## Package 'clusterMI'

July 22, 2025

**Encoding** UTF-8

Type Package

Title Cluster Analysis with Missing Values by Multiple Imputation

Version 1.5

Date 2025-02-24

**Description** Allows clustering of incomplete observations by addressing missing values using multiple imputation. For achieving this goal, the methodology consists in three steps, following Audigier and Niang 2022 <doi:10.1007/s11634-022-00519-1>. I) Missing data imputation using dedicated models. Four multiple imputation methods are pro-

posed, two are based on joint modelling and two are fully sequential methods, as discussed in Audigier et al. (2021) <doi:10.48550/arXiv.2106.04424>. II) cluster analysis of imputed data sets. Six clustering methods are available (distances-based or model-based), but custom methods can also be easily used. III) Partition pooling. The set of partitions is aggregated using Non-negative Matrix Factorization based method. An associated instability measure is computed by boot-

strap (see Fang, Y. and Wang, J., 2012 <doi:10.1016/j.csda.2011.09.003>). Among applications, this instability measure can be used to choose a number of clusters with missing values. The package also proposes several diagnostic tools to tune the number of imputed data sets, to tune the number of iterations in fully sequential imputation, to check the fit of imputation models, etc.

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## **Depends** R (>= 3.5.0)

**Imports** stats, graphics, parallel, mice, micemd, mclust, mix, fpc, knockoff, withr, glmnet, ClusterR, FactoMineR, diceR, NPBayesImputeCat, e1071, Rfast, cat, utils, ggplot2, gridExtra, reshape2, methods, Rcpp

## RoxygenNote 7.3.2

Suggests knitr, rmarkdown, stargazer, VIM, missMDA, clustrd, clusterCrit, bookdown, R.rsp

VignetteBuilder R.rsp

LazyData true

LinkingTo Rcpp, RcppArmadillo

RcppModules IO\_module

NeedsCompilation yes

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**Repository** CRAN

Date/Publication 2025-02-24 17:20:08 UTC

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clusterMI-package clusterMI: Cluster Analysis with Missing Values by Multiple Imputation

#### Description

clusterMI is an R package to perform clustering with missing values. For achieving this goal, multiple imputation is used. The package offers various multiple imputation methods dedicated to clustered individuals, as discussed in Audigier et al. (2021) <arXiv:2106.04424>. In addition, it allows pooling results both in terms of partition and instability, as proposed in Audigier and Niang (2022) <doi:10.1007/s11634-022-00519-1>. Among applications, this instability measure can be used to choose a number of clusters with missing values.

## References

Audigier, V. and Niang, N., Clustering with missing data: which equivalent for Rubin's rules? Advances in Data Analysis and Classification <doi:10.1007/s11634-022-00519-1>, 2022.

Audigier, V., Niang, N., & Resche-Rigon, M. (2021). Clustering with missing data: which imputation model for which cluster analysis method?. arXiv preprint <arXiv:2106.04424>.

## chooseB

Audigier, V. (2024). Clustering on incomplete data using clusterMI. 10emes Rencontres R, Vannes, France. hal preprint <hal:04550305>.

Bar-Hen, A. and Audigier, V., An ensemble learning method for variable selection: application to high dimensional data and missing values, Journal of Statistical Computation and Simulation, <doi:10.1080/00949655.2022.2070621>, 2022.

Fang, Y. and Wang, J., Selection of the number of clusters via the bootstrap method. Computational Statistics and Data Analysis, 56, 468-477 <doi:10.1016/j.csda.2011.09.003> 2012.

#### Examples

```
data(wine, package = "clusterMI")
require(parallel)
set.seed(123456)
ref <- wine$cult</pre>
nb.clust <- 3
wine.na <- wine
wine.na$cult <- NULL</pre>
wine.na <- prodna(wine.na)</pre>
# imputation
m < -5 \# number of imputed data sets. Should be larger in practice
res.imp <- imputedata(data.na = wine.na, nb.clust = nb.clust, m = m)</pre>
# cluster analysis by kmeans and pooling
nnodes <- 2 # Number of CPU cores for parallel computing</pre>
res.pool <- clusterMI(res.imp, nnodes = nnodes)</pre>
res.pool$instability
table(ref, res.pool$part)
# choice of nb.clust
```

res.nbclust <- choosenbclust(res.pool)
res.nbclust\$nb.clust</pre>

chooseB

Diagnostic plot for the number of iterations used in the varselbest function

#### Description

chooseB plots the proportion of times an explanatory variable is selected according to the number of iterations (B).

## chooseB

#### Usage

```
chooseB(
  res.varselbest,
  plotvar = NULL,
  linewidth = 1,
  linetype = "dotdash",
  xlab = "B",
  ylab = "Proportion",
  nrow = 2,
  ncol = 2,
  graph = TRUE
)
```

## Arguments

res.varselbest	an output from the varselbest function
plotvar	index of variables for which a curve is ploted
linewidth	a numerical value setting the widths of lines
linetype	what type of plot should be drawn
xlab	a title for the x axis
ylab	a title for the y axis
nrow	argument of gtable. Default value is 2.
ncol	argument of gtable. Default value is 2.
graph	a boolean. If FALSE, no graphics are ploted. Default value is TRUE

#### Details

varselbest performs variable selection on random subsets of variables and, then, combines them to recover which explanatory variables are related to the response, following Bar-Hen and Audigier (2022) <doi:10.1080/00949655.2022.2070621>. More precisely, the outline of the algorithm are as follows: let consider a random subset of sizeblock among p variables. Then, any selection variables scheme can be applied. By resampling B times, a sample of size sizeblock among the p variables, we may count how many times a variable is considered as significantly related to the response and how many times it is not. The number of iterations B should be large so that the proportion of times a variable is selected becomes stable. chooseB plots the values of proportion according to the number of iterations.

## Value

a list of matrices where each row corresponds to the vector of proportions (for all explanatory variables) obtained for a given value of B

#### References

Bar-Hen, A. and Audigier, V., An ensemble learning method for variable selection: application to high dimensional data and missing values, Journal of Statistical Computation and Simulation, <doi:10.1080/00949655.2022.2070621>, 2022.

## choosem

#### See Also

varselbest

#### Examples

```
data(wine, package = "clusterMI")
```

```
require(parallel)
ref <- wine$cult
nb.clust <- 3
wine.na<-wine
wine.na$cult <- NULL
wine.na <- prodna(wine.na)</pre>
```

```
nnodes <- 2 # Number of CPU cores for parallel computing B <- 80 # Number of iterations for variable selection
```

```
# variable selection
```

*Graphical investigation for the number of datasets generated by multiple imputation* 

## Description

For an object generated by the function clusterMI, the choosem function browses the sequence of the contributory partitions and computes the consensus partition at each step. Then, the rand index between successive consensus partitions is plotted.

#### Usage

choosem(output, graph = TRUE, nnodes = 1)

## Arguments

output	an output from the clusterMI function
graph	a boolean indicating if a graphic is plotted
nnodes	number of CPU cores for parallel computing. By default nnodes = 1.

## Details

The number of imputed datasets (m) should be sufficiently large to improve the partition accuracy. The choosem function can be used to check if this number is suitable. This function computes the consensus partition by considering only the first imputed datasets. By this way, a sequence of m consensus partitions is obtained. Then, the rand index between successive partitions is computed and reported in a graph. The rand index measures the proximity between two partitions. If the rand index between the last consensus partitions of the sequence reaches its maximum values (1), then it means last imputed dataset does not modify the consensus partition. Consequently, the number of imputed datasets can be considered as sufficiently large.

#### Value

A list of two objects

part	m-columns matrix that contains in column p the consensus partition using only the p first imputed datasets
rand	a m-1 vector given the rand index between the m successive consensus partitions

## References

Audigier, V. and Niang, N., Clustering with missing data: which equivalent for Rubin's rules? Advances in Data Analysis and Classification <doi:10.1007/s11634-022-00519-1>, 2022.

#### See Also

clusterMI, imputedata

#### Examples

```
data(wine, package = "clusterMI")
set.seed(123456)
ref <- wine$cult
nb.clust <- 3
wine.na <- wine
wine.na$cult <- NULL
wine.na <- prodna(wine.na)
#imputation
m <- 5 # number of imputed data sets. Should be larger in practice
res.imp <- imputedata(data.na = wine.na, nb.clust = nb.clust, m = m)
#pooling
nnodes <- 2 # number of CPU cores for parallel computing
res.pool <- clusterMI(res.imp, instability = FALSE, nnodes = nnodes)
res.choosem <- choosem(res.pool)</pre>
```

choosemaxit

## Description

The choosemaxit function plots the within and between variance for each variable (specified in plotvars) against the iteration number for each of the replications (specified in plotm).

## Usage

```
choosemaxit(
  output,
  plotvars = NULL,
  plotm = 1:5,
  size = 0.5,
  linewidth = 1,
  linetype = "dotdash",
  xlab = "iterations",
  ylab = "var",
  title = "Within and between variance plots",
  nvar_by_row = 5
)
```

## Arguments

output	an outpout from the imputedata function
plotvars	index of variables for which a curve is plotted
plotm	a vector indicating which imputed datasets must be plotted
size	size of points
linewidth	a numerical value setting the widths of lines
linetype	what type of plot should be drawn
xlab	a title for the x axis
ylab	a title for the y axis
title	the main title
nvar_by_row	the number of variables that are plotted per window. Default value is 5.

## Value

No return value

## Examples

choosenbclust *Tune the number of clusters according to the partition instability* 

## Description

choosenbclust reports the cluster instability according to the number of clusters chosen.

#### Usage

```
choosenbclust(output, grid = 2:5, graph = TRUE, verbose = TRUE, nnodes = NULL)
```

## Arguments

output	an output from the clusterMI function
grid	a vector indicating the grid of values tested for nb.clust. By default 2:5
graph	a boolean indicating if a graphic is plotted
verbose	if TRUE, choosenbclust will print messages on console
nnodes	number of CPU cores for parallel computing. By default, the value used in the call to the clusterMI function

#### Details

The choosenbclust function browses a grid of values for the number of clusters and for each one imputes the data and computes the instability.

## Value

a list of two objects

nb.clust	the number of clusters in grid minimizing the instability
crit	a vector indicating the instability for each value in the grid

## chooser

## References

Audigier, V. and Niang, N., Clustering with missing data: which equivalent for Rubin's rules? Advances in Data Analysis and Classification <doi:10.1007/s11634-022-00519-1>, 2022.

## See Also

#### imputedata

## Examples

```
data(wine, package = "clusterMI")
require(parallel)
set.seed(123456)
ref <- wine$cult
nb.clust <- 3
wine.na <- wine
wine.na$cult <- NULL
wine.na <- prodna(wine.na)
# imputation
res.imp <- imputedata(data.na=wine.na, nb.clust = nb.clust, m = 5)
# pooling
nnodes <- 2 # number of CPU cores for parallel computing
res.pool <- clusterMI(res.imp, nnodes = nnodes, instability = FALSE)
# choice of nb.clust
choosenbclust(res.pool)</pre>
```

chooser

Kfold cross-validation for specifying threshold r

## Description

chooser returns a list specifying the optimal threshold r for each outcome as well as the associated set of explanatory variables selected, and the cross-validation error for each value of the grid

## Usage

```
chooser(
  res.varsel,
  K = 10,
  seed = 12345,
  listvar = NULL,
```

chooser

```
grid.r = seq(0, 1, 1/1000),
graph = TRUE,
printflag = TRUE,
nb.clust = NULL,
nnodes = NULL,
sizeblock = NULL,
method.select = NULL,
B = NULL,
modelNames = NULL,
nbvarused = NULL,
path.outfile = NULL
```

## Arguments

)

res.varsel	an output from the varselbest function
К	an integer given the number of folds
seed	a integer
listvar	a vector of characters specifiying variables (outcomes) for which cross-validation should be done. By default, all variables that have been considered for varselbest are used.
grid.r	a grid for the tuning parameter r
graph	a boolean. If TRUE, cross-validation results are printed
printflag	a boolean. If TRUE, messages are printed
nb.clust	number of clusters. By default, the same as the one used in varselbest
nnodes	an integer specifying the number of nodes for parallel computing. By default, the same as the one used in varselbest
sizeblock	number of sampled variables at each iteration. By default, the same as the one used in varselbest
<pre>method.select</pre>	variable selection method used. By default, the same as the one used in varselbest
В	number of iterations. By default, the same as the one used in varselbest
modelNames	mixture model specification for imputation of subsets. By default, the same as the one used in varselbest
nbvarused	a maximal number of selected variables (can be required for a dataset with a large number of variables)
path.outfile	

#### Details

varselbest performs variable selection on random subsets of variables and, then, combines them to recover which explanatory variables are related to the response. More precisely, the outline of the algorithm are as follows: let consider a random subset of sizeblock among p variables. By choosing sizeblock small, this subset is low dimensional, allowing treatment of missing values by standard imputation method for clustered individuals. Then, any selection variable scheme can be applied (lasso, stepwise and knockoff are proposed by tuning the method.select argument). By

#### chooser

resampling B times, a sample of size sizeblock among the p variables, we may count how many times, a variable is considered as significantly related to the response and how many times it is not. We need to define a threshold (r) to conclude if a given variable is significantly related to the response. chooser aims at finding the optimal value for the threshold r using Kfold cross-validation.

## Value

A list where each object refers to an outcome variable called in the listvar argument. Each element is composed of three objects

r	the optimal value for the threshold
error	the cross-validation error for each value in grid.r
selection	the subset of selected variables for the optimal threshold

#### References

Bar-Hen, A. and Audigier, V., An ensemble learning method for variable selection: application to high dimensional data and missing values, Journal of Statistical Computation and Simulation, <doi:10.1080/00949655.2022.2070621>, 2022.

Schafer, J. L. (1997) Analysis of Incomplete Multivariate Data. Chapman & Hall, Chapter 9.

#### Examples

```
data(wine, package = "clusterMI")
require(parallel)
```

```
set.seed(123456)
ref <- wine$cult
nb.clust <- 3
wine.na <- wine
wine.na$cult <- NULL
wine.na <- prodna(wine.na)
nnodes <- 2 # parallel::detectCores()
B <- 100 # Number of iterations
m <- 5 # Number of imputed data sets</pre>
```

```
nnodes = nnodes)
```

```
# frequency of selection
propselect <- res.varsel$proportion[listvar, ]</pre>
```

```
#predictormatrix with the default threshold value
predictmat <- res.varsel$predictormatrix</pre>
```

clusterMI

*Cluster analysis and pooling after multiple imputation* 

#### Description

From a list of imputed datasets clusterMI performs cluster analysis on each imputed data set, estimates the instability of each partition using bootstrap (following Fang, Y. and Wang, J., 2012 <doi:10.1016/j.csda.2011.09.003>) and pools results as proposed in Audigier and Niang (2022) <doi:10.1007/s11634-022-00519-1>.

#### Usage

```
clusterMI(
  output,
 method.clustering = "kmeans",
 method.consensus = "NMF",
  scaling = TRUE,
  nb.clust = NULL,
 Cboot = 50,
 method.hclust = "average",
 method.dist = "euclidean",
 modelNames = NULL,
 modelName.hc = "VVV",
  nstart.kmeans = 100,
  iter.max.kmeans = 10,
 m.cmeans = 2,
  samples.clara = 500,
  nnodes = 1,
  instability = TRUE,
  verbose = TRUE,
 parameter.nmf = list(method.init = c("BOK", "kmeans"), threshold = 10^(-5), printflag =
    FALSE, parameter.kmeans = list(nstart = 100, iter.max = 50, algorithm =
    c("Hartigan-Wong", "Lloyd", "Forgy", "MacQueen"), trace = FALSE),
   parameter.minibatchkmeans = list(batch_size = 10, num_init = 1, max_iters = 50,
```

```
init_fraction = 1, initializer = "kmeans++", early_stop_iter = 10, verbose = FALSE,
    CENTROIDS = NULL, tol = 1e-04, tol_optimal_init = 0.3, seed = 1))
)
```

## Arguments

<b>tt</b>	an autout farm the impute date familier
output	an output from the imputedata function
method.cluster	a single string specifying the clustering algorithm used ("kmeans", "pam", "clara", "hclust" or "mixture", "cmeans")
method.consens	us
	a single string specifying the consensus method used to pool the contributory partitions ("NMF" or "CSPA")
scaling	boolean. If TRUE, variables are scaled. Default value is TRUE
nb.clust	an integer specifying the number of clusters. If two distinct values are consid- ered for analysis and pooling steps, then a 2 length vector can be provided to specify the two numbers respectively.
Cboot	an integer specifying the number of bootstrap replications. Default value is 50
method.hclust	character string defining the clustering method for hierarchical clustering (re- quired only if method.clustering = "hclust")
method.dist	character string defining the method use for computing dissimilarity matrices in hierarchical clustering (required only if method.clustering = "hclust")
modelNames	character string indicating the models to be fitted in the EM phase of clustering (required only if method.clustering = "mixture"). By default modelNames = NULL.
modelName.hc	A character string indicating the model to be used in model-based agglomera- tive hierarchical clustering.(required only if method.clustering = "mixture"). By default modelNames.hc = "VVV".
nstart.kmeans	how many random sets should be chosen for kmeans initialization. Default value is 100 (required only if method.clustering = "kmeans")
iter.max.kmean	
	how many iterations should be chosen for kmeans. Default value is 10 (required only if method.clustering = "kmeans")
m.cmeans	degree of fuzzification in cmeans clustering. By default m.cmeans = 2
samples.clara	number of samples to be drawn from the dataset when performing clustering using clara algorithm. Default value is 500.
nnodes	number of CPU cores for parallel computing. By default, nnodes = 1
instability	a boolean indicating if cluster instability must be computed. Default value is TRUE
verbose	a boolean. If TRUE, a message is printed at each step. Default value is TRUE
parameter.nmf	a list of arguments for consensus by NMF. See the fastnmf help page.

#### Details

clusterMI performs cluster analysis (according to the method.clustering argument) and pooling after multiple imputation. For achieving this goal, the clusterMI function uses as an input an output from the imputedata function and then

- 1. applies the cluster analysis method on each imputed data set
- 2. pools contributory partitions using non-negative matrix factorization
- 3. computes the instability of each partition by bootstrap
- 4. computes the total instability

Step 1 can be tuned by specifying the cluster analysis method used (method.clustering argument). If method.clustering = "kmeans" or "pam", then the number of clusters can be specified by tuning the nb.clust argument. By default, the same number as the one used for imputation is used. The number of random initializations can also be tuned through the nstart.kmeans argument. If method.clustering = "hclust" (hierarchical clustering), the method used can be specified (see hclust). By default "average" is used. Furthermore, the number of clusters can be specified, but it can also be automatically chosen if nb.clust < 0. If method.clustering = "mixture" (model-based clustering using gaussian mixture models), the model to be fitted can be tuned by modifying the modelNames argument (see Mclust). If method.clustering = "cmeans" (clustering using the fuzzy c-means algorithm), then the fuzziness parameter can be modified by tuning them.cmeans argument. By default, m.cmeans = 2.

Step 2 performs consensus clustering by Non-Negative Matrix Factorization, following Li and Ding (2007) <doi:10.1109/ICDM.2007.98>.

Step 3 applies the nselectboot function on each imputed data set and returns the instability of each cluster obtained at step 1. The method is based on bootstrap sampling, followong Fang, Y. and Wang, J. (2012) <doi:10.1016/j.csda.2011.09.003>. The number of iterations can be tuned using the Cboot argument.

Step 4 averages the previous instability measures given a within instability (Ubar), computes a between instability (B) and a total instability (T = B + Ubar). See Audigier and Niang (2022) <doi:10.1007/s11634-022-00519-1> for details.

All steps can be performed in parallel by specifying the number of CPU cores (nnodes argument). Steps 3 and 4 are more time consuming. To compute only steps 1 and 2 use instability = FALSE.

#### Value

A list with three objects

part	the consensus partition
instability	a list of four objects: U the within instability measure for each imputed data set, Ubar the associated average, B the between instability measure, Tot the total instability measure
call	the matching call

## fastnmf

## References

Audigier, V. and Niang, N. (2022) Clustering with missing data: which equivalent for Rubin's rules? Advances in Data Analysis and Classification <doi:10.1007/s11634-022-00519-1>

Fang, Y. and Wang, J. (2012) Selection of the number of clusters via the bootstrap method. Computational Statistics and Data Analysis, 56, 468-477. <doi:10.1016/j.csda.2011.09.003>

T. Li, C. Ding, and M. I. Jordan (2007) Solving consensus and semi-supervised clustering problems using nonnegative matrix factorization. In Proceedings of the 2007 Seventh IEEE International Conference on Data Mining, ICDM'07, page 577-582, USA. IEEE Computer Society. <doi:10.1109/ICDM.2007.98>

## See Also

hclust, nselectboot, Mclust, imputedata, cmeans

#### Examples

```
data(wine, package = "clusterMI")
require(parallel)
set.seed(123456)
ref <- wine$cult</pre>
nb.clust <- 3
m <- 5 # number of imputed data sets. Should be larger in practice
wine.na <- wine
wine.na$cult <- NULL</pre>
wine.na <- prodna(wine.na)</pre>
#imputation
res.imp <- imputedata(data.na = wine.na, nb.clust = nb.clust, m = m)</pre>
#analysis by kmeans and pooling
nnodes <- 2 # parallel::detectCores()</pre>
res.pool <- clusterMI(res.imp, nnodes = nnodes)</pre>
res.pool$instability
table(ref, res.pool$part)
```

fastnmf

Consensus clustering using non-negative matrix factorization

#### Description

From a list of partitions fastnmf pools partition as proposed in Li and Ding (2007) <doi:10.1109/ICDM.2007.98>.

## Usage

```
fastnmf(
  listpart,
  nb.clust,
  method.init = c("BOK", "kmeans"),
  threshold = 10^(-5),
  printflag = TRUE,
  parameter.kmeans = list(nstart = 100, iter.max = 50, algorithm = c("Hartigan-Wong",
        "Lloyd", "Forgy", "MacQueen"), trace = FALSE),
  parameter.minibatchkmeans = list(batch_size = 10, num_init = 1, max_iters = 50,
        init_fraction = 1, initializer = "kmeans++", early_stop_iter = 10, verbose = FALSE,
        CENTROIDS = NULL, tol = 1e-04, tol_optimal_init = 0.3, seed = 1)
)
```

#### Arguments

listpart	a list of partitions	
nb.clust	an integer specifying the number of clusters	
method.init	a vector giving initialisation methods used among "BOK", "kmeans", "mini- batchkmeans" "sample". See details.	
threshold	a real specifying when the NMF algorithm is stoped. Default value is 10 <sup>(-5)</sup>	
printflag	a boolean. If TRUE, nmf will print messages on console. Default value is TRUE	
parameter.kmeans		
	a list of arguments for kmeans function. See keans help page.	
parameter.minibatchkmeans		
	list of arguments for MiniBatchKmeans function. See MiniBatchKmeans help	

page.

#### Details

fastnmf performs consensus clustering using non-negative matrix factorization following Li and Ding (2007) <doi:10.1109/ICDM.2007.98>. The set of partitions that are aggregated needs to be given as a list where each element is a vector of numeric values. Note that the number of classes for each partition can vary. The number of classes for the consensus partition should be given using the nb.clust argument. The NMF algorithm is iterative and required an initial partition. This latter is specified by method.init. method.init = "BOK" means the partition considered is a partition from listpart which minimizes the NMF criterion. Alternative methods are "kmeans", "minibatchkmeans" or "sample". If method.init = "kmeans" (or "minibatchkmeans"), then clustering on the average of connectivity matrices is performed by kmeans (or "minibatchkmeans"). Mini Batch Kmeans could be faster than kmeans if the number of individuals is large. If method.init = "sample", then a random partition is drawn. If method.init is a vector of several characters, then several initialization methods are considered and the best method is returned. By default, method.init = c("BOK", "kmeans").

#### Value

For each initialisation method, a list of 5 objets is returned

### fastnmf

Htilde	A fuzzy disjunctive table
S	A positive matrix
Mtilde	The average of connectivity matrices
crit	A vector with the optimized criterion at each iteration
cluster	the consensus partition in nb.clust classes

In addition, the best initialisation method is returned

#### References

T. Li, C. Ding, and M. I. Jordan (2007) Solving consensus and semi-supervised clustering problems using nonnegative matrix factorization. In Proceedings of the 2007 Seventh IEEE International Conference on Data Mining, ICDM'07, page 577-582, USA. IEEE Computer Society. <doi:10.1109/ICDM.2007.98>

## See Also

kmeans MiniBatchKmeans

#### Examples

```
data(wine, package = "clusterMI")
require(clustrd)
set.seed(123456)
ref <- wine$cult</pre>
nb.clust <- 3
m <- 3 # number of imputed data sets. Should be larger in practice</pre>
wine.na <- wine
wine.na$cult <- NULL</pre>
wine.na <- prodna(wine.na)</pre>
#imputation
res.imp <- imputedata(data.na = wine.na, nb.clust = nb.clust, m = m)</pre>
#analysis using reduced kmeans
## apply the cluspca function on each imputed data set
res.ana.rkm <- lapply(res.imp$res.imp,</pre>
                       FUN = cluspca,
                       nclus = nb.clust,
                       ndim = 2,
                       method= "RKM")
## extract the set of partitions (under "list" format)
res.ana.rkm <-lapply(res.ana.rkm,"[[","cluster")</pre>
# pooling by NMF
res.pool.rkm <- fastnmf(res.ana.rkm, nb.clust = nb.clust)</pre>
## extract the partition corresponding to the best initialisation
```

imputedata

## Description

imputedata returns a list of imputed datasets by using imputation methods dedicated to individuals clustered in (unknown) groups

## Usage

```
imputedata(
   data.na,
   method = "JM-GL",
   nb.clust = NULL,
   m = 20,
   maxit = 50,
   Lstart = 100,
   L = 20,
   method.mice = NULL,
   verbose = TRUE,
   seed = 1234,
   bootstrap = FALSE
)
```

## Arguments

data.na	an incomplete dataframe
method	a single string specifying the imputation method used among "FCS-homo", "FCS-hetero", "JM-DP", "JM-GL". By default method = "JM-GL". See the details section
nb.clust	number of clusters
m	number of imputed datasets. By default, $m = 20$ .
maxit	number of iterations for FCS methods (only used for method = FCS-homo or method = FCS-hetero)
Lstart	number of iterations for the burn-in period (only used if method ="JM-DP" or "JM-GL")
L	number of skipped iterations to keep one imputed data set after the burn-in pe- riod (only used if method ="JM-DP" or "JM-GL")
method.mice	a vector of strings (or a single string) giving the imputation method for each variable (only used for method = FCS-homo or method = FCS-hetero). Default value is "pmm" (predictive mean matching) for FCS-homo and "mice.impute.2l.jomo" for FCS-hetero
predictmat	predictor matrix used for FCS imputation (only used for method = FCS-homo or method = FCS-hetero)

#### imputedata

verbose	a boolean. If TRUE, a message is printed at each iteration. Use verbose = FALSE for silent imputation
seed	a positive integer initializing the random generator
bootstrap	a boolean. Use bootstrap = TRUE for proper imputation with FCS methods (Mclust sometimes fails with multiple points)

## Details

The imputedata offers various multiple imputation methods dedicated to clustered individuals. In particular, two fully conditional imputation methods are proposed (FCS-homo and FCS-hetero) which essentially differ by the assumption about the covariance in each cluster (constant or not respectively). The imputation requires a pre-specified number of clusters (nb.clust). See choosenbclust if this number is unknown. The imputedata function alternates clustering and imputation given the partition of individuals. When the clustering is performed, the function calls the mice function from the mice R package to perform imputation. The mice package proposes various methods for imputation which can be specified by tuning the method.mice argument. Note that two other joint modelling methods are also available: JM-GL from the R package mix and JM-DP from the R package DPImputeCont https://github.com/hang-j-kim/DPImputeCont

#### Value

a list of 3 objets

res.imp	a list with the several imputed datasets
res.conv	for FCS methods, an array given the between (and within) inertia of each im- puted variable at each iteration and for each imputed dataset. For JM methods, a matrix given the between inertia for each variable and each imputed dataset.
call	the matching call

#### References

Kim, H. J., Reiter, J. P., Wang, Q., Cox, L. H. and Karr, A. F. (2014), Multiple imputation of missing or faulty values under linear constraints, Journal of Business and Economics Statistics, 32, 375-386 <doi:10.1080/07350015.2014.885435>

Schafer, J. L. (1997) Analysis of Incomplete Multivariate Data. Chapman & Hall, Chapter 9.

Audigier, V., Niang, N., & Resche-Rigon, M. (2021). Clustering with missing data: which imputation model for which cluster analysis method?. arXiv preprint <arXiv:2106.04424>.

#### See Also

mice choosenbclust choosemaxit varselbest imp.mix

## Examples

```
data(wine, package = "clusterMI")
set.seed(123456)
wine.na <- wine
wine.na$cult <- NULL</pre>
```

```
wine.na <- prodna(wine.na)
nb.clust <- 3 # number of clusters
m <- 20 # number of imputed data sets
res.imp <- imputedata(data.na = wine.na, nb.clust = nb.clust, m = m)
lapply(res.imp$res.imp, summary)</pre>
```

overimpute

## Overimputation diagnostic plot

## Description

over impute assesses the fit of the predictive distribution after performing multiple imputation with the imputedata function

## Usage

```
overimpute(
  res.imputedata,
  plotvars = NULL,
  plotinds = NULL,
  nnodes = 2,
  path.outfile = NULL,
  alpha = 0.1,
  mfrow = NULL,
  mar = c(5, 4, 4, 2) - 1.9
)
```

## Arguments

res.imputedata	an output from the imputedata function
plotvars	column index of the variables overimputed
plotinds	row index of the individuals overimputed
nnodes	an integer indicating the number of nodes for parallel calculation. Default value is 2
path.outfile	a vector of strings indicating the path for redirection of print messages. De- fault value is NULL, meaning that silent imputation is performed. Otherwise, print messages are saved in the files path.outfile/output.txt. One file per node is generated.
alpha	alpha level for prediction intervals
mfrow	a vector of the form c(nr, nc)
mar	a numerical vector of the form c(bottom, left, top, right)

#### overimpute

#### **Details**

This function imputes each observed value from each conditional imputation model obtained from the imputedata function. The comparison between the "overimputed" values and the observed values is made by building a confidence interval for each observed value using the quantiles of the overimputed values (see Blackwell et al. (2015) <doi:10.1177/0049124115585360>). Note that confidence intervals built with quantiles require a large number of imputations. If the model fits well the data, then the 90% confidence interval should contain the observed value in 90% of the cases. The function overimpute takes as an input an output of the imputedata function (res.imputedata argument), the indices of the incomplete continuous variables that are plotted (plotvars), the indices of individuals (can be useful for time consuming imputation methods), the number of CPU cores for parallel computation, and the path for exporting print message generated during the parallel process (path.outfile).

## Value

A list of two matrices

res.plot	7-columns matrix that contains (1) the variable which is overimputed, (2) the observed value of the observation, (3) the mean of the overimputations, (4) the lower bound of the confidence interval of the overimputations, (5) the upper bound of the confidence interval of the overimputations, (6) the proportion of the other variables that were missing for that observation in the original data, and (7) the color for graphical representation
res.values	a matrix with overimputed values for each cell. The number of columns corre- sponds to the number of values generated (i.e. the number of imputed datasets)

#### References

Blackwell, M., Honaker, J. and King. G. 2015. A Unified Approach to Measurement Error and Missing Data: Overview and Applications. Sociological Methods and Research, 1-39. <doi:10.1177/0049124115585360>

#### Examples

## prodna

prodna	Introduce missing values using a missing completely at random mech-
	anism

## Description

prodna generates an incomplete dataset by removing a proportion of observed values

## Usage

prodna(X, pct = 0.3)

## Arguments

Х	a data frame (or matrix).
pct	proportion of missing values. By default $pct = 0.3$ .

## Value

an incomplete data frame

## Examples

```
n <- 1000
p <- 5
X <- matrix(runif(n*p), nrow = n, ncol = p)
summary(X)
X.na <- prodna(X)
colMeans(is.na(X.na))</pre>
```

varselbest

## Description

varselbest performs variable selection from an incomplete dataset (see Bar-Hen and Audigier (2022) <doi:10.1080/00949655.2022.2070621>) in order to specify the imputation models to use for FCS imputation methods

#### Usage

```
varselbest(
 data.na = NULL,
  res.imputedata = NULL,
 listvar = NULL,
  nb.clust = NULL,
 nnodes = 1,
 sizeblock = 5,
 method.select = "knockoff",
 B = 200,
  r = 0.3,
 graph = TRUE,
 printflag = TRUE,
 path.outfile = NULL,
 mar = c(2, 4, 2, 0.5) + 0.1,
 cex.names = 0.7,
 modelNames = NULL
)
```

#### Arguments

data.na	a dataframe with only numeric variables
res.imputedata	an output from imputedata
listvar	a character vector indicating for which subset of incomplete variables variable selection must be performed. By default all column names.
nb.clust	the number of clusters used for imputation
nnodes	number of CPU cores for parallel computing. By default, nnodes = 1
sizeblock	an integer indicating the number of variables sampled at each iteration
method.select	a single string indicating the variable selection method applied on each subset of variables
В	number of iterations, by default $B = 200$
r	a numerical vector (or a single real number) indicating the threshold used for each variable in listvar. Each value of r should be between 0 and 1. See details.

graph	a boolean. If TRUE two graphics are plotted per variable in listvar: a graphic reporting the variable importance measure of each explanatory variable and a graphic reporting the influence of the number iterations (B) on the importance measures
printflag	a boolean. If TRUE, a message is printed at each iteration. Use printflag = FALSE for silent selection.
path.outfile	a vector of strings indicating the path for redirection of print messages. De- fault value is NULL, meaning that silent imputation is performed. Otherwise, print messages are saved in the files path.outfile/output.txt. One file per node is generated.
mar	a numerical vector of the form c(bottom, left, top, right). Only used if graph = TRUE
cex.names	expansion factor for axis names (bar labels) (only used if graph = TRUE)
modelNames	a vector of character strings indicating the models to be fitted in the EM phase of clustering

## Details

varselbest performs variable selection on random subsets of variables and, then, combines them to recover which explanatory variables are related to the response. More precisely, the outline of the algorithm are as follows: let consider a random subset of sizeblock among p variables. By choosing sizeblock small, this subset is low dimensional, allowing treatment of missing values by standard imputation method for clustered individuals. Then, any selection variable scheme can be applied (lasso, stepwise and knockoff are proposed by tuning the method.select argument). By resampling B times, a sample of size sizeblock among the p variables, we may count how many times, a variable is considered as significantly related to the response and how many times it is not. We need to define a threshold (r) to conclude if a given variable is significantly related to the response.

#### Value

a list of four objects	
predictormatri	x
	a numeric matrix containing 0 and 1 specifying on each line the set of predictors to be used for each target column of the incomplete dataset.
res.varsel	a list given details on the variable selection procedure (only required for check- ing convergence by the chooseB function)
proportion	a numeric matrix of proportion indicating on each line the variable importance of each predictor
call	the matching call

## References

Bar-Hen, A. and Audigier, V., An ensemble learning method for variable selection: application to high dimensional data and missing values, Journal of Statistical Computation and Simulation, <doi:10.1080/00949655.2022.2070621>, 2022.

wine

## See Also

mice,clusterMI, imputedata,knockoff,glmnet,imp.mix

## Examples

```
data(wine, package = "clusterMI")
require(parallel)
set.seed(123456)
ref <- wine$cult</pre>
nb.clust <- 3
wine.na <- wine</pre>
wine.na$cult <- NULL</pre>
wine.na <- prodna(wine.na)</pre>
nnodes <- 2 # parallel::detectCores()</pre>
B <- 150 # Number of iterations
m <- 5 \# Number of imputed data sets
# variable selection
res.varsel <- varselbest(data.na = wine.na,</pre>
                           nb.clust = nb.clust,
                           listvar = c("alco","malic"),
                           B = B,
                           nnodes = nnodes)
predictmat <- res.varsel$predictormatrix</pre>
# imputation
res.imp.select <- imputedata(data.na = wine.na, method = "FCS-homo",</pre>
                       nb.clust = nb.clust, predictmat = predictmat, m = m)
```

wine

Chemical analysis of wines from three different cultivars

## Description

Data are the results of a chemical analysis of wines grown in the same region in Italy but derived from three different cultivars. The analysis determined the quantities of 13 constituents found in each of the three types of wines

#### Usage

data(wine)

## Format

A data frame with 178 rows and 14 variables:

cult Cultivar
alco Alcohol
malic Malic acid
ash Ash
alca Alcalinity of ash
mg Magnesium
phe Total phenols
fla Flavanoids
nfla Nonflavanoid phenols
pro Proanthocyanins
col Color intensity
hue Hue
ratio OD280/OD315 of diluted wines
prol Proline

## Source

https://archive.ics.uci.edu/ml/datasets/wine

## References

M. Forina, C. Armanino, M. Castino and M. Ubigli. Vitis, 25:189-201 (1986)

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