Impact of Missing Data on Mixtures and Clustering

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Impact of Missing Data on Mixtures and Clustering

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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...

Outline

Outline

Missing data: notations

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

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

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

Typology of the missingness mechanisms

- Missing completely at random (MCAR):

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

- Missing at random (MAR):

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

- 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

Mixture model and clustering

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

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

  - $\pi_k = \mathrm{p}(z_{ik}=1)$, $\pi = (\pi_1,\ldots,\pi_K)$
  - $f_k(.;\lambda_k) = \phi(.;\mu_k,\Sigma_k)$ is the d-variate **Gaussian distribution** with mean vector μ_k and covariance matrix Σ_k
  - $\theta = (\ (\pi)_k\ ,(\lambda)_k\ )$ is the whole mixture parameter
- Clustering: MAP principle from the mixture output to estimate the partition

Outline

Degeneracy genesis: unbounded likelihood

- d-variate Gaussian mixture

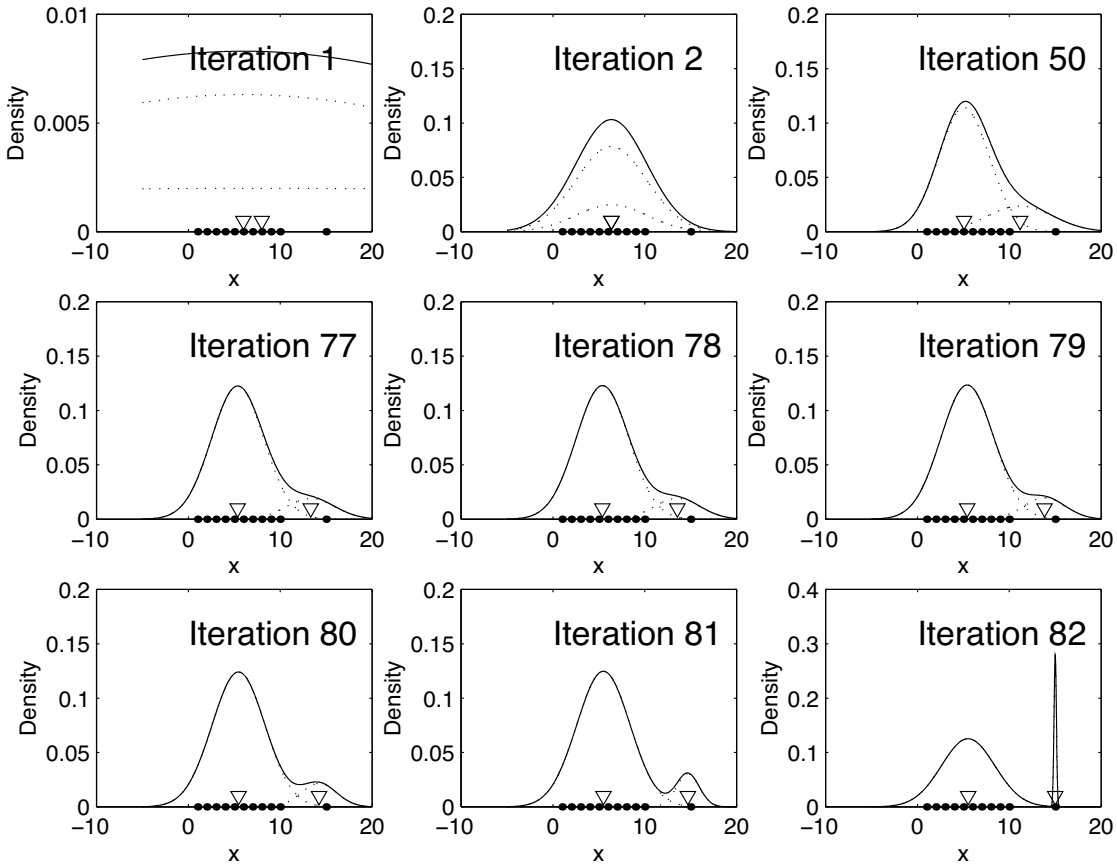
$$f(y_i;\theta) = \sum_{k=1}^{K} \pi_k \underbrace{\frac{1}{(2\pi)^{d/2}|\Sigma_k|^{1/2}} \exp\Big(-\frac{1}{2}(y_i-\mu_k)^T\Sigma_k^{-1}(y_i-\mu_k)\Big)}_{\phi(y_i;\mu_k,\Sigma_k)}$$

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

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

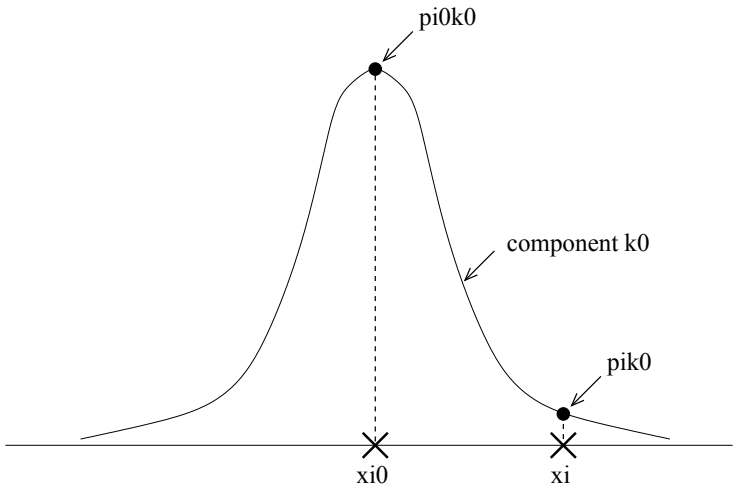
[Kiefer and Wolfowitz, 1956] [Day, 1969]

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}

$\Leftrightarrow$

$\|u_0\| \to 0$

[Biernacki and Chrétien, 2003]

[Ingrassia and Rocci, 2009]

Proposition 1: Existence of a bassin 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

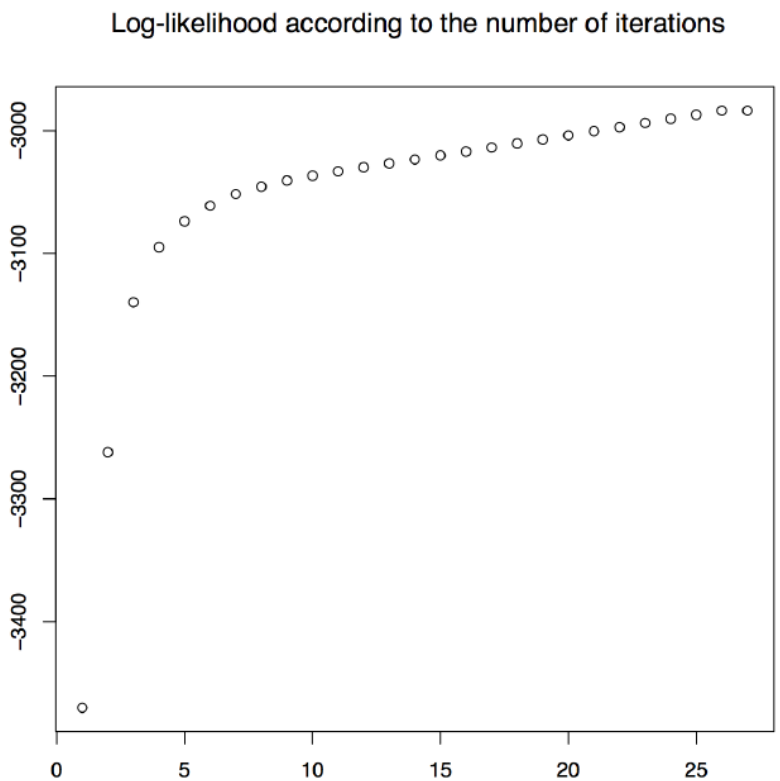
$\exists \epsilon > 0$, $\alpha > 0$ *and* $\beta > 0$ *s.t. if* $\|u_0\| \leq \epsilon$ *then, with probability 1,*

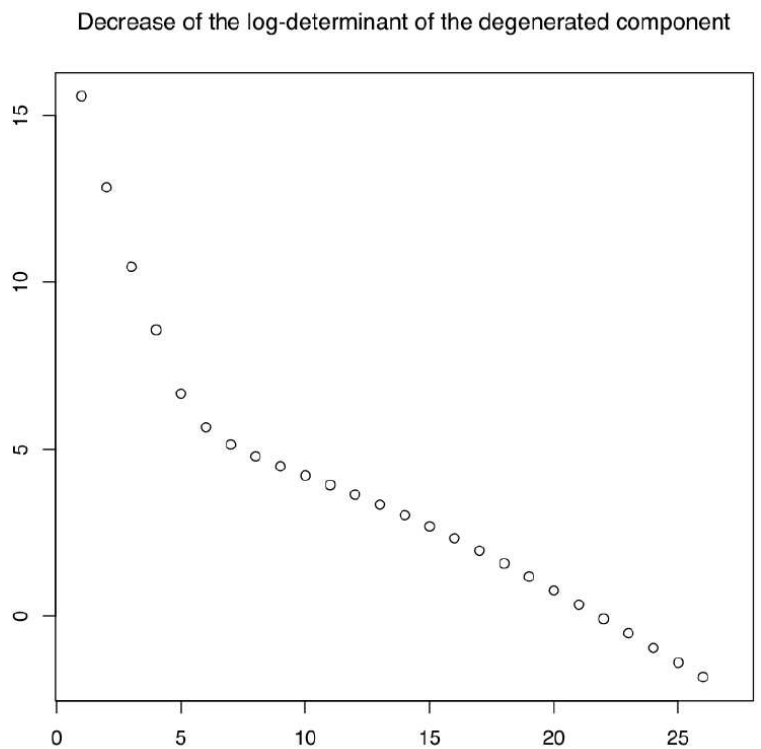
$$|\Sigma_{k_0}^+| \leq \alpha / |\Sigma_{k_0}| \cdot \exp\Big(- \beta / |\Sigma_{k_0}| \Big).$$

Outline

EM behaviour illustration

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





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

Outline

Proposed MNAR models in clustering

Question we address now

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

Hypothesis 1: conditional independence

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

Hypothesis 2: linear function within canonical link functions ρ

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

- $\psi = (\alpha, \beta)$ where $\alpha = (\alpha_{11}, \ldots, \alpha_{1d}, \ldots, \alpha_{K1}, \ldots, \alpha_{Kd})^T \in \mathbb{R}^{Kd}$ and $\beta = (\beta_{11}, \ldots, \beta_{1d}, \ldots, \beta_{K1}, \ldots, \beta_{Kd})^T \in \mathbb{R}^{Kd}$
- 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$z^j y^k$	✓	✓	✓	✓	$2Kd$
MNARyz^j	✓	✗	✓	✓	$(K+1)d$
MNAR$y^k z$	✓	✓	✗	✓	$K(d+1)$
MNARyz	✓	✗	✗	✓	$(K+d)$
MNARy	✓	✗	✗	✗	d
MNARy^k	✓	✓	✗	✗	Kd
MNARz	✗	✗	✗	✓	K
MNARz^j	✗	✗	✓	✓	Kd

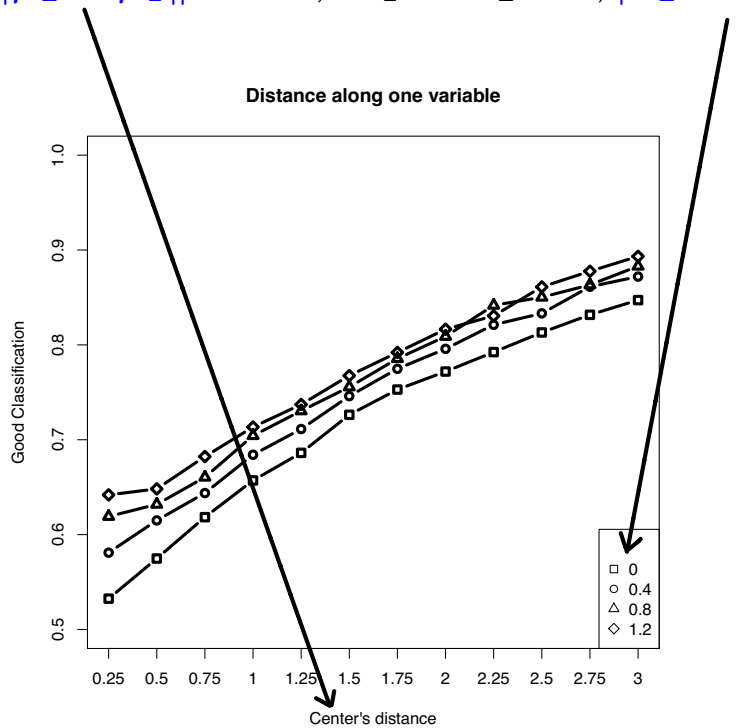
Remarks:

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

MNARz analysis: pattern c gives information on partition z!

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

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



Both μ_k and α_k act on the Bayes error

Reinterpretation of the MNARz and MNARz^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 $\tilde{y}^{\text{obs}}$ 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 $\tilde{y}^{\text{obs}}$ under MAR model is the one associated to the dataset y^{obs} under MNARz or MNARz^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 $j \in \{1, \ldots, d\}$ fixed, where $\mathcal{F}_j = \{f_{1j}, \ldots, f_{Kj}\}$ and $\mathcal{R} = \{\rho_1, \ldots, \rho_K\} = \{\rho(.; \psi_1), \ldots, \rho(.; \psi_K)\}$. The total ordering is s.t. $\forall k < \ell$, $F_k = \rho_k f_{kj} \preceq F_\ell = \rho_\ell f_{\ell j}$ implies

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

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
- MNARz and MNARz^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	
MNARz MNARz^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 "generically" MNAR or not

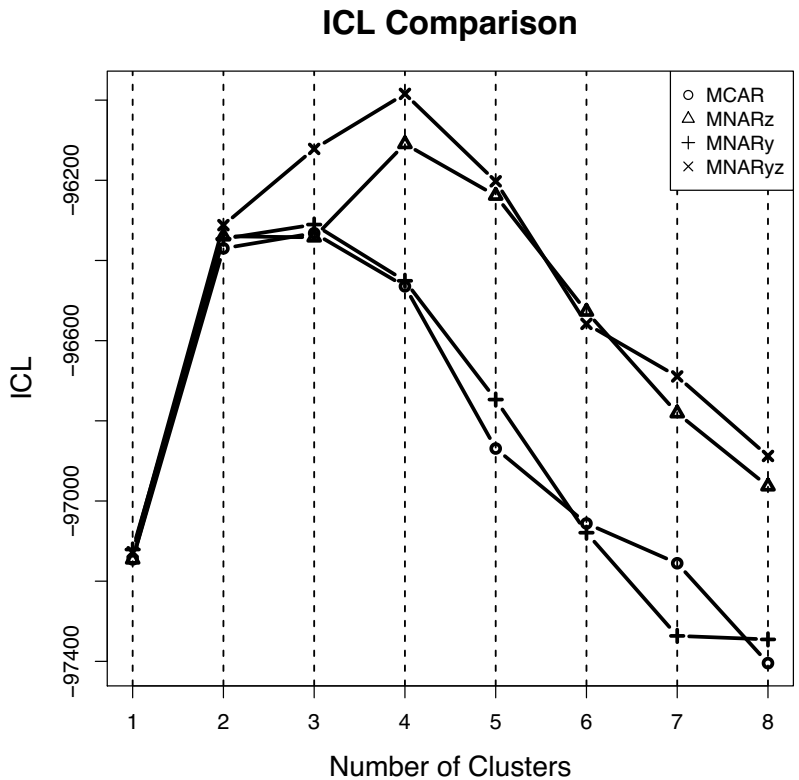
Outline

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 illustation of the effect of c through MNARz and MNARyz

Outline

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
- MNAR: interest of the simple but meaningful model MNARz, link with usual methods

Ongoing works

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

Thanks!