Multiple imputation for clustering on incomplete data

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Clustering

Data $\mathbf{X} = (x_{ij})_{\substack{1 \leq i \leq n \\ 1 \leq j \leq p}}$ a continuous data set

Each individual i belongs to a unique cluster $\mathcal{C}_i \in \{1, ..., K\}$.

Aim identify $\mathcal{C}_i$ for each i based on individual profiles $(\mathbf{x}_i)_{1 \leq i \leq n}$

Methods

Distance-based

- k-means
- fuzzy C-means
- hierarchical clustering
- pam

Model-based

- gaussian mixture models
- mixture of multivariate t-distributions

Clustering with missing values

However, $\mathbf{X}$ is frequently **incomplete**... $\mathbf{x}_i = (\mathbf{x}_i^{obs}, \mathbf{x}_i^{miss})$

Ad-hoc methods

- removing incomplete observations
- removing incomplete variables
- single imputation

Direct methods

- k-means (Chi et al., 2016; Honda et al., 2011; Wagstaff, 2004)
- fuzzy C-means (Zhang et al., 2016; Hathaway and Bezdek, 2001)
- Gaussian mixture (Miao et al., 2016; Marbac et al., 2019; de Chaumaray and Marbac, 2020)

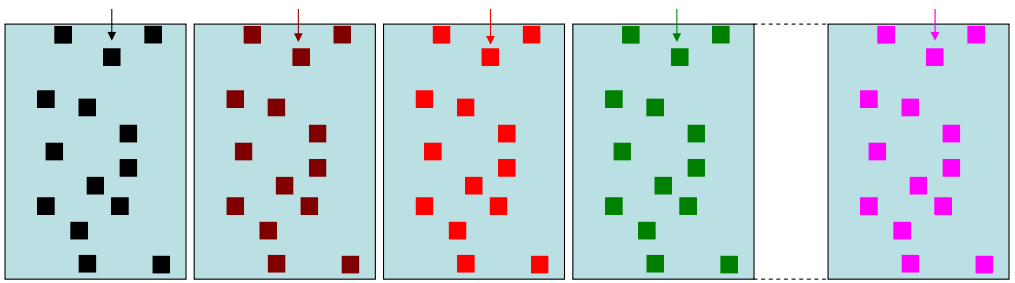
Multiple Imputation (MI)

- a popular method
- could be used for any clustering method

Multiple imputation (Rubin, 1987)

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

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



2. Apply the cluster analysis to each imputed data set: Ψ_m, V_m

3. Combine the results to obtain one partition Ψ and one associated instability measure V

Outline

Fully conditional specification

Two families of imputation models: JM and FCS

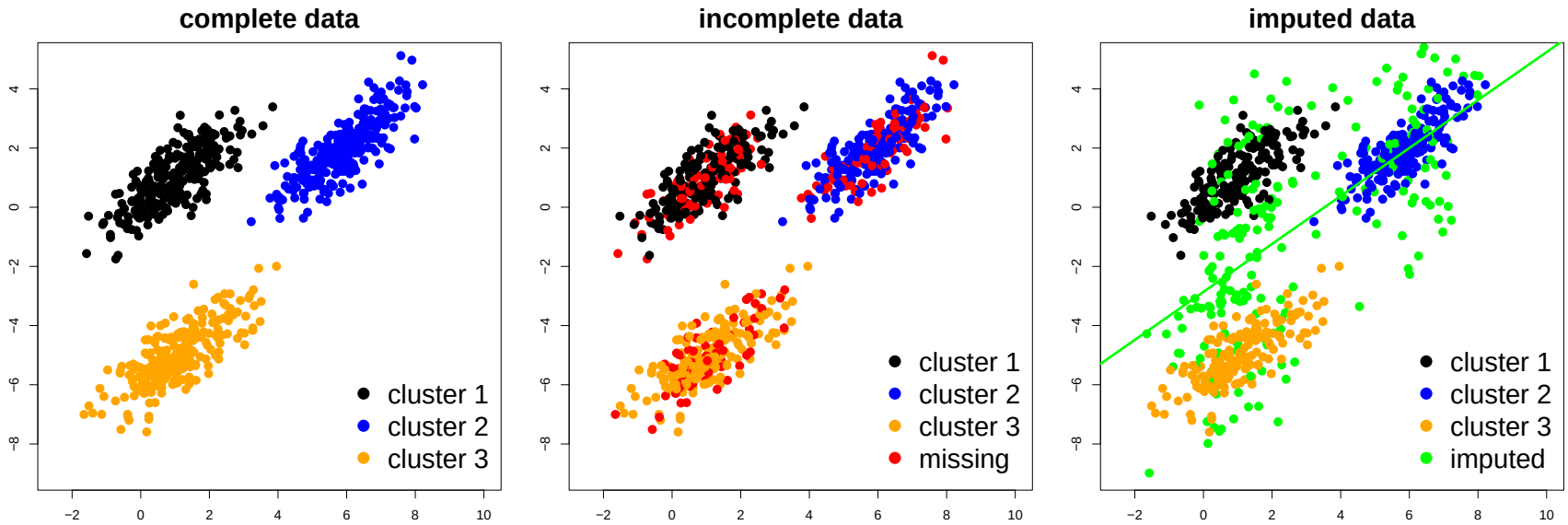
A conditional distribution is specified for each (incomplete) variable

Ex : $P\left(X_j|X_{-j};\zeta_j\right) = \mathcal{N}(X_{-j}\beta, \sigma^2) \quad \zeta_j = (\beta, \sigma)$

To impute the mth data set

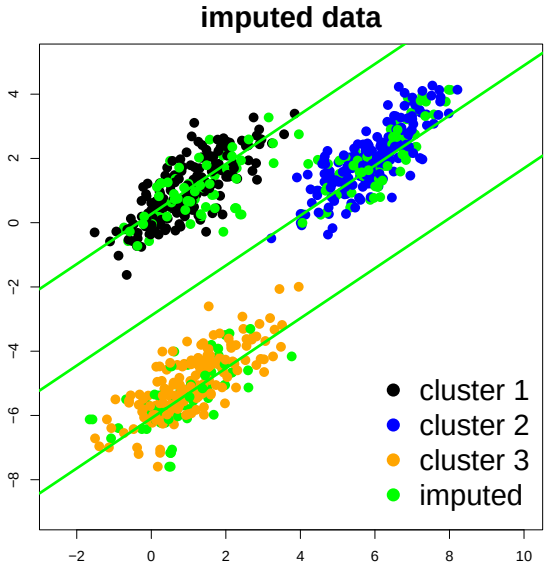
- initialize missing values of $\mathbf{X}$
- for j in 1 ... p
  a. generate ζ_j based on observed individuals on X_j
  b. impute X_j^{miss} according to $P\left(X_j|X_{-j};\zeta_j\right)$
- repeat until convergence

Imputation model for clustering: the issue



FCS-homo (Audigier et al., 2021)

Addressing the issue by using regression models including the class variable W as explanatory variable



FCS-homo

- generating X_j^{miss} given W is performed using regression models including a intercept specific to each cluster

$$P\left(X_j|X_{-j}, W; \zeta_j\right) = \mathcal{N}(X_{-j}\beta + \mu_w, \sigma^2) \qquad \zeta_j = (\beta, \sigma, \mu_w)$$

- generating W given X by linear discriminant analysis

$$P\left(W = w|X; \zeta_W\right) \propto exp(\delta_{w,x}) \qquad \zeta_W = (\boldsymbol{\pi}, \boldsymbol{\mu}, \Sigma)$$

Properties

FCS-homo

- addresses the cluster structure
- assumes homoscedastic regression models
- required a pre-defined number of clusters

Can be easily modified

- to account for heteroscedasticity (van Buuren, 2011)
- to improve sparsity (Zahid and Heumann, 2019)
- to address outliers (Templ et al., 2011)
- to use semi-parametric models (Morris et al., 2014)
- ...

Analysis

Apply the cluster analysis to each imputed data set: Ψ_m, V_m

$\Psi_m \rightarrow$ kmeans, GMM, ... for V_m Fang and Wang (2012) proposed:

- generate C bootstrap pairs $\left(\mathbf{X}_c, \tilde{\mathbf{X}}_c\right)_{1 \leq c \leq C}$ from $\mathbf{X}$
- perform cluster analysis from $\left(\mathbf{X}_c, \tilde{\mathbf{X}}_c\right)_{1 \leq c \leq C}$ to obtain $\left(\Psi_c, \tilde{\Psi}_c\right)$
- classify individuals of $\mathbf{X}$ from Ψ_c and $\tilde{\Psi}_c$ to obtain $\left(\Psi'_c, \tilde{\Psi}'_c\right)$
- the instability V is assessed by averaging the proportions of disagreements

$$V = \frac{1}{C} \sum_{c=1}^{C} \delta(\Psi'_c, \tilde{\Psi}'_c)/n^2$$

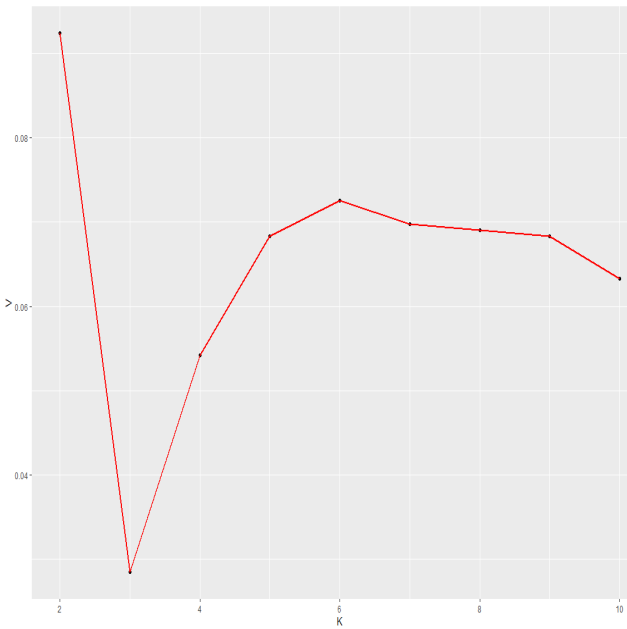


Figure: Instability (V) according to the number of clusters (K)

Pooling

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

Faucheux et al. (2020); Bruckers et al. (2017); Basagana et al. (2013); Audigier and Niang (2022) proposed consensus clustering methods

Theoretically, NMF based methods are appealing

- $(\mathbf{U}_m)_{1\leq m\leq M}$ connectivity matrices associated to $(\Psi_m)_{1\leq m\leq M}$
- $\bar{\mathbf{U}} = \frac{1}{M}\sum_{m=1}^{M}\mathbf{U}_m$

$$\underset{\mathbf{U}\in\mathcal{U}}{argmin} \parallel \mathbf{U} - \bar{\mathbf{U}} \parallel_F^2$$

The solution of this optimization problem can be obtained using NMF (Li et al., 2007).

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

Audigier and Niang (2022) proposed

$$V = \frac{1}{M}\sum_{m=1}^{M} V_m + \frac{1}{M^2}\sum_{m=1}^{M}\sum_{m'=1}^{M}\delta\left(\Psi_m, \Psi_{m'}\right)/n^2$$

Outline

Real data sets

Data

			Variables				Size of cluster	
	n	p	Type	Number for which Shapiro rejects normality	K	Silhouette Index	(min)	(max)
wine	178	13	Real	7	3	0.57	48	71
ovarian	216	100	Real	64	2	0.50	95	121
iris	150	4	Real	1	3	0.52	50	50
glass	214	9	Real	9	2	0.56	51	163
breast cancer	699	9	Discrete	9	2	0.59	241	458

- Gaussian assumption seems not observed
- p large
- n_k small compared to p
- partitions not obvious

Simulation design

Data sets generation

- 25% missing values (MCAR or a MAR mechanism)
- 200 missing data patterns per mechanism

Data sets analysis

- missing values are addressed by MI (FCS-homo, $M = 20$)
- cluster analysis by k-means, fuzzy c-means or GMM
- pooling using NMF

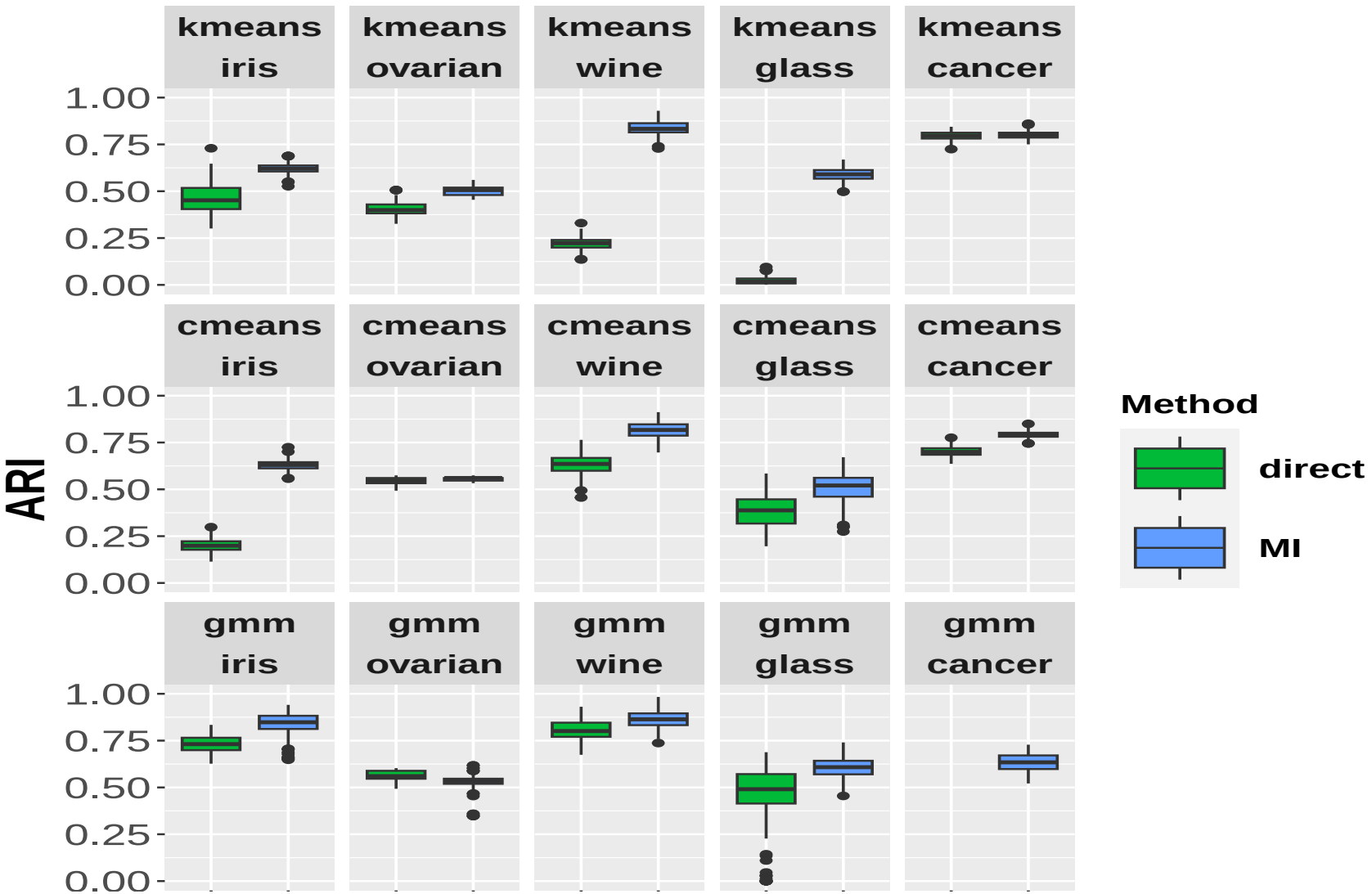
Evaluation

Competitive direct methods

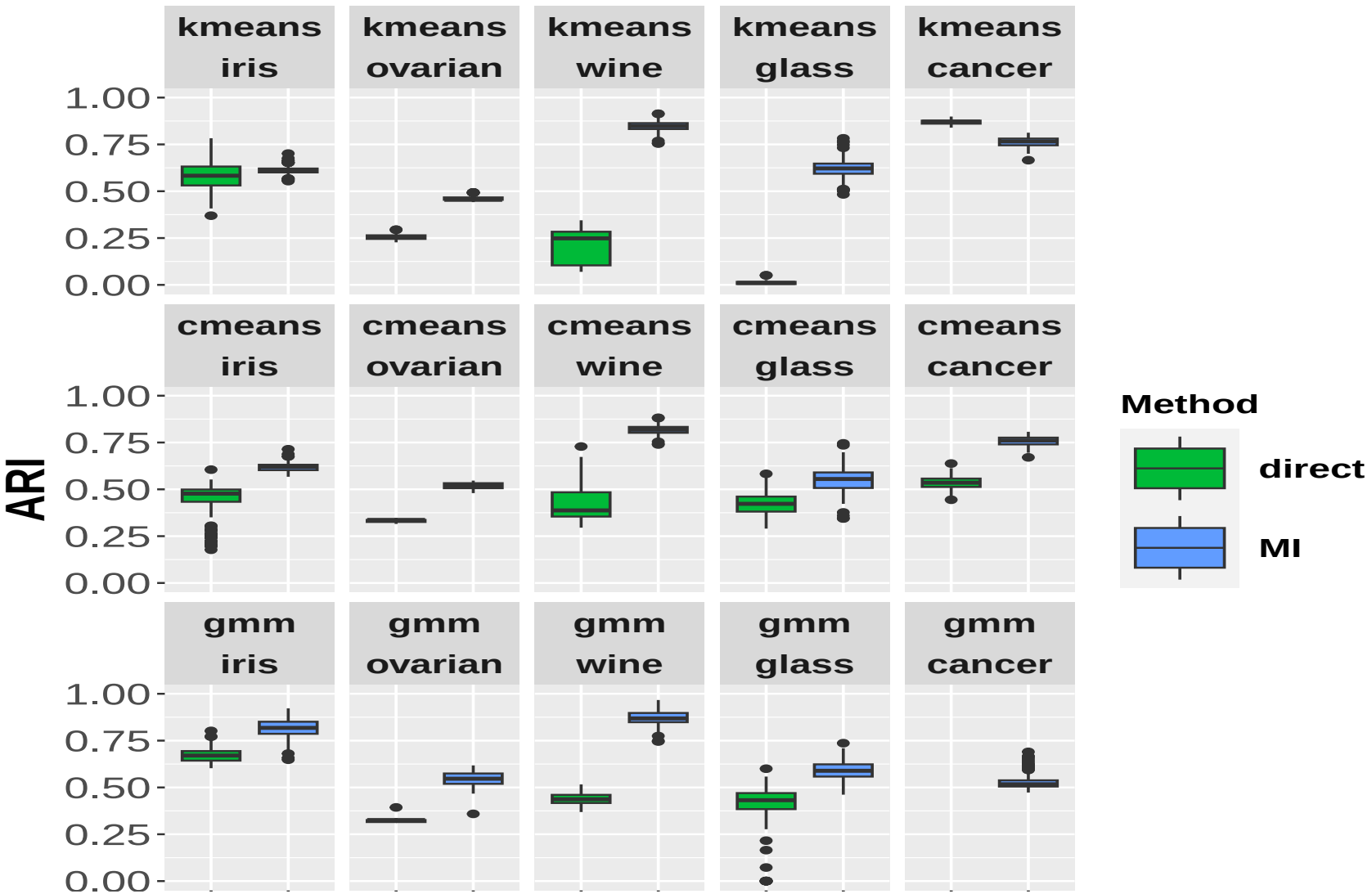
- k-POD (Chi et al., 2016) from the *kpodclustr* R package
- FCM by optimal completion strategy (Hathaway and Bezdek, 2001)
- Ignorable-GMM (Marbac et al., 2019) from the *VarSelLCM* R package

Criteria: Adjusted Rand Index

Real data, MCAR



Real data, MAR



Summary

Based on **real datasets**

- MI generally outperforms direct methods for kmeans and fuzzy cmeans and GMM
- Observed under MCAR and MAR mechanisms

Based on **simulated data** under mixture model distribution

- MI outperforms direct methods for kmeans and fuzzy c means
- MI and direct methods provide similar ARI for GMM
- Differences between MI and direct method highlighted for kmeans with more separated clusters
- Similar results by modifying the number of clusters, the cluster size, the balance between clusters sizes and the heteroscedasticity

Conclusion

This study shows

- MI is a **competitive method** for addressing missing values in clustering (for model-based or distance-based methods)
- Good performances on **real data**

In practice

- The number of clusters can be easily estimated
- MI method is available in the clusterMI R package

Some perspectives

- Addressing mixed data
- Developing indices for clustering with missing values

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