Package 'VarSelLCM'

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Type Package

Title Variable Selection for Model-Based Clustering of Mixed-Type Data Set with Missing Values

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Description Full model selection (detection of the relevant features and estimation of the number of clusters) for model-based clustering (see reference here <doi:10.1007/s11222-016-9670-1>). Data to analyze can be continuous, categorical, integer or mixed. Moreover, missing values can occur and do not necessitate any pre-processing. Shiny application permits an easy interpretation of the results.

License GPL (>= 2)

Depends R (>= 3.3)

Imports methods, Rcpp (>= 0.11.1), parallel, mgcv, ggplot2, shiny

URL http://varsellcm.r-forge.r-project.org/

LinkingTo Rcpp, RcppArmadillo

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LazyLoad yes

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Description

Model-based clustering with variable selection and estimation of the number of clusters. Data to analyze can be continuous, categorical, integer or mixed. Moreover, missing values can occur and do not necessitate any pre-processing. Shiny application permits an easy interpretation of the results.

Details

Package: VarSelLCM
Type: Package
Version: 2.1.2
Date: 2018-06-04
License: GPL-3

LazyLoad: yes

URL: http://varsellcm.r-forge.r-project.org/

The main function to use is VarSelCluster. Function VarSelCluster carries out the model selection (according to AIC, BIC or MICL) and maximum likelihood estimation.

Function VarSelShiny runs a shiny application which permits an easy interpretation of the clustering results.

Function VarSelImputation permits the imputation of missing values by using the model parameters.

Standard tool methods (e.g., summary, print, plot, coef, fitted, predict...) are available for facilitating the interpretation.

Author(s)

Matthieu Marbac and Mohammed Sedki. Maintainer: Mohammed Sedki <mohammed.sedki@u-psud.fr>

References

Marbac, M. and Sedki, M. (2017). Variable selection for model-based clustering using the integrated completed-data likelihood. Statistics and Computing, 27 (4), 1049-1063.

Marbac, M. and Patin, E. and Sedki, M. (2018). Variable selection for mixed data clustering: Application in human population genomics. Journal of classification, to appear.

```
## Not run:
# Package loading
require(VarSelLCM)

# Data loading:
# x contains the observed variables
# z the known statu (i.e. 1: absence and 2: presence of heart disease)
data(heart)
```

```
ztrue <- heart[,"Class"]</pre>
x \leftarrow heart[,-13]
# Cluster analysis without variable selection
res_without <- VarSelCluster(x, 2, vbleSelec = FALSE, crit.varsel = "BIC")</pre>
# Cluster analysis with variable selection (with parallelisation)
res_with <- VarSelCluster(x, 2, nbcores = 2, initModel=40, crit.varsel = "BIC")</pre>
# Comparison of the BIC for both models:
# variable selection permits to improve the BIC
BIC(res_without)
BIC(res_with)
# Comparison of the partition accuracy.
# ARI is computed between the true partition (ztrue) and its estimators
\# ARI is an index between 0 (partitions are independent) and 1 (partitions are equals)
# variable selection permits to improve the ARI
# Note that ARI cannot be used for model selection in clustering, because there is no true partition
ARI(ztrue, fitted(res_without))
ARI(ztrue, fitted(res_with))
# Estimated partition
fitted(res_with)
# Estimated probabilities of classification
head(fitted(res_with, type="probability"))
# Summary of the probabilities of missclassification
plot(res_with, type="probs-class")
# Confusion matrices and ARI (only possible because the "true" partition is known).
# ARI is computed between the true partition (ztrue) and its estimators
# ARI is an index between 0 (partitions are independent) and 1 (partitions are equals)
# variable selection permits to improve the ARI
# Note that ARI cannot be used for model selection in clustering, because there is no true partition
# variable selection decreases the misclassification error rate
table(ztrue, fitted(res_without))
table(ztrue, fitted(res_with))
ARI(ztrue, fitted(res_without))
ARI(ztrue, fitted(res_with))
# Summary of the best model
summary(res_with)
# Discriminative power of the variables (here, the most discriminative variable is MaxHeartRate)
plot(res_with)
# More detailed output
print(res_with)
# Print model parameter
coef(res_with)
```

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```
# Boxplot for the continuous variable MaxHeartRate
plot(x=res_with, y="MaxHeartRate")
# Empirical and theoretical distributions of the most discriminative variable
# (to check that the distribution is well-fitted)
plot(res_with, y="MaxHeartRate", type="cdf")
# Summary of categorical variable
plot(res_with, y="Sex")
# Probabilities of classification for new observations
predict(res_with, newdata = x[1:3,])
# Imputation by posterior mean for the first observation
not.imputed <- x[1,]
imputed <- VarSelImputation(res_with, x[1,], method = "sampling")</pre>
rbind(not.imputed, imputed)
# Opening Shiny application to easily see the results
VarSelShiny(res_with)
## End(Not run)
```

AIC

AIC criterion.

Description

This function gives the AIC criterion of an instance of VSLCMresults. AIC is computed according to the formula

$$AIC = log - likelihood - \nu$$

where ν denotes the number of parameters in the fitted model.

Usage

```
## S4 method for signature 'VSLCMresults'
AIC(object)
```

Arguments

object

instance of VSLCMresults.

References

Akaike, H. (1974), "A new look at the statistical model identification", IEEE Transactions on Automatic Control, 19 (6): 716-723.

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Examples

```
# Data loading:
data(heart)

# Cluster analysis without variable selection
res <- VarSelCluster(heart[,-13], 2, vbleSelec = FALSE)

# Get the AIC value
AIC(res)</pre>
```

ARI

Adjusted Rand Index

Description

This function computes the Adjusted Rand Index

Usage

```
ARI(x, y)
```

Arguments

x vector defining a partition.

y vector defining a partition of whose length is equal to the length of x.

Value

numeric

References

L. Hubert and P. Arabie (1985) Comparing Partitions, Journal of the Classification, 2, pp. 193-218.

```
x \leftarrow sample(1:2, 20, replace=TRUE)

y \leftarrow x

y[1:5] \leftarrow sample(1:2, 5, replace=TRUE)

ARI(x, y)
```

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BIC

BIC criterion.

Description

This function gives the BIC criterion of an instance of VSLCMresults. BIC is computed according to the formula

$$BIC = log - likelihood - 0.5 * \nu * log(n)$$

where ν denotes the number of parameters in the fitted model and n represents the sample size.

Usage

```
## S4 method for signature 'VSLCMresults'
BIC(object)
```

Arguments

object

instance of VSLCMresults.

References

Schwarz, G. (1978). Estimating the dimension of a model. Annals of Statistics, 6(2), 461-464.

Examples

```
# Data loading:
data(heart)

# Cluster analysis without variable selection (number of clusters between 1 and 3)
res<- VarSelCluster(heart[,-13], 2, vbleSelec = FALSE)

# Get the BIC value
BIC(res)</pre>
```

coef

Extract the parameters

Description

This function returns an instance of class VSLCMparam which contains the model parameters.

Usage

```
## S4 method for signature 'VSLCMresults'
coef(object)
```

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Arguments

object instance of VSLCMresults.

Examples

```
# Data loading:
data(heart)

# Cluster analysis without variable selection (number of clusters between 1 and 3)
res <- VarSelCluster(heart[,-13], 1:3, vbleSelec = FALSE)

# Get the ICL value
coef(res)</pre>
```

coefficients

Extract the parameters

Description

This function returns an instance of class VSLCMparam which contains the model parameters.

Usage

```
## S4 method for signature 'VSLCMresults'
coefficients(object)
```

Arguments

object instance of VSLCMresults.

```
# Data loading:
data(heart)

# Cluster analysis without variable selection (number of clusters between 1 and 3)
res <- VarSelCluster(heart[,-13], 1:3, vbleSelec = FALSE)

# Get the ICL value
coefficients(res)</pre>
```

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fitted

Extract the partition or the probabilities of classification

Description

This function returns the probabilities of classification or the partition among the observations of an instance of VSLCMresults.

Usage

```
## S4 method for signature 'VSLCMresults'
fitted(object, type = "partition")
```

Arguments

object instance of VSLCMresults.

type the type of prediction: probability of classification (probability) or the partition

(partition)

Examples

```
# Data loading:
data(heart)

# Cluster analysis without variable selection (number of clusters between 1 and 3)
res <- VarSelCluster(heart[,-13], 2, vbleSelec = FALSE)

# Get the ICL value
fitted(res)</pre>
```

fitted.values

Extract the partition or the probabilities of classification

Description

This function returns the probabilities of classification or the partition among the observations of an instance of VSLCMresults.

Usage

```
## S4 method for signature 'VSLCMresults'
fitted.values(object, type = "partition")
```

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Arguments

object instance of VSLCMresults.

type the type of prediction: probability of classification (probability) or the partition

(partition)

Examples

```
# Data loading:
data(heart)

# Cluster analysis without variable selection (number of clusters between 1 and 3)
res <- VarSelCluster(heart[,-13], 2, vbleSelec = FALSE)

# Get the ICL value
fitted.values(res)</pre>
```

heart

Statlog (Heart) Data Set

Description

This dataset is a heart disease database similar to a database already present in the repository (Heart Disease databases) but in a slightly different form.

Details

12 variables are used to cluster the observations

- age (integer)
- sex (binary)
- chest pain type (categorical with 4 levels)
- resting blood pressure (continuous)
- serum cholestoral in mg/dl (continuous)
- fasting blood sugar > 120 mg/dl (binary)
- resting electrocardiographic results (categorical with 3 levels)
- maximum heart rate achieved (continuous)
- exercise induced angina (binary)
- the slope of the peak exercise ST segment (categorical with 3 levels)
- number of major vessels colored by flourosopy (categorical with 4 levels)
- thal: 3 = normal; 6 = fixed defect; 7 = reversable defect (categorical with 3 levels)

1 variable define a "true" partition: Absence (1) or presence (2) of heart disease

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References

UCI Machine Learning Repository [http://archive.ics.uci.edu/ml]. Irvine, CA: University of California, School of Information and Computer Science: http://archive.ics.uci.edu/ml/datasets/statlog+(heart)

Examples

```
data(heart)
```

ICL

ICL criterion

Description

This function gives the ICL criterion for an instance of VSLCMresults.

Usage

```
ICL(object)
```

Arguments

object

VSLCMresults

References

Biernacki, C., Celeux, G., and Govaert, G. (2000). Assessing a mixture model for clustering with the integrated completed likelihood. IEEE transactions on pattern analysis and machine intelligence, 22(7), 719-725.

```
# Data loading:
data(heart)

# Cluster analysis without variable selection
res <- VarSelCluster(heart[,-13], 2, vbleSelec = FALSE)

# Get the ICL value
ICL(res)</pre>
```

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MICL

MICL criterion

Description

This function gives the MICL criterion for an instance of VSLCMresults.

Usage

```
MICL(object)
```

Arguments

object

VSLCMresults

References

Marbac, M. and Sedki, M. (2017). Variable selection for model-based clustering using the integrated completed-data likelihood. Statistics and Computing, 27 (4), 1049-1063.

Examples

```
## Not run:
# Data loading:
data("heart")

# Cluster analysis with variable selection
object <- VarSelCluster(heart[,-13], 2, vbleSelec = TRUE, crit.varsel = "MICL")

# Get the MICL value
MICL(object)

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

plot

Plots of an instance of VSLCMresults

Description

This function proposes different plots of an instance of VSLCMresults. It permits to visualize:

- the discriminative power of the variables (type="bar" or type="pie"). The larger is the discriminative power of a variable, the more explained are the clusters by this variable.
- the probabilities of misclassification (type="probs-overall" or type="probs-class").
- the distribution of a signle variable (y is the name of the variable and type="boxplot" or type="cdf").

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Usage

```
## S4 method for signature 'VSLCMresults, character'
plot(x, y, type = "boxplot", ylim = c(1,
    x@data@d))
```

Arguments

x instance of VSLCMresults.

y character. The name of the variable to ploted (only used if type="boxplot" or

type="cdf").

type character. The type of plot ("bar": barplot of the disciminative power, "pie":

pie of the discriminative power, "probs-overall": histogram of the probabilities of misclassification, "probs-class": histogram of the probabilities of misclassification per cluster, "boxplot": boxplot of a single variable per cluster, "cdf":

distribution of a single variable per cluster).

ylim numeric. Define the range of the most discriminative variables to considered

(only use if type="pie" or type="bar")

```
## Not run:
require(VarSelLCM)
# Data loading:
# x contains the observed variables
# z the known statu (i.e. 1: absence and 2: presence of heart disease)
data(heart)
ztrue <- heart[,"Class"]</pre>
x \leftarrow heart[,-13]
# Cluster analysis with variable selection (with parallelisation)
res_with <- VarSelCluster(x, 2, nbcores = 2, initModel=40)</pre>
# Summary of the probabilities of missclassification
plot(res_with, type="probs-class")
# Discriminative power of the variables (here, the most discriminative variable is MaxHeartRate)
plot(res_with)
# Boxplot for the continuous variable MaxHeartRate
plot(res_with, y="MaxHeartRate")
# Empirical and theoretical distributions (to check that the distribution is well-fitted)
plot(res_with, y="MaxHeartRate", type="cdf")
# Summary of categorical variable
plot(res_with, y="Sex")
## End(Not run)
```

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predict

Prediction of the cluster memberships

Description

This function gives the probabilities of classification for new observations by using the mixture model fit with the function VarSelCluster.

Usage

```
## S4 method for signature 'VSLCMresults'
predict(object, newdata, type = "probability")
```

Arguments

object instance of VSLCMresults.

newdata data.frame of the observations to classify.

type the type of prediction: probability of classification (probability) or the partition

(partition)

Value

Returns a matrix of the probabilities of classification.

print

Print function.

Description

This function gives the print of an instance of VSLCMresults.

Usage

```
## S4 method for signature 'VSLCMresults'
print(x)
```

Arguments

Х

instance of VSLCMresults.

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summary	Summary function.	
Summar y	Summer y function.	

Description

This function gives the summary of an instance of VSLCMresults.

Usage

```
## S4 method for signature 'VSLCMresults'
summary(object)
```

Arguments

object instance of VSLCMresults.

VarSelCluster

Variable selection and clustering.

Description

This function performs the model selection and the maximum likelihood estimation. It can be used for clustering only (i.e., all the variables are assumed to be discriminative). In this case, you must specify the data to cluster (arg. x), the number of clusters (arg. g) and the option vbleSelec must be FALSE. This function can also be used for variable selection in clustering. In this case, you must specify the data to analyse (arg. x), the number of clusters (arg. g) and the option vbleSelec must be TRUE. Variable selection can be done with BIC, MICL or AIC.

Usage

```
VarSelCluster(x, gvals, vbleSelec = TRUE, crit.varsel = "BIC",
  initModel = 50, nbcores = 1, discrim = rep(1, ncol(x)), nbSmall = 250,
  iterSmall = 20, nbKeep = 50, iterKeep = 1000, tolKeep = 10^(-6))
```

Arguments

x	data.frame/matrix. Rows correspond to observations and columns correspond to variables. Continuous variables must be "numeric", count variables must be "integer" and categorical variables must be "factor"
gvals	numeric. It defines number of components to consider.
vbleSelec	logical. It indicates if a variable selection is done
crit.varsel	character. It defines the information criterion used for model selection. Without variable selection, you can use one of the three criteria: "AIC", "BIC" and "ICL". With variable selection, you can use "AIC", BIC" and "MICL".

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initModel	numeric. It gives the number of initializations of the alternated algorithm maximizing the MICL criterion (only used if crit.varsel="MICL")
nbcores	numeric. It defines the numerber of cores used by the alogrithm
discrim	numeric. It indicates if each variable is discrimiative (1) or irrelevant (0) (only used if vbleSelec=0)
nbSmall	numeric. It indicates the number of SmallEM algorithms performed for the ML inference
iterSmall	numeric. It indicates the number of iterations for each SmallEM algorithm
nbKeep	numeric. It indicates the number of chains used for the final EM algorithm
iterKeep	numeric. It indicates the maximal number of iterations for each EM algorithm
tolKeep	numeric. It indicates the maximal gap between two successive iterations of EM algorithm which stops the algorithm

Value

Returns an instance of VSLCMresults.

References

Marbac, M. and Sedki, M. (2017). Variable selection for model-based clustering using the integrated completed-data likelihood. Statistics and Computing, 27 (4), 1049-1063.

Marbac, M. and Patin, E. and Sedki, M. (2018). Variable selection for mixed data clustering: Application in human population genomics. Journal of Classification, to appear.

```
## Not run:
# Package loading
require(VarSelLCM)
# Data loading:
# x contains the observed variables
# z the known statu (i.e. 1: absence and 2: presence of heart disease)
data(heart)
ztrue <- heart[,"Class"]</pre>
x \leftarrow heart[,-13]
# Cluster analysis without variable selection
res_without <- VarSelCluster(x, 2, vbleSelec = FALSE, crit.varsel = "BIC")</pre>
# Cluster analysis with variable selection (with parallelisation)
res_with <- VarSelCluster(x, 2, nbcores = 2, initModel=40, crit.varsel = "BIC")</pre>
# Comparison of the BIC for both models:
# variable selection permits to improve the BIC
BIC(res_without)
BIC(res_with)
# Confusion matrices and ARI (only possible because the "true" partition is known).
```

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```
# ARI is computed between the true partition (ztrue) and its estimators
# ARI is an index between 0 (partitions are independent) and 1 (partitions are equals)
# variable selection permits to improve the ARI
# Note that ARI cannot be used for model selection in clustering, because there is no true partition
# variable selection decreases the misclassification error rate
table(ztrue, fitted(res_without))
table(ztrue, fitted(res_with))
ARI(ztrue, fitted(res_without))
ARI(ztrue, fitted(res_with))
# Estimated partition
fitted(res_with)
# Estimated probabilities of classification
head(fitted(res_with, type="probability"))
# Summary of the probabilities of missclassification
plot(res_with, type="probs-class")
# Summary of the best model
summary(res_with)
# Discriminative power of the variables (here, the most discriminative variable is MaxHeartRate)
plot(res_with)
# More detailed output
print(res_with)
# Print model parameter
coef(res_with)
# Boxplot for the continuous variable MaxHeartRate
plot(x=res_with, y="MaxHeartRate")
# Empirical and theoretical distributions of the most discriminative variable
# (to check that the distribution is well-fitted)
plot(res_with, y="MaxHeartRate", type="cdf")
# Summary of categorical variable
plot(res_with, y="Sex")
# Probabilities of classification for new observations
predict(res_with, newdata = x[1:3,])
# Imputation by posterior mean for the first observation
not.imputed \leftarrow x[1,]
imputed <- VarSelImputation(res_with, x[1,], method = "sampling")</pre>
rbind(not.imputed, imputed)
# Opening Shiny application to easily see the results
VarSelShiny(res_with)
```

VarSelImputation

```
## End(Not run)
```

VarSelImputation

Imputation of missing values

Description

This function permits imputation of missing values in a dataset by using mixture model. Two methods can be used for imputation:

- posterior mean (method="postmean")
- sampling from the full conditionnal distribution (method="sampling")

Usage

```
VarSelImputation(obj, newdata, method = "postmean")
```

Arguments

obj an instance of VSLCMresults which defines the model used for imputation.

newdata data.frame Dataset containing the missing values to impute.

method character definiting the method of imputation: "postmean" or "sampling"

```
# Data loading
data("heart")

# Clustering en 2 classes
results <- VarSelCluster(heart[,-13], 2)

# Data where missing values will be imputed
newdata <- heart[1:2,-13]
newdata[1,1] <- NA
newdata[2,2] <- NA

# Imputation
VarSelImputation(results, newdata)</pre>
```

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VarSelShiny

Shiny app for analyzing results from VarSelCluster

Description

Shiny app for analyzing results from VarSelCluster

Usage

```
VarSelShiny(X)
```

Arguments

Χ

an instance of VSLCMresults returned by function VarSelCluster.

Examples

```
## Not run:
# Data loading
data("heart")
# Clustering en 2 classes
results <- VarSelCluster(heart[,-13], 2)
# Opening Shiny application to easily see the results
VarSelShiny(results)
## End(Not run)</pre>
```

VSLCMcriteria-class

Constructor of VSLCMcriteria class

Description

```
loglikelihood numeric. Log-likelihood
AIC numeric. Value of the AIC criterion.
BIC numeric. Value of the BIC criterion.
ICL numeric. Value of the ICL criterion.
MICL numeric. Value of the MICL criterion.
nbparam integer. Number of parameters.
```

cvrate numeric. Rate of convergence of the alternated algorithm for optimizing the MICL criterion.

degeneracyrate numeric. Rate of degeneracy for the selected model.

discrim numeric. Discriminative power of each variable.

```
getSlots("VSLCMcriteria")
```

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VSLCMdata-class

Constructor of VSLCMdata class

Description

n number of observations

d number of variables

withContinuous logical indicating if some variables are continuous

withInteger logical indicating if some variables are integer

withCategorica logical indicating if some variables are categorical

dataContinuous instance of VSLCMdataContinuous containing the continuous data

dataInteger instance of VSLCMdataContinuous containing the integer data

dataCategorical instance of VSLCMdataContinuous containing the categorical data

var.names labels of the variables

Examples

```
getSlots("VSLCMdata")
```

VSLCMmodel-class

Constructor of VSLCMmodel class

Description

g numeric. Number of components.

omega logical. Vector indicating if each variable is irrelevant (1) or not (0) to the clustering.

names.relevant character. Names of the relevant variables.

names.irrelevant character. Names of the irrelevant variables.

```
getSlots("VSLCMmodel")
```

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VSLCMparam-class

Constructor of VSLCMparam class

Description

```
    pi numeric. Proportions of the mixture components.
    paramContinuous VSLCMparamContinuous. Parameters of the continuous variables.
    paramInteger VSLCMparamInteger. Parameters of the integer variables.
    paramCategorical VSLCMparamCategorical. Parameters of the categorical variables.
```

Examples

```
getSlots("VSLCMparam")
```

VSLCMparamCategorical-class

Constructor of VSLCMparamCategorical class

Description

```
pi numeric. Proportions of the mixture components.alpha list. Parameters of the multinomial distributions.
```

Examples

```
getSlots("VSLCMparamCategorical")
```

VSLCMparamContinuous-class

Constructor of VSLCMparamContinuous class

Description

```
pi numeric. Proportions of the mixture components.mu matrix. Mean for each component (column) and each variable (row).sd matrix. Standard deviation for each component (column) and each variable (row).
```

```
getSlots("VSLCMparamContinuous")
```

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VSLCMparamInteger-class

Constructor of VSLCMparamInteger class

Description

```
pi numeric. Proportions of the mixture components.

lambda matrix. Mean for each component (column) and each variable (row).
```

Examples

```
getSlots("VSLCMparamInteger")
```

VSLCMpartitions-class Constructor of VSLCMpartitions class

Description

zMAP numeric. A vector indicating the class membership of each individual by using the MAP rule computed for the best model with its maximum likelihood estimates.

zOPT numeric. Partition maximizing the integrated complete-data likelihood of the selected model. **tik** numeric. Fuzzy partition computed for the best model with its maximum likelihood estimates.

Examples

```
getSlots("VSLCMpartitions")
```

VSLCMresults-class

Constructor of VSLCMresults class

Description

```
data VSLCMdata. Results relied to the data.

criteria VSLCMcriteria. Results relied to the information criteria.

partitions VSLCMpartitions. Results relied to the partitions.

model VSLCMmodel. Results relied to the selected model.

strategy VSLCMstrategy. Results relied to the tune parameters.

param VSLCMparam. Results relied to the parameters.
```

```
getSlots("VSLCMresults")
```

VSLCMstrategy-class 23

VSLCMstrategy-class

Constructor of VSLCMstrategy class

Description

initModel numeric. Number of initialisations for the model selection algorithm.

vbleSelec logical. It indicates if the selection of the variables is performed.

paramEstim logical. It indicates if the parameter estimation is performed.

parallel logical. It indicates if a parallelisation is done.

nbSmall numeric. It indicates the number of small EM.

iterSmall numeric. It indicates the number of iteration for the small EM

nbKeep numeric. It indicates the number of chains kept for the EM.

iterKeep numeric. It indicates the maximum number of iteration for the EM.

tolKeep numeric. It indicates the value of the difference between successive iterations of EM stopping the EM.

Examples

getSlots("VSLCMstrategy")

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