
  operations = NULL,
  RclusTool.env = initParameters(),
  reset = TRUE,
  preprocessed.only = FALSE
)
```

### **Arguments**

```
data.sample sample object.

operations list of data.frames describing all preprocessing operations.

RclusTool.env environment in which all global parameters, raw data and results are stored.

reset boolean: if TRUE (default) the configuration is reset.

preprocessed.only

boolean: if TRUE (default) processing are restricted to the "preprocessed" features.
```

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### **Details**

applyPreprocessing applies a new preprocess to a data.sample object

#### Value

The data.sample sample object on which was applied the operations or NULL if preprocessing operations fail.

#### See Also

loadPreprocessFile

# **Examples**

clusterSummary

Clusters summaries computation

# Description

Save clusters summaries results in a csv file.

computeSemiSupervised

### **Arguments**

```
data.sample list containing features, profiles and clustering results.

label vector of labels.

features.to.keep

vector of features names on which the summaries are computed.

summary.functions

vector of functions names for the summaries computation. Could be 'Min', 'Max', 'Sum', 'Average', 'sd'.
```

# **Details**

clusterSummary computes the clusters summaries (min, max, sum, average, sd) from a clustering result.

#### Value

out data.frame containing the clusters summaries.

### **Examples**

computeSemiSupervised Semi-supervised clustering

# **Description**

Perform semi-supervised clustering based on pairwise constraints, dealing with the number of clusters K, automatically or not.

```
computeSemiSupervised(
  data.sample,
  ML,
  CNL,
```

```
K = 0,
kmax = 20,
method.name = "Constrained_KM",
maxIter = 2,
pca = FALSE,
pca.nb.dims = 0,
spec = FALSE,
use.sampling = FALSE,
sampling.size.max = 0,
scaling = FALSE,
RclusTool.env = initParameters(),
echo = TRUE
```

# **Arguments**

data.sample list containing features, profiles and clustering results.

ML list of ML (must-link) constrained pairs (as row.names of features).

CNL list of CNL (cannot-link) constrained pairs (as row.names of features).

K number of clusters. If K=0 (default), this number is automatically computed

thanks to the Elbow method.

kmax maximum number of clusters.

method.name character vector specifying the constrained algorithm to use. Must be 'Con-

strained\_KM' (default) or 'Constrained\_SC' (Constrained Spectral Clustering).

maxIter number of iterations for SemiSupervised algorithm

pca boolean: if TRUE, Principal Components Analysis is applied to reduce the data

space.

pca.nb.dims number of principal components kept. If pca.nb.dims=0, this number is com-

puted automatically.

spec boolean: if TRUE, spectral embedding is applied to reduce the data space.

use.sampling boolean: if FALSE (default), data sampling is not used.

sampling.size.max

numeric: maximal size of the sampling set.

scaling boolean: if TRUE, scaling is applied.

RclusTool.env environment in which data and intermediate results are stored.

echo boolean: if FALSE (default), no description printed in the console.

#### **Details**

computeSemiSupervised performs semi-supervised clustering based on pairwise constraints, dealing with the number of clusters K, automatically or not

computeSupervised 7

# Value

The function returns a list containing:

label vector of labels.

summary data.frame containing clusters summaries (min, max, sum, average, sd).

nbItems number of observations.

### See Also

```
computeCKmeans, computeCSC, KwaySSSC
```

### **Examples**

 ${\tt computeSupervised}$ 

Supervised classification

### **Description**

Perform supervised classification based on the use of a training set.

```
computeSupervised(
  data.sample,
  prototypes,
  method.name = "K-NN",
  model = NULL,
  RclusTool.env = initParameters()
)
```

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# **Arguments**

data.sample list containing features, profiles and clustering results.

prototypes data.frame containing the features of each prototype associated to a class.

method.name character vector specifying the supervised algorithm to use. Must be 'K-NN'

(K-Nearest Neighbor by default), 'MLP' (MultiLayer Perceptron), 'SVM' (Sup-

port Vector Machine) or 'RF' (Random Forest).

model option to predict directly from model

RclusTool.env environment in which all global parameters, raw data and results are stored.

#### **Details**

computeSupervised performs supervised classification based on the use of a training set

#### Value

The function returns a list containing:

label vector of labels.

summary data.frame containing classes summaries (min, max, sum, average, sd).

nbItems number of observations.

prototypes data.frame containing the features of each prototype associated to a class.

### See Also

readTrainSet

```
rep <- system.file("extdata", package="RclusTool")
featuresFile <- file.path(rep, "sample_example_features.csv")
features <- read.csv(featuresFile, header = TRUE)
features$ID <- NULL
traindir <- file.path(rep, "train_example")
tf <- tempfile()
write.table(features, tf, sep=",", dec=".")

x <- importSample(file.features=tf, dir.save=dirname(tf))
train <- readTrainSet(traindir)
res <- computeSupervised(x, prototypes=train)
plot(features[,3], features[,4], type = "p", xlab = "x", ylab = "y", col = res$label, main = "K-Nearest-Neighbor classification")</pre>
```

computeUnSupervised L

Unsupervised clustering

# **Description**

Perform unsupervised clustering, dealing with the number of clusters K, automatically or not.

### Usage

```
computeUnSupervised(
  data.sample,
  K = 0,
  method.name = "K-means",
  pca = FALSE,
  pca.nb.dims = 0,
  spec = FALSE,
  use.sampling = FALSE,
  sampling.size.max = 0,
  scaling = FALSE,
  RclusTool.env = initParameters(),
  echo = FALSE
)
```

### **Arguments**

data.sample list containing features, profiles and clustering results. number of clusters. If K=0 (default), this number is automatically computed thanks to the Elbow method. method.name character vector specifying the constrained algorithm to use. Must be 'K-means' (default), 'EM' (Expectation-Maximization), 'Spectral', 'HC' (Hierarchical Clustering) or 'PAM' (Partitioning Around Medoids). boolean: if TRUE, Principal Components Analysis is applied to reduce the data рса space. number of principal components kept. If pca.nb.dims=0, this number is compca.nb.dims puted automatically. boolean: if TRUE, spectral embedding is applied to reduce the data space. spec use.sampling boolean: if FALSE (default), data sampling is not used. sampling.size.max numeric: maximal size of the sampling set. scaling boolean: if TRUE, scaling is applied. RclusTool.env environment in which all global parameters, raw data and results are stored. boolean: if FALSE (default), no description printed in the console. echo

10 extractProtos

### **Details**

computeUnSupervised performs unsupervised clustering, dealing with the number of clusters K, automatically or not

#### Value

data.sample list containing features, profiles and updated clustering results (with vector of labels and clusters summaries).

### See Also

computeKmeans, computeEM, spectralClustering, computePcaSample, computeSpectralEmbeddingSample

### **Examples**

extractProtos

Prototypes extraction

# Description

Extract prototypes of each cluster automatically, according to a clustering result, and save them in different directories. In order to catch the whole variability, each cluster is divided into several sub-clusters, and medoids of each sub-cluster are considered as prototypes.

```
extractProtos(
  data.sample,
  method,
  K.max = 20,
  kmeans.variance.min = 0.95,
  user.name = ""
)
```

formatLabelSample 11

# **Arguments**

```
data.sample list containing features, profiles and clustering results.

method character vector specifying the clustering method (already performed) to use.

K.max maximal number of clusters (K.max=20 by default).

kmeans.variance.min
elbow method cumulative explained variance > criteria to stop K-search.

user.name character vector specifying the user name.
```

#### **Details**

extractProtos extracts prototypes automatically according to a clustering result, and save them in different directories

### Value

csv file containing the prototypes

### **Examples**

formatLabelSample

Labels formatting

### **Description**

Format labels for unsupervised classification and add cleaned observations as 'Noise'.

```
formatLabelSample(
  label,
  data.sample,
  new.labels = TRUE,
  use.sampling = FALSE,
  noise.cluster = "Noise"
)
```

imgClassif

### **Arguments**

```
label vector of labels.

data.sample sample object.

new.labels boolean: if TRUE (default), new names are given for each cluster (beginning by 'Cluster').

use.sampling boolean: if TRUE (not default), data.sample$sampling is used to generalize label from sampling set to the whole set.

noise.cluster character name of the cluster "noise".
```

#### **Details**

formatLabelSample formats labels for unsupervised classification and adds cleaned observations as 'Noise'

#### Value

new.labels formatted labels.

# **Examples**

imgClassif

Images clustering

# Description

Sort images (if available) in different directories according to a clustering result.

```
imgClassif(data.sample, imgdir, method, user.name = "")
```

importSample 13

# Arguments

data.sample list containing features, profiles and clustering results.

imgdir character vector specifying the path of the images directory.

method character vector specifying the clustering method (already performed) to use.

user.name character vector specifying the user name.

user thanks character vector specifying the user hance

### **Details**

imgClassif sorts images (if available) in different directories according to a clustering result

### Value

images files in the different directories, csv file containing the detail.

#### See Also

```
sigClassif
```

# **Examples**

importSample

Sample importation

### **Description**

Import the required and the optional files, and build a dataset.

14 importSample

# Usage

```
importSample(
   file.features = "",
   file.meta = "",
   file.profiles = "",
   file.RDS = "",
   file.config = "",
   dir.images = "",
   dir.save = "",
   sepFeat = ",",
   decFeat = ".",
   naFeat = c("", "NA"),
   sepSig = ",",
   decSig = ".",
   naSig = c("", "NA"),
   headerCSV = TRUE,
   RclusTool.env = new.env(),
   ...
)
```

# Arguments

file.features	character vector specifying the csv file containing features data.
file.meta	character vector specifying the txt file containing metadata.
file.profiles	character vector specifying the csv file containing profiles data.
file.RDS	character vector for a RDS file containing a data.sample object. This file is automatically saved when importing a (csv-)file-features. When both a csv-file-features and a RDS file are given, the last one is ignored.
file.config	character vector for the name of the configuration file.
dir.images	character vector containing the path of images directory.
dir.save	character vector specifying path of the working directory to save results; "" to not save any results
sepFeat	character specifying the field separator for the csv file containing features data.
decFeat	character specifying the decimal points for the csv file containing features data.
naFeat	vector containing missing values for the csv file containing features data.
sepSig	character specifying the field separator for the csv file containing profiles data.
decSig	character specifying the decimal point for the csv file containing profiles data.
naSig	vector containing missing values for the csv file containing profiles data.
headerCSV	boolean if TRUE (default) the file contains the names of the variables as its first line.
RclusTool.env	environment in which data and intermediate results are stored.
	parameters adressed to read.csv functions.

loadPreprocessFile 15

### **Details**

function to import sample from CSV files; sample is preprocessed

#### Value

data.sample loaded data.sample.

#### See Also

loadSample

### **Examples**

loadPreprocessFile

Preprocessing loading

# **Description**

Load a csv file configuration with instruction to remove bad observations and builds object config that describes all preprocessings to apply.

### Usage

```
loadPreprocessFile(file.config, ...)
```

# **Arguments**

```
file.config character vector specifying the name of a csv file with preprocessing instructions.

... parameters addressed to read.csv functions.
```

### **Details**

loadPreprocessFile reads a csv file configuration with instruction to remove bad particles and builds object config that describes all preprocessings done

purgeSample

### Value

operations character matrix describing all preprocessing operations.

#### See Also

```
applyPreprocessing
```

### **Examples**

```
instr <- rbind(c("select","x","log",""), c("select","y","log",""))
tf <- tempfile()
write.table(instr, tf, sep=",", col.names = FALSE, row.names = FALSE)
operations <- loadPreprocessFile(tf)</pre>
```

purgeSample

Sample purging

# **Description**

Purge sample from its temporary computing results.

# Usage

```
purgeSample(
  data.sample,
  purge.preprocessing = TRUE,
  purge.clustering = TRUE,
  user.expert = FALSE
)
```

### **Arguments**

```
data.sample sample object

purge.preprocessing

boolean: if TRUE (default), the configuration is reset.

purge.clustering

boolean: if TRUE (default), the clusterings are reset.

user.expert boolean: if FALSE (default), initial classification feature space is PCA.
```

### **Details**

Function to purgeSample from its temporary computing results

### Value

data.sample purged data.sample.

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### **Examples**

RclusToolGUI

Username and user type selection

# Description

Generate a first window to enter the username and to select the user type ('standard' or 'expert').

### Usage

```
RclusToolGUI(RclusTool.env = new.env(), debug = FALSE)
```

### **Arguments**

RclusTool.env environment in which data and results will be stored. If NULL, a local environment will be created.

debug boolean: if TRUE, the debug mode is activated.

# **Details**

function to display the first window of the RclusTool interface (username and user type selection)

### Value

Nothing, just open the graphical user interface.

```
RclusToolGUI()
```

18 readTrainSet

readTrainSet	Training set reading		
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# **Description**

Read a training set built from prototypes, to train a classifier for supervised classification.

### Usage

```
readTrainSet(
   traindir,
   keep_ = FALSE,
   operations = NULL,
   RclusTool.env = initParameters()
)
```

# **Arguments**

traindir character vector specifying the path of the training set.

keep\_ boolean: if FALSE (default), the '\_' directory is not considered in the training

set.

operations list of data.frames describing all preprocessing operations.

RclusTool.env environment in which all global parameters, raw data and results are stored.

### **Details**

readTrainSet reads a training set built from prototypes, to train a classifier for supervised classification

# Value

prototypes data.frame containing the features of each prototype associated to a class.

### See Also

```
dropTrainSetVars
```

```
rep <- system.file("extdata", package="RclusTool")
traindir <- file.path(rep, "train_example")
train <- readTrainSet(traindir)</pre>
```

saveCalcul 19

saveCalcul

Object saving

# **Description**

Save object created after calculation in a csv file.

# Usage

```
saveCalcul(filename.rdata, dat, dir)
```

# Arguments

```
filename.rdata character vector specifying the path and the name of the rdata file.
```

dat object to save.

dir character vector specifying the directory where to save the rdata file.

### **Details**

saveCalcul saves object created after calculation in a csv file

### Value

RDS file containing calculation.

20 saveClustering

saveClustering

Clustering saving

# Description

Save a clustering result in a csv file.

### Usage

```
saveClustering(filename.csv, label, dir)
```

# **Arguments**

```
filename.csv character vector specifying the path and the name of the csv file.
```

label vector of labels.

dir character vector specifying the directory where to save the csv file.

# **Details**

saveClustering saves a clustering result in a csv file

# Value

csv file containing clustering result.

# See Also

```
buildClusteringSample
```

saveCounts 21

saveCounts

Count saving

# **Description**

Save a count result in a csv file.

### Usage

```
saveCounts(filename.csv, counts, dir)
```

# **Arguments**

 $\label{lem:csv} \mbox{file.ame.csv} \quad \mbox{character vector specifying the path and the name of the csv file.}$ 

counts vector of counts.

dir character vector specifying the directory where to save the csv file.

### **Details**

saveCounts saves a count result in a csv file

### Value

csv file containing count result.

22 saveManualProtos

saveManualProtos

Manual prototypes saving

# **Description**

Save the profiles and images of prototypes selected manually by user in a scatterplot.

# Usage

```
saveManualProtos(data.sample, protos)
```

### **Arguments**

```
data.sample list containing features, profiles and clustering results.

protos list of selected prototypes (with index and name).
```

### **Details**

saveManualProtos saves the profiles and images of prototypes selected manually by user in a scatterplot

### Value

profiles and images of prototypes selected, csv file with detail.

savePreprocess 23

COVOD	ranraaaaa	
saver	reprocess	

Preprocessing exportation

# Description

Export all preprocessing operations in a csv file.

### Usage

```
savePreprocess(filename.csv, config, dir)
```

### Arguments

filename.csv character vector specifying the name of the csv file.

config 4-columns character matrix describing all preprocessing operations.

dir character vector specifying the directory of the csv file.

#### **Details**

savePreprocess exports all preprocessing operations in a csv file

### Value

csv file containing preprocessing.

### **Examples**

```
test.file <- tempfile()
config <- matrix(c("select","x",NA,NA,"select","y",NA,NA), byrow=TRUE, ncol=4)
savePreprocess(basename(test.file), config, dirname(test.file))</pre>
```

saveSummary

Clusters summaries saving

# Description

Save clusters summaries results in a csv file.

```
saveSummary(filename.csv, cluster.summary, dir, info = NULL)
```

24 sigClassif

# **Arguments**

```
cluster.summary
data.frame containing the clusters summaries results.

dir
character vector specifying the directory where to save the csv file.
character vector specifying the directory where to save the csv file.
character vector about sample or clustering.
```

### **Details**

saveSummary saves clusters summaries results in a csv file

#### Value

csv file containing clusters summaries results.

#### See Also

**loadSummary** 

### **Examples**

sigClassif

Signals clustering

# **Description**

Sort signals (if available) in different directories according to a clustering result.

```
sigClassif(data.sample, method, user.name = "")
```

# **Arguments**

```
data.sample list containing features, profiles and clustering results.

method character vector specifying the clustering method (already performed) to use.

user.name character vector specifying the user name.
```

### **Details**

sigClassif sorts signals (if available) in different directories according to a clustering result

#### Value

signals plots images in the different directories.

### See Also

```
imgClassif
```

### **Examples**

```
visualizeSampleClustering
```

Interactive figure with 2D scatter-plot

# Description

Open an interactive figure with 2D scatter-plot of all particles with axis choice. Grey color (label=0) is for data to cleaned or to remove in classification process.

### Usage

```
visualizeSampleClustering(
  data.sample,
  label = NULL,
  clustering.name = "proposed clustering",
  cluster.summary = NULL,
  RclusTool.env = initParameters(),
  prototypes = NULL,
  profile.mode = "none",
  selection.mode = "none",
  compare.mode = "off",
  pairs = NULL,
  features.mode = "initial",
  wait.close = FALSE,
  fontsize = 9
)
```

### **Arguments**

data.sample

vector of labels. label clustering.name character vector specifying the clustering method used to get labels. cluster.summary data.frame containing the clusters summaries (as returned by 'clusterSummary'). environment in which all global parameters, raw data and results are stored. RclusTool.env list containing vectors of prototypes indices. prototypes character vector specifying the plot mode of profiles. Must be 'none' (default), profile.mode 'whole sample', 'cluster i' or 'constrained pairs'. selection mode character vector specifying the selection mode of profiles. Must be 'none' (default), 'prototypes' or 'pairs'. character vector specifying the mode of comparison between two clusterings compare.mode results. Must be 'off' (default) or 'on'. list of constrained pairs (must-link and cannot-link). pairs features.mode character vector specifying the plot mode of features (projection in a specific space). Must be 'initial' (default), 'preprocessed', 'pca', 'pca\_full' or 'spectral', or prefixed versions ('sampled', 'scaled') of those space names. wait.close boolean: if FALSE (default), the following steps of the analysis calculations are computed even if the window is not closed.

list containing features, profiles and clustering results.

#### **Details**

fontsize

visualizeSampleClustering opens an interactive figure with 2D scatter-plot of all particles with axis choice

size of font (default is 9)

# Value

prototypes in selection.mode = "prototypes" mode, pairs in selection.mode = "pairs" mode.

#### See Also

```
plotProfile, plotSampleFeatures
```

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