

Clustering on incomplete data using *clusterMI*

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Clustering

Data $X_{n \times p} = (x_{ij})$ a mixed data set

Each individual i belongs to a unique cluster $C_i \in \{1, \dots, K\}$.

Aim identify C_i for each i using individual profiles $(x_i)_{1 \leq i \leq n}$

Methods

Distance-based

- k-means
- k-prototypes partitioning
- hierarchical clustering
- partitioning around medoids (pam)

Model-based

- gaussian mixture models
- latent class models
- model-based clustering of mixed-type data
- mixture of multivariate t -distributions

Clustering with missing values

However, X is frequently **incomplete**... $x_i = (x_i^{obs}, x_i^{miss})$

Ad-hoc methods

removing incomplete observations/variables

Advanced methods

Direct methods

- k-means (Wagstaff, 2004; Honda et al., 2011; Chi et al., 2016)
- gaussian mixture (Miao et al., 2016; Marbac et al., 2019; McCaw et al., 2022)
- k-prototypes (Aschenbruck et al., 2022)

Multiple Imputation (MI)

- a three-stage approach
- references: Faucheux et al. (2020); Bruckers et al. (2017); Basagana et al. (2013); Audigier and Niang (2022)
- could be used for any clustering method

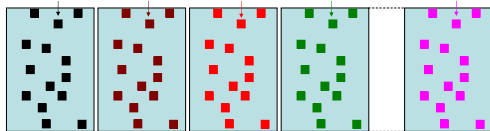
CRAN R packages

		<i>ClustImpute, kpodclustr</i>	<i>MGMM, mixture, MixtureMissing</i>	<i>RMixtComp, MixAll, VarSelLCM</i>	<i>miclust</i>	<i>clusterMI</i>
Clustering methods	kmeans	✓	✗	✗	✓	✓
	pam	✗	✗	✗	✗	✓
	hc	✗	✗	✗	✗	✓
	mixture	✗	✓	✓	✗	✓
Variable type	numeric	✓	✓	✓	✓	✓
	categorical	✗	✗	✓	✗	✓
	mixed	✗	✗	✓	✗	✓
Missing data	mcar	✓	✓	✓	✓	✓
	mar	✓	✓	✓	✓	✓
	mnar	✗	✗	✗	✗	✗
K	automatic ?	✗	✓	✓	✓	✓

Multiple imputation

- 1 Generate a set of M parameters $(\zeta_m)_{1 \leq m \leq M}$ of an **imputation model** to generate M plausible imputed data sets

$$P(X^{miss} | X^{obs}, \zeta_1) \quad \dots \quad P(X^{miss} | X^{obs}, \zeta_M)$$



- 2 Apply the **cluster analysis** to each imputed data set: Ψ_m, U_m
- 3 Combine the results to obtain one partition and one associated instability measure

Outline

① Introduction

② Clustering using *clusterMI*

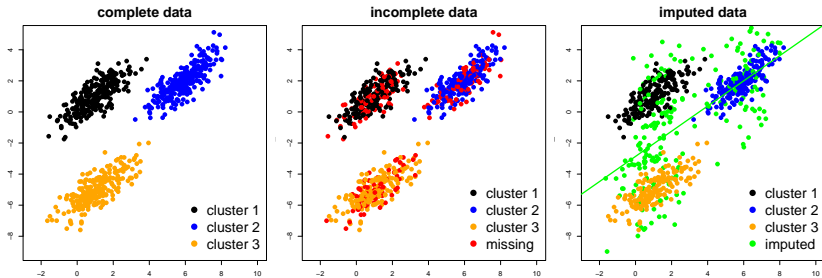
Imputation

Analysis

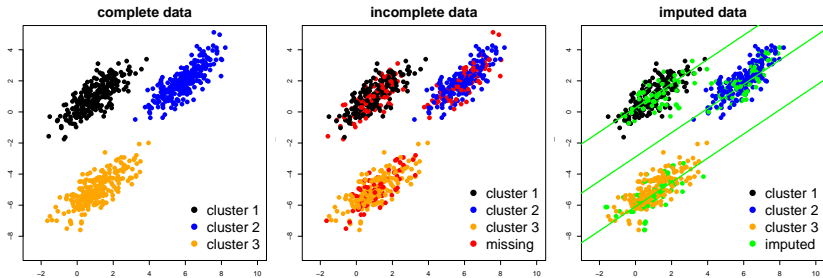
Pooling

③ Conclusion

Imputation model for clustering: the issue



Imputation model for clustering: the solution



Imputation methods in *clusterMI*

Joint Modelling

One joint distribution

- JM-DP (*DPimputeCont*, *NPBayesImputeCat*)
- JM-GL (*mix*)

Fully Conditional Specification

A conditional distribution for each variable

- FCS-homo: linear model including a fixed effect for the cluster
- FCS-hetero: linear mixed effect model (*micemd*)

Properties

	JM-DP	JM-GL	FCS-homo	FCS-hetero
fast	✓	✓	✗	✗
heteroscedasticity	✓	✗	✗	✓
flexibility	✗	✗	✓	✓

```
1 imputedata(data.na, method = "JM-GL", nb.clust = 3)
```

Flexibility of FCS methods

Conditional imputation models can be easily modified

- to address specific data
 - non-gaussian distributions (Morris et al., 2014)
 - mixed data
 - complex relationships (Doove et al., 2014)

```
1 imputedata(data.na, method = "FCS-homo", nb.clust = 3,  
2           method.mice = c("pmm", "logreg", "rf", ...))
```

- to improve sparsity
 - penalized regression (Zahid and Heumann, 2019)
 - variable selection (Bar-Hen and Audigier, 2022)

```
1 imputedata(data.na, method = "FCS-homo", nb.clust = 3,  
2           method.mice = "lasso.norm",  
3           predictmat = matrix(...))
```

Variable selection (Bar-Hen and Audigier, 2022)

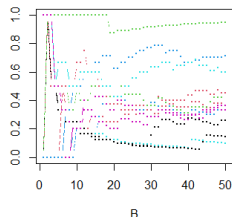
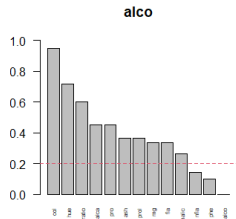
Tune a conditional imputation model for variable X_j

Repeat B times

- Sample k variables among $p - 1$
- Handle missing values by JM-GL
- Apply a selection procedure on the subset

Compute

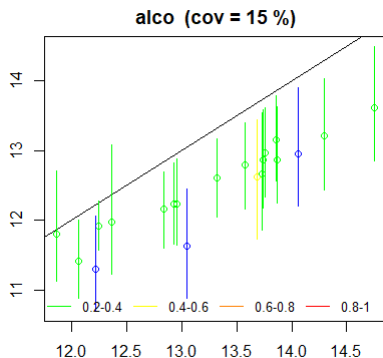
$$\frac{\text{\# times the variable } X_j \text{ is selected}}{\text{\# time } X_j \text{ is present in the instances}}$$



```
1 res.varsel <- varselbest(res.imputedata = res.imp.FCS,  
2                          listvar = "alco", nnodes = 20)  
3 predictmat <- res.varsel$predictormatrix  
4 res.chooser <- chooser(res.varsel = res.varsel)
```

Overimputation (Blackwell et al., 2015)

- 1 perform multiple imputation
- 2 remove several observed values for a given variable
- 3 build 90% intervals using the percentile method



```
1 res.imp.over <- imputedata(data.na,  
2                             nb.clust = 3,  
3                             m = 200)  
4 res.over <- overimpute(res.imp.over,  
5                         nnodes = 20,  
6                         plotvars = "alco",  
7                         plotinds = seq(nrow(data.na)))
```

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Imputation

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Analysis

Apply the **cluster analysis** to each imputed data set

- various pre-implemented methods from **fpc** kmeans, pam, clara, agnes or mixture, cmeans
- or any other method, e.g. reduced kmeans

Obtain $(\Psi_m)_{1 \leq m \leq M}$ and compute $(U_m)_{1 \leq m \leq M}$ (Fang and Wang, 2012)

- generate C bootstrap pairs $(X_c, \tilde{X}_c)_{1 \leq c \leq C}$ from X
- perform cluster analysis from $(X_c, \tilde{X}_c)_{1 \leq c \leq C}$ to obtain $(\Psi_c, \tilde{\Psi}_c)$
- classify individuals of X from Ψ_c and $\tilde{\Psi}_c$ to obtain $(\Psi'_c, \tilde{\Psi}'_c)$
- assess the instability $U = \frac{1}{C} \sum_{c=1}^C \frac{\delta(\Psi'_c, \tilde{\Psi}'_c)}{n^2}$

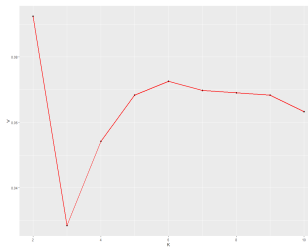


Figure: Instability (U) according to the number of clusters (K)

Pooling

Partitions pooling from $(\Psi_m)_{1 \leq m \leq M}$ using NMF

Principle

- $(\Gamma_m)_{1 \leq m \leq M}$ connectivity matrices associated to $(\Psi_m)_{1 \leq m \leq M}$

- $\bar{\Gamma} = \frac{1}{M} \sum_{m=1}^M \Gamma_m$

$$\operatorname{argmin}_{\Gamma \in \mathcal{G}} \|\Gamma - \bar{\Gamma}\|_F^2$$

Properties

- can be solved using various NMF algorithms
- monotone convergence
- no label switching problem, various choices for K_m are available

Instabilities pooling from $(U_m)_{1 \leq m \leq M}$

$$T = \frac{1}{M} \sum_{m=1}^M U_m + \frac{1}{M^2} \sum_{m=1}^M \sum_{m'=1}^M \delta(\Psi_m, \Psi_{m'}) / n^2$$

Pooling in *clusterMI*

Using the R function `clusterMI`

```
1 > res.pool <- clusterMI(res.imp,  
2                       method.clustering = "kmeans",  
3                       instability = TRUE  
4                       nnodes = nnodes)  
5 > names(res.pool)  
6 [1] "part"          "instability" "call"  
7 > names(res.pool$instability)  
8 [1] "U"          "Ubar" "B"          "Tot"
```

```
1 choosenbclust(res.pool, grid = 2:5)
```

Or at hand for applying any clustering method, e.g. reduced kmeans

```
1 library(clustrd)  
2 res.ana <- lapply(res.imp$res.imp,  
3                 FUN = cluspca,  
4                 nclus = 3, ndim = 2, method= "RKM")  
5 res.ana <- lapply(res.ana, "[[", "cluster")  
6 res.pool <- fastnmf(res.ana, nb.clust = 3)$cluster
```


Conclusion

An **R package** for clustering with missing values

- good **performances**
- flexible imputation methods
- a complete **vignette**

Specificities

- based on multiple imputation
- use dedicated imputation methods
- perform pooling using NMF
- compute instability measure to choose K

Perspectives

- parallel computing for FCS imputation
- add new clustering methods (dbscan, tclust, spectral clustering, ...)
- investigate imputation methods for MNAR mechanisms

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