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Impact of missing data on mixtures and clustering with illustrations in Biology and Medicine

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Impact of missing data on mixtures and clustering with illustrations in Biology and Medicine

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Bucharest, April 21-22, 2023

Take home message

Missing data may change preconceptions

- **Mixtures**: EM has unexpected behaviour concerning degeneracy dynamic
- **Clustering**: the missing data pattern may convey some information on partition

These topics are in the research agenda of Statisticians since:

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

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Outline

1 Introduction

2 Impact of MAR data on the EM algorithm

- Gaussian mixture degeneracy *without* missing data
- Gaussian mixture degeneracy *with* missing data

3 Impact of MAR data on clustering

- A model-based MAR approach
- Biology study illustration

4 Impact of MNAR data on clustering

- A model-based MNAR clustering approach
- Medical study illustration

5 Concluding remarks

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Missing data: notations

- $y = \{y_1 | \dots | y_n\}^T$: **full dataset** with n individuals
- $y_i = (y_{i1}, \dots, y_{id}) \in \mathcal{Y} = \mathbb{R}^d$ with individual $i \in \{1, \dots, n\}$
- $c = \{c_1 | \dots | c_n\}^T \in \{0, 1\}^{n \times d}$: **pattern of missing data** for the full dataset
- $c_i = (c_{i1}, \dots, c_{id}) \in \{0, 1\}^d$: pattern of missing data for individual $i \in \{1, \dots, n\}$

$$c_{ij} = 1 \Leftrightarrow y_{ij} \text{ is missing}$$

- y_i^{obs} : the observed variables values for indiv. i (and $y^{\text{obs}} = \{y_1^{\text{obs}} | \dots | y_n^{\text{obs}}\}^T$)
- y_i^{mis} : the missing variables values for individual i (and $y^{\text{mis}} = \{y_1^{\text{mis}} | \dots | y_n^{\text{mis}}\}^T$)



Typology of the missingness mechanisms

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

$$p(c|y; \psi) = p(c; \psi) \quad \forall y$$

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

$$p(c|y; \psi) = p(c|y^{\text{obs}}; \psi) \quad \forall y^{\text{mis}}$$

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

Ignorable vs. non ignorable model

A missing mechanism is ignorable if likelihoods can be decomposed as

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

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

Inference of θ

“If the missing mechanism is **ignorable** then likelihood-based inferences for θ from $L(\theta; y^{\text{obs}})$ will be the same as likelihood based inference for θ from $L(\theta, \psi; y^{\text{obs}}, c)$.”

[Little and Rubin, 2002 Section 6.2]

- M(C)AR is ignorable
- MNAR is not ignorable

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Mixture model and clustering (Gaussian case)

- **Partition (K clusters):** $z = (z_1 | \dots | z_n)^T \in \{0, 1\}^{n \times K}$ where
 - $z_i = (z_{i1}, \dots, z_{iK}) \in \{0, 1\}^K$
 - $z_{ik} = 1$ if y_i belongs to cluster k , $z_{ik} = 0$ otherwise
- **Mixture model:** y_1, \dots, y_n are i.i.d. from the d -variate Gaussian mixture

$$f(y_i; \theta) = \sum_{k=1}^K \pi_k f_k(y_i; \alpha_k)$$

- $\pi_k = \mathbb{P}(z_{ik} = 1)$
- $f_k(\cdot; \alpha_k) = \phi(\cdot; \mu_k, \Sigma_k)$ is the d -variate **Gaussian distribution** with mean vector μ_k and covariance matrix Σ_k
- $\theta = (\pi_1, \dots, \pi_K, \alpha_1, \dots, \alpha_K)$ is the whole mixture parameter
- **Clustering:** MAP principle from the mixture output to estimate the partition

And also: algorithm estimation (EM, SEM...) and model selection (BIC, ICL...)

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Degeneracy genesis: unbounded likelihood

- d -variate Gaussian mixture

$$f(y_i; \theta) = \sum_{k=1}^K \pi_k \underbrace{\frac{1}{(2\pi)^{d/2} |\Sigma_k|^{1/2}} \exp\left(-\frac{1}{2}(y_i - \mu_k)^T \Sigma_k^{-1} (y_i - \mu_k)\right)}_{\phi(y_i; \mu_k, \Sigma_k)}$$

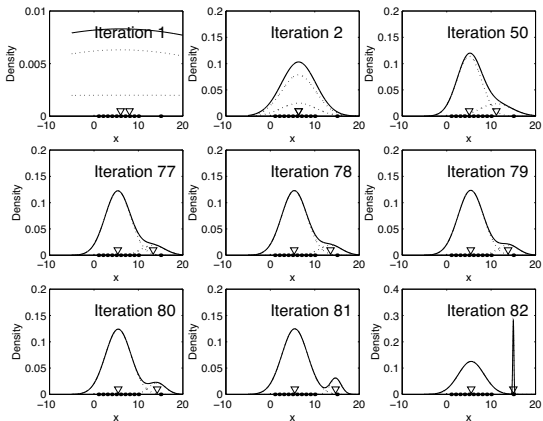
- Sampling: $y_1, \dots, y_n \stackrel{i.i.d.}{\sim} p(\cdot; \theta)$ without any missing data ($y^{\text{obs}} = y$)
- Likelihood: $\ell(\theta; y) = \ln L(\theta; y) = \sum_{i=1}^n \ln f(y_i; \theta)$

$$\text{particular center } \mu_2 = y_i \quad \Rightarrow \quad \lim_{|\Sigma_2| \rightarrow 0} \ell(\theta; y) = +\infty$$

[Kiefer and Wolfowitz, 1956] [Day, 1969]

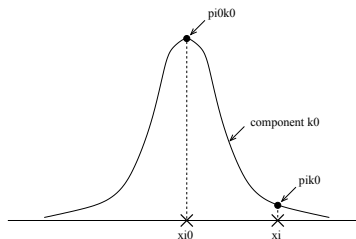


EM behaviour: illustration



- degeneracy may occur even when starting from large variances
- convergence can be slow when far from the degenerate limit
- convergence extremely fast near degeneracy

EM behaviour: results



$$u_0 = \left[\frac{1}{p_{i_0 k_0}}, \{p_{ik_0}\}_{i \neq i_0} \right]$$

degeneracy of component k_0 at y_{i_0}

\Leftrightarrow

$$\|u_0\| \rightarrow 0$$

[Biernacki and Chrétien, 2003]

[Ingrassia and Rocci, 2009]

Proposition 1: Existence of a basin of attraction

$\exists \epsilon > 0$ s.t. if $\|u_0\| \leq \epsilon$ then $\|u_0^+\| = o(\|u_0\|)$ with probability 1.

Proposition 2: Speed towards degeneracy is exponential

$\exists \epsilon > 0, \alpha > 0$ and $\beta > 0$ s.t. if $\|u_0\| \leq \epsilon$ then, with probability 1,

$$|\Sigma_{k_0}^+| \leq \alpha / |\Sigma_{k_0}| \cdot \exp(-\beta / |\Sigma_{k_0}|).$$

Outline

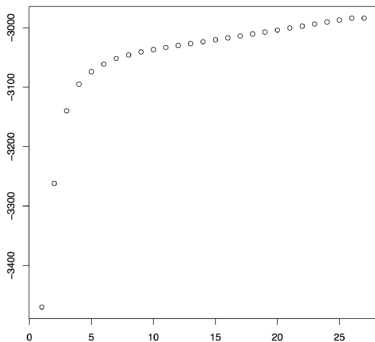
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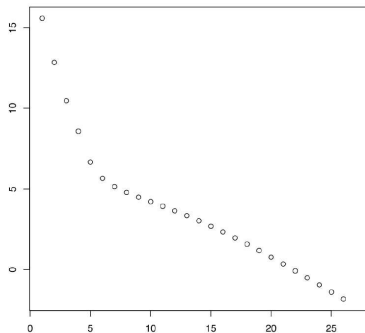
EM behaviour illustration

- Breast cancer tissue of the UCI database repository: 106 units, 9 variables.
- 10% of missing data randomly generated
- $K = 4$ clusters

Log-likelihood according to the number of iterations



Decrease of the log-determinant of the degenerated component





Detail from the illustration

	1	2	3	4	5	6	7	8	9
1	211.00		0.09	30.75	151.98	4.94	14.27	27.24	217.13
2	196.86	0.02	0.09	28.59	82.06	2.87	7.97	27.66	200.75
3	144.00	0.12	0.05	19.65	70.43	3.58		7.57	160.37
4	172.52	0.13	0.04		192.22	5.12	19.32	32.19	174.93
5	121.00	0.17	0.09	24.44	144.47	5.91	22.02	10.59	141.77
6	223.00	0.12	0.08	33.10	197.01	5.95	30.45	12.96	252.48
7		0.17	0.23	34.22	94.35	2.76	31.28	13.88	180.61
8	303.00	0.06	0.04	22.57		4.54	21.83	5.72	321.65
9	250.00	0.09	0.09	29.64	180.76	6.10	26.14	13.96	280.12
10	391.00	0.06	0.01	35.78		7.41	22.13	28.11	400.99
11	176.00	0.09	0.08	20.59	79.71		18.23	9.58	191.99
12	145.00		0.11	21.22	82.46	3.89	20.30	6.17	162.51
13	124.13	0.13	0.11	20.59			18.46	9.12	134.89
14	103.00	0.16	0.29	23.75	78.26	3.29	22.32	8.12	124.98

Table : Data belonging to the degenerated component.

- Cvg. towards a degenerated component (no plateau of the log-likelihood)
- Degeneracy relatively slow: log-likelihood linear according to the nb of it.
- Number of points of the degenerated solution greater than the space dimension d (but the number of complete points lower than d)



Intermediate conclusion on missing data

Like the complete data y case

- Likelihood is unbounded
- EM can be attracted by degenerate solutions

Unlike the complete data y case

- Risk to consider a degenerated solution as valid
- Risk of losing a lot of time in useless iterations

Statisticians should be aware of such dangerous EM behaviour. . .

. . . since missing data are more and more frequent



Understanding degeneracy speed on a toy example

- Univariate framework, no mixture, only one observed data: y
- Maximum likelihood estimator (**Unbounded likelihood!**): $\mu = y, \sigma^2 = 0$
- Suppose equivalently that $n - 1$ data are unobserved (unchanged likelihood)
- Here is one iteration of a (useless) EM algorithm (it. q)

$$\mu^{(q+1)} = \frac{(n-1)\mu^{(q)} + y}{n} \quad \text{and} \quad \sigma^{2(q+1)} = \frac{(n-1)\sigma^{2(q)} + (y - \mu^{(q+1)})^2}{n}$$

Linear grow of the log-likelihood (have a look also when n increases!)

$$\ell(\theta^{(q)}; x) \sim -0.5q \log \frac{n-1}{n}$$

Geometrical convergence rate towards 0 for the variance

$$\sigma^{2(q)} \sim \sigma^{2(0)} \left(\frac{n-1}{n} \right)^q$$



Influence of the missing data rate

% missing data	0	5	10	15	20	25	30
% deg.	16	4	12	11	46	51	100
Average nb of iterations before deg.	2	13	13	82	304	138	215

Table : Frequency and speed of degeneracy (deg.) according to the rate of missing data on the breast cancer data set.

When the rate of missing data increases:

- The rate of degeneracy increases
- The number of iterations before degeneracy seems to (globally) increase

Again, statisticians should be aware of such dangerous EM behaviour...

... since missing data are more and more frequent

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Full mixed data: conditional independence everywhere¹

The aim is to combine continuous, categorical, integer data, ordinal, ranking and functional data

$$y_1 = (y_1^{cont}, y_1^{cat}, y_1^{int}, \dots)$$

The proposed solution is to mixed all types by **inter-type conditional independence**

$$p(y_1; \alpha_k) = p(y_1^{cont}; \alpha_k^{cont}) \times p(y_1^{cat}; \alpha_k^{cat}) \times p(y_1^{int}; \alpha_k^{int}) \times \dots$$

In addition, for symmetry between types, **intra-type conditional independence**

Only need to define the univariate pdf for each variable type!

- **Continuous**: Gaussian
- **Categorical**: multinomial
- **Integer**: Poisson
- ...

¹MixtComp package: <https://cran.r-project.org/web/packages/RMixtComp/index.html>



Missing data: MAR assumption and estimation

Assumption on the missingness mechanism

Missing At Random (MAR): the probability that a variable is missing does not depend on its own value given the observed variables.

Observed log-likelihood...

$$\ell(\theta; y^{\text{obs}}) = \sum_{i=1}^n \log \left(\sum_{k=1}^K \pi_k p(y_i^{\text{obs}}; \alpha_k) \right) = \sum_{i=1}^n \ln \left[\sum_{k=1}^K \pi_k \underbrace{\int_{y_i^{\text{mis}}} p(y_i^{\text{obs}}, y_i^{\text{mis}}; \alpha_k) dy_i^{\text{mis}}}_{\text{MAR assumption}} \right]$$

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SEM algorithm

(implemented in the `MixtComp` package, available on the CRAN repository)

A SEM algorithm to estimate θ by maximizing the **observed**-data log-likelihood

- Initialisation: $\theta^{(0)}$
- Iteration nb q :
 - **E-step**: compute conditional probabilities $p(y^{\text{mis}}, z | y^{\text{obs}}; \theta^{(q)})$
 - **S-step**: draw $(y^{\text{mis}(q)}, z^{(q)})$ from $p(y^{\text{mis}}, z | y^{\text{obs}}; \theta^{(q)})$
 - **M-step**: maximize $\theta^{(q+1)} = \arg \max_{\theta} \ln p(y^{\text{obs}}, y^{\text{mis}(q)}, z^{(q)}; \theta)$
- Stopping rule: iteration number

Properties: simpler than EM and interesting properties!

- Avoid possibly difficult E-step in an EM
- Classical M steps
- Avoids local maxima
- The mean of the sequence $(\theta^{(q)})$ approximates $\hat{\theta}$
- The variance of the sequence $(\theta^{(q)})$ gives confidence intervals



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Prostate cancer data (with missing data)³

- **Individuals:** 506 patients with prostatic cancer grouped on clinical criteria into two Stages 3 and 4 of the disease
- **Variables:** $d = 12$ pre-trial variates were measured on each patient, composed by **eight continuous** variables (age, weight, systolic blood pressure, diastolic blood pressure, serum haemoglobin, size of primary tumour, index of tumour stage and histologic grade, serum prostatic acid phosphatase) and **four categorical** variables with various numbers of levels (performance rating, cardiovascular disease history, electrocardiogram code, bone metastases)
- Some **missing data:** 62 missing values ($\approx 1\%$)

We forget the classes (Stages of the disease) for performing **clustering**

Questions

- How many clusters?
- Which partition?

³Byar DP, Green SB (1980): Bulletin Cancer, Paris 67:477-488

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Two strategies in competition

- **Strategy “mice⁴ + MixtComp”**: MixtComp on the dataset completed by mice

```
> data.imp=mice(data)
> data.comp.mice=complete(data.imp)
```

- **Strategy “full MixtComp”**: MixtComp on the observed (no completed) dataset

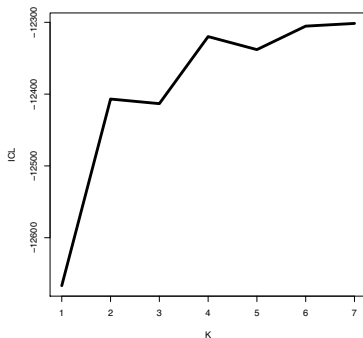
Partition quality with $K = 2$

Strategy	mice + MixtComp	full MixtComp
% misclassified	12.8	8.1

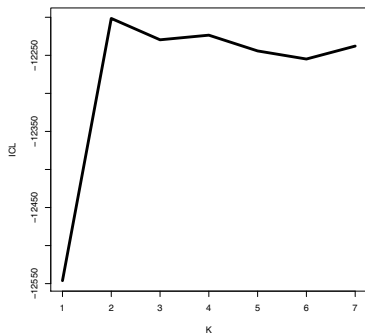
⁴<http://cran.r-project.org/web/packages/mice/mice.pdf>



Choosing K with the ICL criterion



mice + MixtComp
 $\hat{K} = 7$



full MixtComp
 $\hat{K} = 2$

... may lose some cluster information when imputation before clustering

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Outline

- 4 Impact of MNAR data on clustering
 - A model-based MNAR clustering approach
 - Medical study illustration

Proposed MNAR models in clustering

Question we address now

Since MNAR is not ignorable, which distribution $p(c|y, z; \psi)$ to propose?

Hypothesis 1: conditional independence

$$p(c_i | y_i, z_{ik} = 1; \psi) = \prod_{j=1}^d p(c_{ij} | y_i, z_{ik} = 1; \psi)$$

Hypothesis 2: linear function within canonical link functions ρ

$$p(c_{ij} = 1 | y_i, z_{ik} = 1; \psi) = \rho(\alpha_{kj} + \beta_{kj} y_{ij})$$

- $\psi = (\alpha, \beta)$ where $\alpha = (\alpha_{11}, \dots, \alpha_{1d}, \dots, \alpha_{K1}, \dots, \alpha_{Kd})^T \in \mathbb{R}^{Kd}$ and $\beta = (\beta_{11}, \dots, \beta_{1d}, \dots, \beta_{K1}, \dots, \beta_{Kd})^T \in \mathbb{R}^{Kd}$
- ρ is the cdf of any continuous distribution (logit, probit)



A by-product zoology of MNAR models

	Effect on the variable j		Effect on the class membership k		Nb parameters
	Depends on j	Depends on k	Depends on j	Depends on k	Continuous
MNAR $z^j y^k$	✓	✓	✓	✓	$2Kd$
MNAR yz^j	✓	✗	✓	✓	$(K + 1)d$
MNAR $y^k z$	✓	✓	✗	✓	$K(d + 1)$
MNAR yz	✓	✗	✗	✓	$(K + d)$
MNAR y	✓	✗	✗	✗	d
MNAR y^k	✓	✓	✗	✗	Kd
MNAR z	✗	✗	✗	✓	K
MNAR z^j	✗	✗	✓	✓	Kd

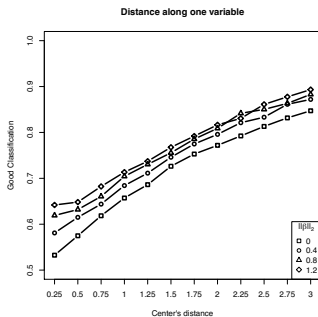
Remarks:

- MNAR $z^j y^k$ is the most complex model
- MNAR z , MNAR z^j : the only effect of missingness is on the class membership, $\psi = (\alpha_{11}, \dots, \alpha_{1d}, \dots, \alpha_{K1}, \dots, \alpha_{Kd})^T$, $p(c_{ij} = 1 \mid y_i, z_{ik} = 1; \psi) = \rho(\alpha_{kj})$
- MCAR is a specific and simple case

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

$$\pi_k = 0.5, \|\mu_2 - \mu_1\| \text{ varies}, \Sigma_1 = \Sigma_2 = \mathbf{I}, |\alpha_2 - \alpha_1| \text{ varies}$$



Both μ_k and α_k act on the Bayes error



Reinterpretation of the MNAR_z and MNAR_z^j models as MAR

Commonly used in Machine Learning [Jones, 1996], [Little and Rubin, 2002], [Josse *et al.*, 2019]

Mixture model for y^{obs} and Bernoulli distribution for C
 \Leftrightarrow MAR mixture model for $\tilde{y}^{\text{obs}} = (y^{\text{obs}}|c)$

For example,

$$y^{\text{obs}} = \begin{pmatrix} ? & 2.6 & 5 \\ \text{blue} & 1.9 & 4 \\ \text{red} & 2.3 & ? \end{pmatrix}, \quad c = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

then \tilde{y}^{obs} is expressed as

$$\tilde{y}^{\text{obs}} = \begin{pmatrix} ? & 2.6 & 5 & 1 & 0 & 0 \\ \text{blue} & 1.9 & 4 & 0 & 0 & 0 \\ \text{red} & 2.3 & ? & 0 & 0 & 1 \end{pmatrix}.$$

Proposition 3: in terms of maximum likelihood

The maximum likelihood estimate associated to the dataset \tilde{y}^{obs} under MAR model is the one associated to the dataset y^{obs} under MNAR_z or MNAR_z^j models.

Identifiability

Previous works: [Teicher, 1963] (without NA), [Miao et al., 2016] (for MNAR data)

Proposition 4

Assume that

- 1 The marginal mixture $\sum_{k=1}^K \pi_k f_k(y_i; \theta_k)$ is identifiable
- 2 There exists a total ordering \preceq of $\mathcal{F}_j \times \mathcal{R}$, for $j \in \{1, \dots, d\}$ fixed, where $\mathcal{F}_j = \{f_{1j}, \dots, f_{Kj}\}$ and $\mathcal{R} = \{\rho_1, \dots, \rho_K\} = \{\rho(\cdot; \psi_1), \dots, \rho(\cdot; \psi_K)\}$. The total ordering is s.t. $\forall k < \ell, F_k = \rho_k f_{kj} \preceq F_\ell = \rho_\ell f_{\ell j}$ implies

$$\lim_{u \rightarrow +\infty} \frac{\rho_\ell(u) f_{\ell j}(u)}{\rho_k(u) f_{kj}(u)} = 0$$

Then the mixture model with one of the MNAR* mechanisms is identifiable up to label swapping

All MNAR models are identifiable (or at least generically identifiable) for probit/logit



Estimation procedure overview

- Use EM or Stochastic EM (SEM) algorithms
- MNAR_z and MNAR_z^j: EM and SEM are very simple
- MNAR_y*: the SE step requires a within Gibbs loop, sometimes involving itself a Sampling Importance Resampling (SIR)

	EM		SEM	
MNAR _z MNAR _z ^j	✓		✓	
	Probit	Logit	Probit	Logit
MNAR _y *	no closed form	no closed form, optim. pb	✓	require algorithms as SIR (costly)



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

CAUTION

- It is just a selection between several proposed MNAR models
- It is not deciding if missingness procedure is “genererically” MNAR or not



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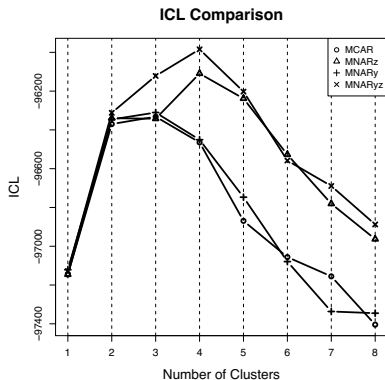
Hospital data description

- 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%

Doctors are convinced that their missing data are MNAR



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

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To conclude

Summary

- Statisticians should properly consider the potential missing data impact both from an **algorithmic** and from a **modeling** point of view
- EM: be careful about degeneracy which seems to exacerbated/masqued
- MAR: the minimal approach to be used by statisticians. . .
- MNAR: interest of the simple but meaningful model MNAR_z, link with usual methods

Ongoing works

- EM: propose mechanism to identify/discard degenerate runs
- MNAR: extend to categorical, count and mixed data

Thanks!