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Dealing with missing data in model-based clustering through a MNAR model

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Final CRoNoS meeting and Workshop on Multivariate Data Analysis and Software
14-16 April 2019, Limassol, Cyprus



Take home message

- 1 The missing data **pattern** may convey some information on clustering
- 2 **Embed the missingness mechanism** directly within the clustering modeling step

Outline

- 1 Introduction
- 2 A model-based MNAR clustering approach
- 3 Inference procedures
- 4 Medical study illustration
- 5 Concluding remarks

Missing data: an inevitable event

The larger the datasets, the more missing data may appear. . .

Two traditional solutions (for obtaining a filled dataset)

- **Discard** individuals with missing data: expect to add **variance** into analysis
- **Impute** missing data: expect to add **bias** modeling into analysis

General guidelines

- Obtaining a non-missing dataset is **not** the final goal
- Missing data management should **take into account the initial analysis target**

Our analysis target: **model-based clustering**

Embed missing data management into this paradigm. . .

Missing data: notations

- $\mathbf{y} = \{\mathbf{y}_1, \dots, \mathbf{y}_n\}$: full dataset with n individuals
- $\mathbf{y}_i = (y_i^1, \dots, y_i^d) \in \mathbb{R}^d$: full individual $i \in \{1, \dots, n\}$
- $\mathbf{c} = \{\mathbf{c}_1, \dots, \mathbf{c}_n\}$: pattern of missing data for the full dataset
- $\mathbf{c}_i = (c_i^1, \dots, c_i^d) \in \{0, 1\}^d$: pattern of missing data for individual $i \in \{1, \dots, n\}$

$$c_i^j = 1 \Leftrightarrow y_i^j \text{ is missing}$$

- $o_i = \{j : c_i^j = 0\}$: the observed variables indexes for individual i
- $\mathbf{y}_i^{o_i}$: the observed variables values for individual i
- $\mathbf{y}^o = \{\mathbf{y}_1^{o_1}, \dots, \mathbf{y}_n^{o_n}\}$: the observed values in \mathbf{y}
- $m_i = \{j : c_i^j = 1\}$: the missing variables indexes for individual i
- $\mathbf{y}_i^{m_i}$: the missing variables values for individual i
- $\mathbf{y}^m = \{\mathbf{y}_1^{m_1}, \dots, \mathbf{y}_n^{m_n}\}$: the missing values in \mathbf{y}

$\mathbf{y} = \{\mathbf{y}^o, \mathbf{y}^m\}$ is the full dataset with its observed and missing parts

Missing data: typology of the missing mechanisms

- Missing completely at random (**MCAR**):

$$P(\mathbf{c}|\mathbf{y}; \psi) = P(\mathbf{c}; \psi) \quad \forall \mathbf{y}$$

- Missing at random (**MAR**):

$$P(\mathbf{c}|\mathbf{y}; \psi) = P(\mathbf{c}|\mathbf{y}^o; \psi) \quad \forall \mathbf{y}^m$$

- Missing not at random (**MNAR**): the mechanism is not MCAR nor MAR

Clustering: model-based approach

- **Partition with K clusters:** $\mathbf{z} = (\mathbf{z}_1, \dots, \mathbf{z}_n)$ where
 - $\mathbf{z}_i = (z_i^1, \dots, z_i^K) \in \{0, 1\}^K$
 - $z_i^k = 1$ if \mathbf{y}_i belongs to cluster k , $z_i^k = 0$ otherwise
- **Gaussian mixture:** $\mathbf{y}_1, \dots, \mathbf{y}_n$ are i.i.d. from the mixture

$$f(\mathbf{y}_i; \boldsymbol{\theta}) = \sum_{k=1}^K \pi_k \phi_k(\mathbf{y}_i; \boldsymbol{\theta}_k)$$

where:

- $\pi_k = P(z_i^k = 1)$
- $\phi_k(\cdot; \boldsymbol{\theta}_k)$: d -variate Gaussian pdf with mean vector and covariance matrix
 $\boldsymbol{\theta}_k = (\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$, d -multinomial pdf with $\boldsymbol{\theta}_k = p_k$ probabilities vector or mixed pdf.
- $\boldsymbol{\theta} = (\pi_1, \dots, \pi_K, \boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_K)$

Question we address in this work

Which distribution $P(\mathbf{c}|\mathbf{y}, \mathbf{z}; \boldsymbol{\psi})$ to propose in this clustering context?

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Logistic model: a natural and flexible candidate

$$P(\mathbf{c}|\mathbf{y}, \mathbf{z}; \boldsymbol{\psi}) = \prod_{i=1}^n \prod_{j=1}^d P(c_i^j | \mathbf{y}, \mathbf{z}; \boldsymbol{\psi})$$

- **MCAR**, with $\boldsymbol{\psi} = \alpha_0$

$$\text{logit}(P(c_i^j = 1 | \mathbf{y}, \mathbf{z}; \boldsymbol{\psi})) = \alpha_0$$

- **MNARz** (**MNARz^j**), with $\boldsymbol{\psi} = (\alpha_0, \beta_1^{1\dots d}, \dots, \beta_K^{1\dots d})$

$$\text{logit}(P(c_i^j = 1 | \mathbf{y}, \mathbf{z}; \boldsymbol{\psi})) = \alpha_0 + \sum_{k=1}^K \beta_k^j z_i^k$$

- **MNARY**, with $\boldsymbol{\psi} = (\alpha_0, \alpha_1, \dots, \alpha_d)$

$$\text{logit}(P(c_i^j = 1 | \mathbf{y}, \mathbf{z}; \boldsymbol{\psi})) = \alpha_0 + \alpha_j y_i^j$$

- **MNARYz**, with $\boldsymbol{\psi} = (\alpha_0, \alpha_1, \dots, \alpha_d, \beta_1, \dots, \beta_K)$

$$\text{logit}(P(c_i^j = 1 | \mathbf{y}, \mathbf{z}; \boldsymbol{\psi})) = \alpha_0 + \alpha_j y_i^j + \sum_{k=1}^K \beta_k z_i^k$$

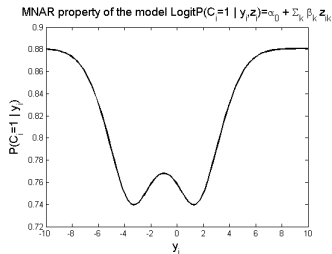
MNARz analysis: it depends on \mathbf{y} through \mathbf{z} !

$$P(c_i^j = 1 | \mathbf{y}; \boldsymbol{\theta}, \boldsymbol{\psi}) = \sum_{k=1}^K P(c_i^j = 1 | \mathbf{y}, \mathbf{z}; \boldsymbol{\psi}) P(\mathbf{z} | \mathbf{y}; \boldsymbol{\theta})$$

Example of a univariate Gaussian model with the three components

$$0.2N(\cdot; 0, 1) + 0.3N(\cdot; 1, 2) + 0.5N(\cdot; 2, 3)$$

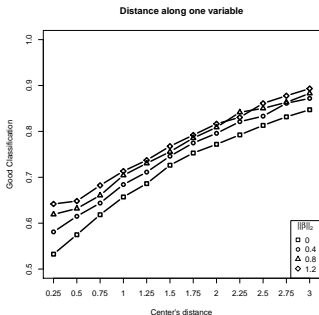
and with parameters of the logit expression: $\alpha_0 = 1, \beta_1 = 1, \beta_2 = -1, \beta_3 = 1$



MNARz analysis: pattern \mathbf{c} gives information on partition \mathbf{z} !

Draw Bayes error of a MNARz model with two components and 20% of missing data

$$\pi_k = 0.5, \|\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1\| \text{ varies}, \boldsymbol{\Sigma}_1 = \boldsymbol{\Sigma}_2 = \mathbf{I}, |\beta_2 - \beta_1| \text{ varies}$$



Both $\boldsymbol{\mu}_k$ and β_k act on the Bayes error

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Ignorable vs. non ignorable model

A missing mechanism is ignorable if likelihoods can be decomposed as

$$L(\boldsymbol{\theta}, \boldsymbol{\psi}; \underbrace{\mathbf{y}^o, \mathbf{c}}_{\text{observed data}}) = L(\boldsymbol{\psi}; \mathbf{c} | \mathbf{y}^o) \times L(\boldsymbol{\theta}; \mathbf{y}^o)$$

Some simple algebra show that this occurs when missing mechanism is not MNAR

Inference of $\boldsymbol{\theta}$

“If the missing mechanism is **ignorable** then likelihood-based inferences for $\boldsymbol{\theta}$ from $L(\boldsymbol{\theta}; \mathbf{y}^o)$ will be the same as likelihood based inference for $\boldsymbol{\theta}$ from $L(\boldsymbol{\theta}, \boldsymbol{\psi}; \mathbf{y}^o, \mathbf{c})$.”
([Little and Rubin, 2002] Section 6.2)

- MCAR is ignorable
- MNAR_z, MNAR_y and MNAR_{yz} are non ignorable

EM algorithm: looks simple

Decomposition of $Q(\theta, \psi; \hat{\theta}, \hat{\psi})$

The expected complete log-likelihood conditional related to observed data is:

$$E \left[L(\theta, \psi; \mathbf{c}, \mathbf{y}, \mathbf{z}); \hat{\theta}, \hat{\psi} | \mathbf{y}^o, \mathbf{c} \right] = Q_Y(\theta; \hat{\theta}, \hat{\psi}) + Q_C(\psi; \hat{\theta}, \hat{\psi})$$

$$Q_Y(\theta; \hat{\theta}, \hat{\psi}) = \sum_{i=1}^n \sum_{k=1}^K \tau_i^k E \left[\log(\pi_k \phi_k(\mathbf{y}_i; \theta_k)) | \mathbf{y}_i^{oi}, \mathbf{c}_i; \hat{\theta}, \hat{\psi} \right]$$

$$Q_C(\psi; \hat{\theta}, \hat{\psi}) = \sum_{i=1}^n \sum_{k=1}^K \tau_i^k E \left[\log(P(\mathbf{c}_i | z_i^k = 1, \mathbf{y}_i; \theta, \psi)) | \mathbf{y}_i^{oi}, \mathbf{c}_i; \hat{\theta}, \hat{\psi} \right]$$

$$\tau_i^k = P(z_i^k = 1 | \mathbf{c}_i, \mathbf{y}_i^{oi}; \hat{\theta}, \hat{\psi}) = \frac{\hat{\pi}_k \phi_k(\mathbf{y}_i^{oi}; \theta_k^{oi}) P(\mathbf{c}_i | z_i^k = 1, \mathbf{y}_i^{oi}; \hat{\psi})}{\sum_{h=1}^K \hat{\pi}_h \phi_h(\mathbf{y}_i^{oi}) P(\mathbf{c}_i | z_i^h = 1, \mathbf{y}_i^{oi}; \hat{\psi})}$$

EM and/or SEM algorithms

- **MCAR** (and also **MAR**...): classical formula! (EM , SEM)

$$\tau_i^k \propto \hat{\pi}_k \phi_k(\mathbf{y}_i^{oi}; \theta_k^{oi})$$

- **MNARz**: needs some new calculus but still simple (EM , SEM)

$$\tau_i^k \propto \hat{\pi}_k \phi_k(\mathbf{y}_i^{oi}; \theta_k^{oi}) \prod_{j=1}^d (1 + \exp(-r_i^j \hat{\beta}_k))^{-1} \text{ where } r_i^j = \begin{cases} 1 & \text{if } c_i^j = 1 \\ -1 & \text{otherwise} \end{cases}$$

- **MNARy**: needs approximations (EM , SEM)

$$P(c_i^j | \mathbf{y}_i^{oi}, z_i^k = 1; \boldsymbol{\psi}) = \begin{cases} \int_{-\infty}^{+\infty} \frac{1}{1 + \exp(-(\alpha_j y_i^j))} \phi_k(y_i^j; \theta_k^j) dy_i^j & \text{if } c_i^j = 1 \\ \frac{1}{1 + \exp(\alpha_j y_i^j)} & \text{otherwise} \end{cases}$$

- In the Gaussian case, there is **no closed form** [Pirjol, 2013] (same for MNARyz)
- But **SEM is still simple** in that case thanks to random drawing instead of expectation

Link with some usual procedures!

Concatenation [Jones, 1996]: model equivalence

$$\text{MNARz}^j(\mathbf{y}^o, \mathbf{c}) \iff \text{MCAR}(\mathbf{y}^o | \mathbf{c})$$

$$\text{MNARz}(\mathbf{y}^o, \mathbf{c}) \iff \text{MCAR} \left(\mathbf{y}^o \mid \left(\sum_{j=1}^d \mathbf{c}^j \right) \right)$$

“All Available Cases” [Little and Rubin, 2002]: estimation equivalence

In case of **conditional independence** between variables, whatever MCAR or MNAR*:

$$\text{Classical (S)EM} \iff \text{(S)EM without estimating missing } \mathbf{y}^m$$

... an opportunity to reduce the computing time

What about model selection?

Can select between MCAR and MNAR* with any information criterion (BIC, ICL)

Even if the missing mechanism is ignorable for MCAR...

... need to model c to compare a MCAR and a MNAR model

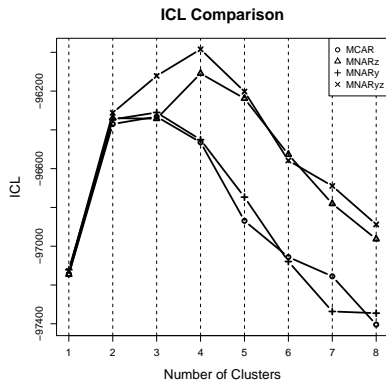
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Hospital Data

- Number of patients: $n = 5\,146$
- Number of features: $d = 7$
 - Age
 - Size
 - Weight
 - Cardiac frequency
 - Hemoglobin concentration
 - Temperature
 - Minimum Diastolic and Systolic Blood Pressure
- Percentage of missing data: 6.4%

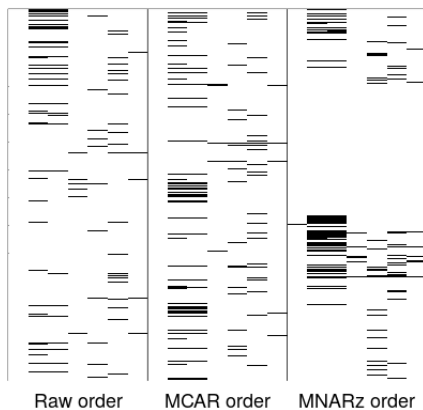
ICL comparison



- MCAR, MNARy and MNARz are equivalent until $K = 3$
- MNARz and MNARyz clearly indicate presence of an additional cluster ($K = 4$)

It seems to be an illustration of the effect of c through MNARz and MNARyz

Missing Pattern



It seems that MNARz modelling leads to a missing free cluster

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Summary

- Interest to put a model on c
- Interest of the simple but meaningful model MNAR z
- Link between our models and usual methods

Ongoing works

- Deeper analysis of the previous results with doctors. . .
- Implement the proposed models/algo. in the Mixmod software^a
- Use **mixed data** algorithms for medical study with **the same MNAR* models**

^a<http://www.mixmod.org>

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