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

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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

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

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

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

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

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

Missing data: typology of the missing mechanisms

- Missing completely at random (MCAR):

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

- Missing at random (MAR):

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

- 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

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

where:

- $\pi_k = P(z_i^k = 1)$
- $\phi_k(.; \theta_k)$: d-variate Gaussian pdf with mean vector and covariance matrix $\theta_k = (\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$, d-multinomial pdf with $\theta_k = p_k$ probabilities vector or mixed pdf.
- $\boldsymbol{\theta} = (\pi_1, \dots, \pi_K, \theta_1, \dots, \theta_K)$

Question we address in this work

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

Outline

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 $\boldsymbol{\psi} = \alpha_0$

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

- MNAR**z** (MNAR**z**^{j}), with $\boldsymbol{\psi} = (\alpha_0, \beta_1^{1...d}, \ldots, \beta_K^{1...d})$

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

- MNAR**y**, with $\boldsymbol{\psi} = (\alpha_0, \alpha_1, \ldots, \alpha_d)$

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

- MNAR**yz**, with $\boldsymbol{\psi} = (\alpha_0, \alpha_1, \ldots, \alpha_d, \beta_1, \ldots, \beta_K)$

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

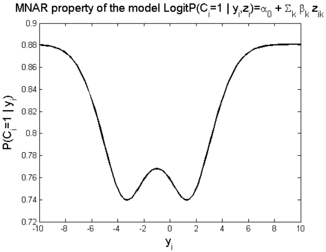
MNAR**z** analysis: it depends on **y** through **z**!

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

Example of a univariate Gaussian model with the three components

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

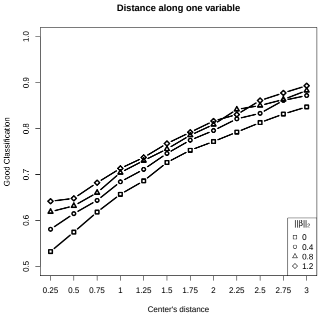
and with parameters of the logit expression: $\alpha_0 = 1, \beta_1 = 1, \beta_2 = -1, \beta_3 = 1$



MNAR**z** analysis: pattern **c** gives information on partition **z**!

Draw Bayes error of a MNAR**z** 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

Outline

Ignorable *vs.* non ignorable model

A missing mechanism is ignorable if likelihoods can be decomposed as

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

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 $L(\boldsymbol{\theta}, \psi; \mathbf{y}^o, \mathbf{c})$." ([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 $Q(\boldsymbol{\theta}, \boldsymbol{\psi}; \widehat{\boldsymbol{\theta}}, \widehat{\boldsymbol{\psi}})$

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

$$E\left[L(\boldsymbol{\theta}, \boldsymbol{\psi}; \mathbf{c}, \mathbf{y}, \mathbf{z}); \widehat{\boldsymbol{\theta}}, \widehat{\boldsymbol{\psi}} | \mathbf{y}^o, \mathbf{c}\right] = Q_y(\boldsymbol{\theta}; \widehat{\boldsymbol{\theta}}, \widehat{\boldsymbol{\psi}}) + Q_c(\boldsymbol{\psi}; \widehat{\boldsymbol{\theta}}, \widehat{\boldsymbol{\psi}})$$

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

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

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

EM and/or SEM algorithms

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

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

- MNAR**z**: needs some new calculus but still simple .... (EM , SEM)

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

- MNAR**y**: needs approximations .... (~~EM~~ , SEM)

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

  - In the Gaussian case, there is **no closed form** [Pirjol, 2013] (same for MNAR**yz**)
  - 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

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

$$\text{MNARz}(\mathbf{y}^o, \mathbf{c}) \iff \text{MCAR}\left(\quad \left(\mathbf{y}^o \middle| \left(\sum_{j=1}^{d} \mathbf{c}_{\cdot}^{j}\right)\right) \quad \right)$$

"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. . .

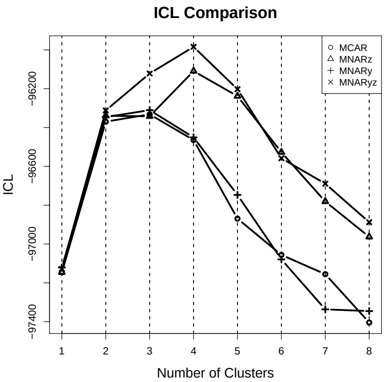
. . . need to model **c** to compare a MCAR and a MNAR model

Outline

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%

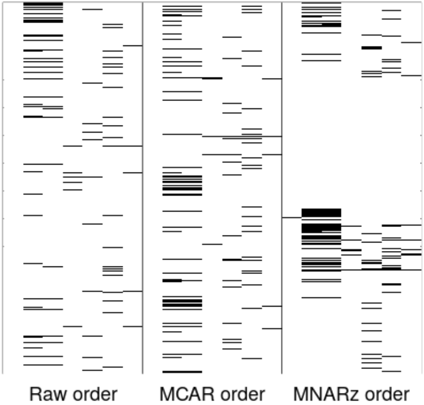
ICL comparison



- MCAR, MNAR**y** and MNAR**z** are equivalent until $K = 3$
- MNAR**z** and MNAR**yz** clearly indicate presence of an additional cluster ($K = 4$)

It seems to be an illustation of the effect of **c** through MNAR**z** and MNAR**yz**

Missing Pattern



It seems that MNARz modelling leads to a missing free cluster

Outline

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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