## How to handle missing values?

Model-based approaches

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#### Overview

- 1. Introduction
- 2. Statistical framework in missing-data literature Missing-data pattern Missing-data mechanism
- 3. EM algorithm for handling missing values

# Your viewpoint



## Missing values are everywhere!

- unanswered questions in a survey,
- lost data,
- sensing machines that fail,
- aggregation of dataset, ...

#### Take-home message

Growing masses of data + Multiplication of sources

⇒ Not available values, NA

The more data we have, the more missing data we have!

Trauma.center	Heart	Death	Anticoagulant.	Glascow	/
	rate		therapy	score	•••
Pitie-Salpêtrière	88	0	No	3	
Beaujon	103	0	NA	5	
Bicêtre	NA	0	Yes	6	
Bicêtre	NA	0	No	NA	
Lille	62	0	Yes	6	
Lille	NA	0	No	NA	
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250 clinical variables (heterogeneous)

1 patient; in total: 30 000 patients

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23 different hospitals

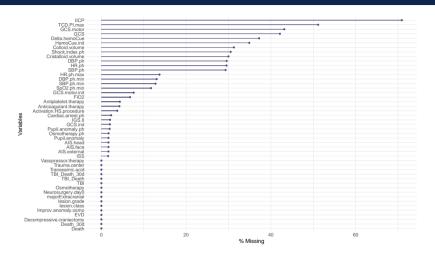


Figure: Percentage of missing values for 40 variables.

## Traumabase® dataset

- now **30 000** patients (in 2018: 10 000).
- 250 heterogeneous variables: continuous, categorical, ordinal,...
- 23 different hospitals
- missing values everywhere (1% to 90% NA in each variable).
- Imputation: provide a complete dataset to the doctors.
- **Estimation:** explain the level of platelet with pre-hospital characteristics.
- **Prediction:** predict the administration or not of the tranexomic acid.
- **Clustering:** identify relevant groups of patients sharing similarities.

Question: How to deal with missing values? A first naive idea?

### What we should not do

```
Pitie-Salpêtrière
                           No
                  88
    Beaujon
                  103
    Bicêtre
                           Yes
                  NA
    Bicêtre
                           No
                  NA
     Lille
                  62
                         Yes
     Lille
                           No
                  NA
```

#### Discarding individuals with missing values is not a solution

Loss of information .

Traumabase<sup>®</sup>: only 5% of the rows are kept.

Bias in the analysis.

Kept observations: sub-population **not necessarily representative** of the overall population.

#### Example:

• We consider a bivariate Gaussian variable.  $X \sim \mathcal{N}(\mu, \Sigma)$ , with

$$\mu = \begin{pmatrix} 5 \\ -1 \end{pmatrix}$$
 and  $\Sigma = \begin{pmatrix} 1 & 0.5 \\ 0.5 & 1 \end{pmatrix}$ 

- $X_2$  is missing.
- We estimate  $\mu_2$  with the empirical mean in the complete case.
- see Rmarkdown!

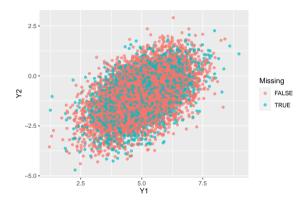


Figure: The sub-population is representative of the overall population.

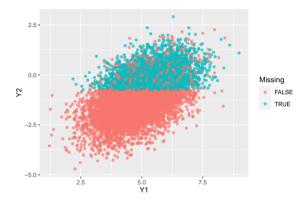


Figure: The sub-population is **not** representative of the overall population.

## Need for assumption

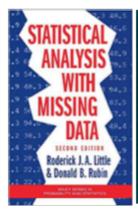
**Example:** survey with two variables, Income and Age, with missing values only on Income.

- Poor and rich respondents would be less incline to reveal their income.
- There are missing values for the smallest and highest values of Income.
- Even though Age and Income are related, the process that causes the missing data is not fully explained by Age.
- Knowing the value of Age is not enough to retrieve the value of Income.

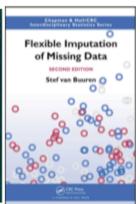
#### Take-home message

- Knowing **why** the data is missing is an important issue.
- The process that causes the missing data should be modeled in some situations.

#### Main references







## Goal of this course<sup>1</sup>

This is only an **introduction** to missing data.

- Dangers of naive methods in the analysis,
- Importance of the missing-data mechanism (type of missing data),
- EM algorithm for handling missing data (+ R code session),
- To be continued next week (other methods, comparison of the methods on a real dataset).

<sup>&</sup>lt;sup>1</sup>Inspired by the courses of Pierre-Alexandre Mattei (2019-2020) and Julie Josse (2020) on missing values.

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## A statistical framework for incomplete data

$$X = \underbrace{\begin{pmatrix} 30 & 100 & 61 \\ 85 & 31 & 50 \end{pmatrix}}_{\text{not observed}} \qquad X^{\text{NA}} = \underbrace{\begin{pmatrix} 30 & \text{NA} & 61 \\ \text{NA} & \text{NA} & 50 \end{pmatrix}}_{\text{observed}}$$

We observe also where are the missing values in  $X^{NA}$ .

#### Definition: missing-data pattern (mask)

 $M \in \{0,1\}^{n \times d}$ : indicates where are the missing values in  $X^{NA}$ .

$$\forall i, j, \quad M_{ij} = egin{cases} 1 & ext{if } X_{ij}^{ ext{NA}} ext{ is missing,} \\ 0 & ext{otherwise.} \end{cases}$$

## A statistical framework for incomplete data

$$X = \underbrace{\begin{pmatrix} 30 & 100 & 61 \\ 85 & 31 & 50 \end{pmatrix}}_{\text{not observed}} \qquad X^{\text{NA}} = \underbrace{\begin{pmatrix} 30 & \text{NA} & 61 \\ \text{NA} & \text{NA} & 50 \end{pmatrix}}_{\text{observed}} \qquad M = \underbrace{\begin{pmatrix} 0 & 1 & 0 \\ 1 & 1 & 0 \end{pmatrix}}_{\text{observed}}$$

#### Question: What to model?

- model  $p(X^{NA})$ : too difficult because the entries  $X_{ij}^{NA} \in \mathbb{R} \cup \{NA\}$  (semi-discrete set).
- model p(X, M): entries are in a well-behaved mathematical set  $\mathbb{R}^{n \times d} \cup \{1, 0\}^{n \times d}$

# Model the joint distribution (X, M)

We want to model the **joint** distribution of the data X and the missing-data pattern M.

The observations are assumed to be i.i.d., i.e.  $(X_1, M_1), \ldots, (X_n, M_n)$  have the same distribution and are independent

$$p(X,M) = \prod_{i=1}^{n} p(X_i, M_i).$$

# Model the joint distribution (X, M)

We want to model the **joint** distribution of the data X and the missing-data pattern M.

#### Selection model factorization

$$p(X,M) = p(X)p(M|X)$$

where

- p(X): distribution of the data,
- p(M|X): conditional distribution of the missing-data pattern given the data, it is the **missing-data mechanism**.

Parametric approach:

$$p(X, M; \theta, \phi) = p(X; \theta)p(M|X; \phi)$$

where  $\theta \in \Omega_{\theta}$  and  $\phi \in \Omega_{\phi}$ .

# Missing-data mechanism (Rubin, 1976)

#### Missing Completely At Random (MCAR)

$$p(M|X;\phi)=p(M;\phi)$$

#### Missing At Random (MAR)

 $X^{\mathrm{obs}}$ : observed component of X.

$$p(M|X;\phi) = p(M|X^{\text{obs}};\phi)$$

#### Missing Not At Random (MNAR)

The MAR assumption does not hold. The missingness can depend on the missing data value itself.

Question: Which mechanism is realistic? How to choose the right mechanism for real data?

## Example of models

$$p(X, M; \theta, \phi) = p(X; \theta)p(M|X; \phi)$$

- For p(X): models seen in the rest of the course, e.g. mixture model, single Gaussian, variational autoencoder, . . .
- For p(M|X): typically Logit or Probit distribution.

$$p(M_{ij}|X_{ij};\phi) = [(1+e^{-\phi_{1j}(X_{ij}-\phi_{2j})})^{-1}]^{M_{ij}}[1-(1+e^{-\phi_{1j}(X_{ij}-\phi_{2j})})^{-1}]^{(1-M_{ij})}.$$

But it is a **strong assumption**. We will see that in some situations, the missing-data mechanism can be *ignored* (not modelled).

## Likelihood approach with incomplete data

- Goal of the **parametric estimation**: model the joint distribution (X, M) parametrized by  $\theta, \phi \in \Omega_{\theta} \times \Omega_{\phi}$ .
- Likelihood-approach without missing data: maximizing the full likelihood

$$L_{\text{full}}(\theta, \phi; X, M) = p(X; \theta)p(M|X; \phi)$$

- Split X into two components  $X^{\text{obs}}$  (observed features),  $X^{\text{mis}}$  (missing features).
- Likelihood-approach with missing data: maximizing the full observed likelihood

$$L_{\mathrm{full,obs}}(\theta,\phi;X^{\mathrm{obs}},M) = \int L_{\mathrm{full}}(\theta,\phi;X,M)dX^{\mathrm{mis}}$$

## Ignorable mechanisms

Question: How can we ignore the missing-data mechanism?

## Ignorable mechanisms

For MCAR and MAR data, we can **ignore** the missing-data mechanism:

$$L_{\mathrm{full,obs}}(\theta,\phi;X^{\mathrm{obs}},M) \propto L_{\mathrm{ign}}(\theta;X^{\mathrm{obs}}) = \int p(X;\theta) dX^{\mathrm{mis}} = p(X^{\mathrm{obs}};\theta)$$

#### Take-home message

- M(C)AR: one can ignore the mechanism.
- MNAR: one should consider the mechanism.

## Link with the logistic regression

Ignorability in missing-data analysis: to model (X, M), we can in some cases ignore the mechanism (M|X), by treating  $\phi$  as a nuisance parameter.

- $\rightarrow$  Similar trick for logistic regression.
  - $p(x, y) = p(y|x; \theta)p(x)$  with p(x) which does not involve  $\theta$ .
  - Likelihood written as  $L_{\text{full}}(\theta; x, y) = p(y|x; \theta)p(x)$ .
  - Goal: estimate  $\theta$ .
  - We do not model p(x) because  $\hat{\theta} \in \operatorname{argmax}_{\theta} L_{\operatorname{full}}(\theta; x, y) = \operatorname{argmax}_{\theta} p(y|x; \theta)$

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## Setting

- Goal: estimate  $\theta \in \Omega_{\theta}$ , when X contain **MCAR** or **MAR** values.
- We can maximize the fully observed **log**-likelihood (logarithm more convenient):

$$\hat{\theta} = \operatorname{argmax}_{\theta} \ell_{\operatorname{ign}}(\theta; X^{\operatorname{obs}}) = \log(p(X^{\operatorname{obs}}; \theta))$$

• When it has no closed form, a solution can be to use the EM algorithm. Idea: consider the missing variables as latent variables.

# Expectation Maximization algorithm (Dempster et al., 1977)

Starting from an initial point  $\theta^0$ , the EM algorithm proceeds two steps **iteratively**:

• E-step: computation of the expected full log-likelihood knowing the observed data and a current value of the parameters.

$$Q(\theta; \theta^r) = \mathbb{E}[\ell_{\text{full}}(X; \theta) | X^{\text{mis}}, \theta^r]$$

• M-step: maximization of  $Q(\theta; \theta^r)$  over  $\theta$ .

$$\theta^{r+1} = \operatorname{argmax}_{\theta} Q(\theta; \theta^r)$$

Consider a Gaussian bivariate variable  $X = (X_{.1}^T, X_{.2}^T) \in \mathbb{R}^{n \times 2}$ .

$$X \sim \mathcal{N}(\mu, \Sigma),$$

with 
$$\mu = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}$$
 and  $\Sigma = \begin{pmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{12} & \sigma_{22} \end{pmatrix}$ .

 $X_{.2}$  contain some **M(C)AR missing values**. Without loss of generality, assume that  $X_{i2}$  is missing, with  $r < i \le n$ .

**Question:** First, we want to know if it is possible to maximize the observed log-likelihood directly. Write the observed log-likelihood.

Question: Write the observed log-likelihood.

Tip: use the classical formula  $X_{i2}|X_{i1} \sim \mathcal{N}(\mathbb{E}[X_{i2}|X_{i1}], \mathrm{Var}(X_{i2}|X_{i1}))$  with

$$\mathbb{E}[X_{i2}|X_{i1}] = \mu_2 + \frac{\sigma_{21}}{\sigma_{11}}(X_{i1} - \mu_1)$$

$$\operatorname{Var}(X_{i2}|X_{i1}) = \sigma_{22} - \frac{\sigma_{21}^2}{\sigma_{11}}$$

Question: Write the observed log-likelihood.

In this simple setting, directly maximizing the log-likelihood is possible.

$$\ell(X_{.1}, X_{.2}^{\text{obs}}; \mu, \Sigma) = -\frac{n}{2} \log(\sigma_{11}^2) - \frac{1}{2} \sum_{i=1}^{n} \frac{(X_{i1} - \mu_1)^2}{\sigma_{11}^2} - \frac{r}{2} \log\left(\sigma_{22} - \frac{\sigma_{21}^2}{\sigma_{11}}\right)^2 - \frac{1}{2} \sum_{i=1}^{r} \frac{(X_{i2} - \mu_2 + \frac{\sigma_{21}}{\sigma_{11}}(X_{i1} - \mu_1))^2}{\left(\sigma_{22} - \frac{\sigma_{21}^2}{\sigma_{11}}\right)^2}$$

More fun: let us derive the EM algorithm!

**E-step:** computation of the expected full log-likelihood knowing the observed data and a current value of the parameters.

$$Q(\theta; \theta^r) = \mathbb{E}[\ell_{\text{full}}(X; \theta) | X^{\text{mis}}, \theta^r]$$

**Question:** Write the full log-likelihood (easy question).

**Question:** Write  $Q(\theta; \theta^r)$ . What quantities should be computed in the E-step?

**M-step:** maximization of  $Q(\theta; \theta^r)$  over  $\theta$ .

$$\theta^{r+1} = \operatorname{argmax}_{\theta} Q(\theta; \theta^r)$$

#### References



Little, Roderick JA and Rubin, Donald B (2019) Statistical analysis with missing data John Wiley & Sons.