

# What is a good imputation under MAR missingness

---

**Julie Josse**

Head of the Inria-Inserm team **PreMeDICaL**:

"**Precision Medicine by Data Integration & Causal Learning**"

December 16, 2024

Näf et al. (2024)  
(<https://arxiv.org/abs/2403.19196>)



Jeffrey Näf  
(Postdoc Inria)



Erwan Scornet  
(Prof. Sorbonne Univ.)

# Traumabase: an observational French registry on trauma<sup>2</sup>

- ▷ 40000 patients
- ▷ 250 continuous and categorical variables
- ▷ 40 trauma centers, 4000 new patients/ year

Center	Accident	Age	Sex	Lactate	Blood Pres.	Shock	Platelet	...
Beaujon	fall	54	m	NM	180	yes	292 000	
Pitie	gun	26	m	NA	131	no	323 000	
Beaujon	moto	63	m	3.9	NR	yes	318 000	
Pitie	moto	30	w	Imp	107	no	211 000	
⋮								⋮

<sup>1</sup>Zaffran, J., Dieuleveut, Romano. Conformal Prediction with Missing Values. *ICML 2023*.

<sup>2</sup>[www.traumabase.eu](http://www.traumabase.eu) - <https://www.traumatrix.fr/>

# Traumabase: an observational French registry on trauma<sup>2</sup>

- ▷ 40000 patients
- ▷ 250 continuous and categorical variables
- ▷ 40 trauma centers, 4000 new patients/ year

Center	Accident	Age	Sex	Lactate	Blood Pres.	Shock	Platelet	...
Beaujon	fall	54	m	NM	180	yes	292 000	
Pitie	gun	26	m	NA	131	no	323 000	
Beaujon	moto	63	m	3.9	NR	yes	318 000	
Pitie	moto	30	w	Imp	107	no	211 000	
⋮								

⇒ **Explain and Predict** hemorrhagic shock, need for neurosurgery and need for a trauma center given pre-hospital features.

Ex: logistic regression/ random forests + **Quantify uncertainty**<sup>1</sup>

Clinical trial will be launched end 2024: real-time implementation of models in the ambulance via a mobile data collection application

<sup>1</sup>Zaffran, J., Dieuleveut, Romano. Conformal Prediction with Missing Values. *ICML 2023*.

<sup>2</sup>[www.traumabase.eu](http://www.traumabase.eu) - <https://www.traumatrix.fr/>

# Solutions to handle missing values in the covariates

Abundant literature: Creation of **Rmistic platform**<sup>3</sup> (> 150 packages)

Inferential aim: **Estimate parameters & their variance, i.e.  $\hat{\beta}$ ,  $\hat{V}(\hat{\beta})$**   
to get confidence intervals with the appropriate coverage

---

<sup>3</sup>Mayer, J. et al. A unified platform for missing values methods and workflows. *R journal*. 2022.

<sup>4</sup>Jiang, J. et al. Logistic Regression with Missing Covariates *CSDA*. 2019. - **misaem package**

<sup>5</sup>J. et al. Consistency of supervised learning with missing values. *Stats papers*. 2018-2024.

<sup>6</sup>Le morvan, J. et al. What's a good imputation to predict with missing values? *Neurips2021*.

# Solutions to handle missing values in the covariates

Abundant literature: Creation of **Rmistic platform**<sup>3</sup> (> 150 packages)

Inferential aim: **Estimate parameters & their variance, i.e.**  $\hat{\beta}$ ,  $\hat{V}(\hat{\beta})$   
to get confidence intervals with the appropriate coverage

**Modify the estimation process to deal with missing values**

Maximum likelihood inference: Expectation Maximization algorithms<sup>4</sup>

---

<sup>3</sup>Mayer, J. et al. A unified platform for missing values methods and workflows. *R journal*. 2022.

<sup>4</sup>Jiang, J. et al. Logistic Regression with Missing Covariates *CSDA*. 2019. - **misaem package**

<sup>5</sup>J. et al. Consistency of supervised learning with missing values. *Stats papers*. 2018-2024.

<sup>6</sup>Le morvan, J. et al. What's a good imputation to predict with missing values? *Neurips2021*.

# Solutions to handle missing values in the covariates

Abundant literature: Creation of **Rmistic platform**<sup>3</sup> (> 150 packages)

Inferential aim: **Estimate parameters & their variance**, i.e.  $\hat{\beta}$ ,  $\hat{V}(\hat{\beta})$   
to get confidence intervals with the appropriate coverage

**Modify the estimation process to deal with missing values**

Maximum likelihood inference: Expectation Maximization algorithms<sup>4</sup>

**(Multiple) imputation to get a complete data set. Ex: (M)ICE**

---

<sup>3</sup>Mayer, J. et al. A unified platform for missing values methods and workflows. *R journal*. 2022.

<sup>4</sup>Jiang, J. et al. Logistic Regression with Missing Covariates *CSDA*. 2019. - **misaem package**

<sup>5</sup>J. et al. Consistency of supervised learning with missing values. *Stats papers*. 2018-2024.

<sup>6</sup>Le morvan, J. et al. What's a good imputation to predict with missing values? *Neurips2021*.

# Solutions to handle missing values in the covariates

Abundant literature: Creation of **Rmistic platform**<sup>3</sup> (> 150 packages)

Inferential aim: **Estimate parameters & their variance**, i.e.  $\hat{\beta}$ ,  $\hat{V}(\hat{\beta})$   
to get confidence intervals with the appropriate coverage

**Modify the estimation process to deal with missing values**

Maximum likelihood inference: Expectation Maximization algorithms<sup>4</sup>

**(Multiple) imputation to get a complete data set. Ex: (M)ICE**

Matrix completion aim: **Predict the missing values** as well as possible.  
Solutions: using low rank matrix approximation

Predictive aim: **Predict an outcome** with missing values in covariates.<sup>5,6</sup>  
Solutions: using deterministic (e.g. constant) imputation or Missing Incorporated in Attributes for trees based methods (**grf package**)

<sup>3</sup>Mayer, J. et al. A unified platform for missing values methods and workflows. *R journal*. 2022.

<sup>4</sup>Jiang, J. et al. Logistic Regression with Missing Covariates *CSDA*. 2019. - **misaem package**

<sup>5</sup>J. et al. Consistency of supervised learning with missing values. *Stats papers*. 2018-2024.

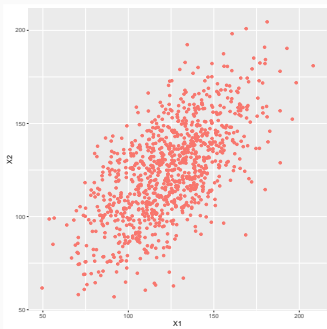
<sup>6</sup>Le morvan, J. et al. What's a good imputation to predict with missing values? *Neurips2021*.



# Single imputation by the mean

$$\triangleright (x_{i1}, x_{i2}) \underset{\text{i.i.d.}}{\sim} \mathcal{N}_2((\mu_{x_1}, \mu_{x_2}), \Sigma_{x_1 x_2})$$

$X_1$	$X_2$
-0.56	-1.93
-0.86	-1.50
.....	...
2.16	0.7
0.16	0.74



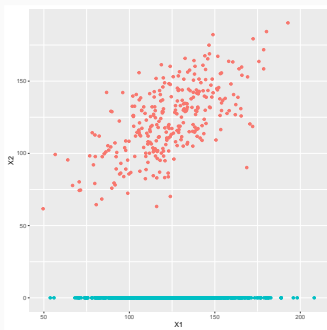
$$\begin{aligned}\mu_{x_2} &= 0 \\ \sigma_{x_2} &= 1 \\ \rho &= 0.6\end{aligned}$$

$\hat{\mu}_{x_2} = -0.01$
$\hat{\sigma}_{x_2} = 1.01$
$\hat{\rho} = 0.66$

# Single imputation by the mean

- ▷  $(x_{i1}, x_{i2}) \underset{\text{i.i.d.}}{\sim} \mathcal{N}_2((\mu_{x_1}, \mu_{x_2}), \Sigma_{x_1 x_2})$
- ▷ 70 % of missing entries completely at random on  $X_2$

$X_1$	$X_2$
-0.56	NA
-0.86	NA
.....	...
2.16	0.7
0.16	NA



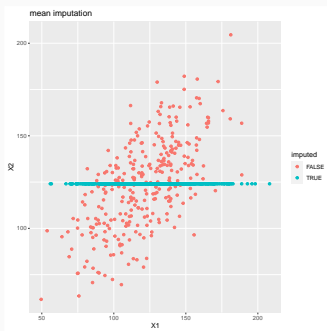
$$\begin{aligned}\mu_{x_2} &= 0 \\ \sigma_{x_2} &= 1 \\ \rho &= 0.6\end{aligned}$$

$\hat{\mu}_{x_2} = 0.18$
$\hat{\sigma}_{x_2} = 0.9$
$\hat{\rho} = 0.6$

# Single imputation by the mean

- ▷  $(x_{i1}, x_{i2}) \underset{\text{i.i.d.}}{\sim} \mathcal{N}_2((\mu_{x_1}, \mu_{x_2}), \Sigma_{x_1 x_2})$
- ▷ 70 % of missing entries completely at random on  $X_2$
- ▷ Estimate parameters on the mean imputed data

$X_1$	$X_2$
-0.56	<b>0.01</b>
-0.86	<b>0.01</b>
.....	...
2.16	0.7
0.16	<b>0.01</b>



$$\begin{aligned}\mu_{x_2} &= 0 \\ \sigma_{x_2} &= 1 \\ \rho &= 0.6\end{aligned}$$

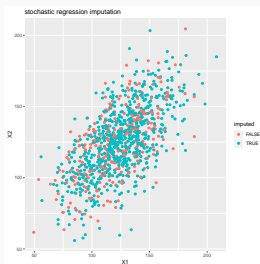
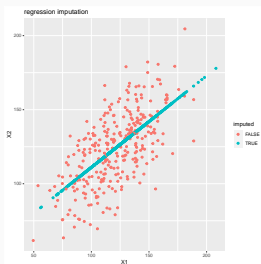
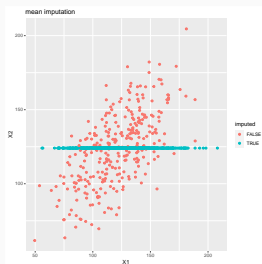
$\hat{\mu}_{x_2} = 0.01$
$\hat{\sigma}_{x_2} = 0.5$
$\hat{\rho} = 0.30$

Mean imputation deforms joint and marginal distributions

# Objective: to impute while preserving distribution

Assuming a bivariate gaussian distribution  $x_{i2} = \beta_0 + \beta_1 x_{i1} + \varepsilon_i$ ,  $\varepsilon_i \sim \mathcal{N}(0, \sigma^2)$

- ▷ Regression imputation: Estimate  $\beta$  (here with complete data) and impute  $\hat{x}_{i2} = \hat{\beta}_0 + \hat{\beta}_1 x_{i1} \Rightarrow$  variance underestimated and correlation overestimated
- ▷ Stochastic reg. imputation: Estimate  $\beta$  and  $\sigma$  - impute from the predictive  $\hat{x}_{i2} \sim \mathcal{N}(\beta_0 + \hat{\beta}_1 x_{i1}, \hat{\sigma}^2) \Rightarrow$  preserve distributions



$$\mu_{x_2} = 0$$

$$\sigma_{x_2} = 1$$

$$\rho = 0.6$$

0.01
0.5
0.30

0.01
0.72
0.78

0.01
0.99
0.59

# Impute while preserving distribution. Multivariate case

## Assuming a joint distribution

- ▷ Gaussian model  $x_i \sim \mathcal{N}(\mu, \Sigma)$
- ▷ Low rank :  $X_{n \times d} = \mu_{n \times d} + \varepsilon$   $\varepsilon_{ij} \stackrel{\text{iid}}{\sim} \mathcal{N}(0, \sigma^2)$  with  $\mu$  of low rank
  - ⇒ Different regularization depending on noise regime<sup>7</sup>
  - ⇒ Count data,<sup>8</sup> ordinal data, categorical data, blocks/multilevel data
- ▷ Optimal transport,<sup>9</sup> deep generative models: GAIN,<sup>10</sup> MIWAE,<sup>11</sup> etc.<sup>12,13</sup>

<sup>7</sup>J. & Wager. Stable autoencoding for regularized low-rank matrix estimation. *JMLR*. 2016.

<sup>8</sup>Robin, Klopp, J., Moulines, Tibshirani. Main effects & interac. in mixed data. *JASA*. 2019.

<sup>9</sup>Muzelec, Cuturi, Boyer, J. Missing Data Imputation using Optimal Transport. *ICML*. 2020.

<sup>10</sup>Yoon et al. GAIN: Missing data imputation using generative adversarial nets. *ICML*. 2018.

<sup>11</sup>Mattei & Frellsen. Miwae: Deep generative model. & imput. of incomplete data. *ICML*. 2018.

<sup>12</sup>Deng et al. Extended missing data imput. via gans. *Data Mining & Knowledge Discovery*. 2022.

<sup>13</sup>Fang Bao. Fragmgan gan for fragmentary data imputation. *Stat.theory & Related Fields*. 2023.

<sup>14</sup>van Buuren, S. Flexible Imputation of Missing Data. Chapman Hall/CRC Press. 2018.

<sup>15</sup>Stekhoven & Bühlmann. MissForest–non-parametric imputation for mixed data. *Bioinfo*. 2012.

# Impute while preserving distribution. Multivariate case

## Assuming a joint distribution

- ▷ Gaussian model  $x_i \sim \mathcal{N}(\mu, \Sigma)$
- ▷ Low rank :  $X_{n \times d} = \mu_{n \times d} + \varepsilon \varepsilon_{ij}^{\text{iid}} \sim \mathcal{N}(0, \sigma^2)$  with  $\mu$  of low rank
  - ⇒ Different regularization depending on noise regime<sup>7</sup>
  - ⇒ Count data,<sup>8</sup> ordinal data, categorical data, blocks/multilevel data
- ▷ Optimal transport,<sup>9</sup> deep generative models: GAIN,<sup>10</sup> MIWAE,<sup>11</sup> etc.<sup>12,13</sup>

## Iterating conditional models (joint distribution implicitly defined)

- ▷ with parametric regression (M)ICE: (Multiple) Imput. by Chained Equations<sup>14</sup>
- ▷ iterative imputation of each variable by random forests<sup>15</sup>

<sup>7</sup>J. & Wager. Stable autoencoding for regularized low-rank matrix estimation. *JMLR*. 2016.

<sup>8</sup>Robin, Klopp, J., Moulines, Tibshirani. Main effects & interac. in mixed data. *JASA*. 2019.

<sup>9</sup>Muzelec, Cuturi, Boyer, J. Missing Data Imputation using Optimal Transport. *ICML*. 2020.

<sup>10</sup>Yoon et al. GAIN: Missing data imputation using generative adversarial nets. *ICML*. 2018.

<sup>11</sup>Mattei & Frellsen. Miwae: Deep generative model. & imput. of incomplete data. *ICML*. 2018.

<sup>12</sup>Deng et al. Extended missing data imput. via gans. *Data Mining & Knowledge Discovery*. 2022.

<sup>13</sup>Fang Bao. Fragmgan gan for fragmentary data imputation. *Stat.theory & Related Fields*. 2023.

<sup>14</sup>van Buuren, S. Flexible Imputation of Missing Data. Chapman Hall/CRC Press. 2018.

<sup>15</sup>Stekhoven & Bühlmann. MissForest–non-parametric imputation for mixed data. *Bioinfo*. 2012.

# Missing values mechanism: Rubin's taxonomy<sup>16,17</sup>

- Random Variables:

- ▷  $X^* \in \mathbb{R}^d$ : complete unavailable data,  $X \in \mathbb{R}^d$ : observed data with NA
- ▷  $M \in \{0, 1\}^d$ : missing pattern, or mask,  $M_j = 1$  if and only if  $X_j$  is missing

- Realizations: For a pattern  $m$ ,  $o(x, m) = (x_j)_{j \in \{1, \dots, d\}: m_j=0}$  the observed elements of  $x$  and while  $o^c(x, m) = (x_j)_{j \in \{1, \dots, d\}: m_j=1}$ , the missing elements.

$$x^* = (1, 2, 3, 8, 5)$$

$$x = (1, \text{NA}, 3, 8, \text{NA})$$

$$m = (0, 1, 0, 0, 1)$$

$$o(x, m) = (1, 3, 8), \quad o^c(x^*, m) = (2, 5)$$

<sup>16</sup>Rubin. Inference and missing data. *Biometrika*. 1976.

<sup>17</sup>What Is Meant by "Missing at Random"? Seaman, et al. *Statistical Science*. 2013.

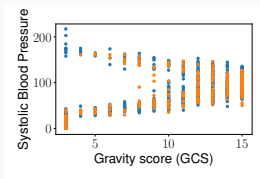
# Missing values mechanism: Rubin's taxonomy<sup>16,17</sup>

- Random Variables:

- ▷  $X^* \in \mathbb{R}^d$ : complete unavailable data,  $X \in \mathbb{R}^d$ : observed data with NA
- ▷  $M \in \{0, 1\}^d$ : missing pattern, or mask,  $M_j = 1$  if and only if  $X_j$  is missing

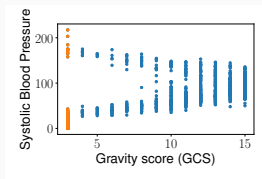
For a pattern  $m$ ,  $o(x, m) = (x_j)_{j \in \{1, \dots, d\}: m_j=0}$  the observed elements of  $x$  and while  $o^c(x, m) = (x_j)_{j \in \{1, \dots, d\}: m_j=1}$ , the missing elements.

Ex: Simulated missing values according to the 3 mechanisms (Orange points will be missing) in Systolic Blood Pressure - GCS is always observed



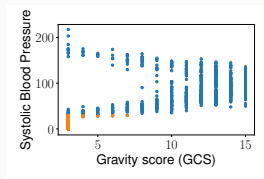
Missing Completely at Random (MCAR)

$$m \in \mathcal{M}, x \in \mathcal{X}, \\ \mathbb{P}(M = m|x) = \mathbb{P}(M = m)$$



Missing at Random (MAR)

$$\forall m \in \mathcal{M}, x \in \mathcal{X} \\ \mathbb{P}(M = m|x) = \mathbb{P}(M = m|o(x, m))$$



Missing Not At Random (MNAR)

If not MAR: it is MNAR

<sup>16</sup>Rubin. Inference and missing data. *Biometrika*. 1976.

<sup>17</sup>What Is Meant by "Missing at Random"? Seaman, et al. *Statistical Science*. 2013.



# Two views to model the joint distribution of $(X, M)$

**Selection Model**<sup>18</sup>:  $p^*(M = m, x) = \mathbb{P}(M = m | x)p^*(x)$

## Definition (SM-MAR)

$$\mathbb{P}(M = m | x) = \mathbb{P}(M = m | o(x, m)) \text{ for all } m \in \mathcal{M}, x \in \mathcal{X}.$$

The proba. of any  $m$  occurring only depends on the obs part of  $x$ .

**Pattern Mixture Model**<sup>19</sup>:  $p^*(M = m, x) = p^*(x | M = m)\mathbb{P}(M = m)$

## Definition (PMM-MAR)

$$p^*(o^c(x, m) | o(x, m), M = m) = p^*(o^c(x, m) | o(x, m)).$$

for all  $m \in \mathcal{M}, x \in \mathcal{X}$ . The conditional distrib. of missing given obs. in pattern  $m$  is equal to the unconditional one.<sup>20</sup>

<sup>18</sup>Heckman. Sample selection bias as a specification error. *Econometrica*. 1979

<sup>19</sup>Little. Pattern-mixture models for multivariate incomplete data. *JASA*. 1993

<sup>20</sup>Molenberghs et al. Every MNAR model has a MAR counterpart with equal fit. *JRSSB*. 2008

# Two views to model the joint distribution of $(X, M)$

**Selection Model**<sup>18</sup>:  $p^*(M = m, x) = \mathbb{P}(M = m | x)p^*(x)$

## Definition (SM-MAR)

$$\mathbb{P}(M = m | x) = \mathbb{P}(M = m | o(x, m)) \text{ for all } m \in \mathcal{M}, x \in \mathcal{X}.$$

The proba. of any  $m$  occurring only depends on the obs part of  $x$ .

**Pattern Mixture Model**<sup>19</sup>:  $p^*(M = m, x) = p^*(x | M = m)\mathbb{P}(M = m)$

## Definition (PMM-MAR)

$$p^*(o^c(x, m) | o(x, m), M = m) = p^*(o^c(x, m) | o(x, m)).$$

for all  $m \in \mathcal{M}, x \in \mathcal{X}$ . The conditional distrib. of missing given obs. in pattern  $m$  is equal to the unconditional one.<sup>20</sup>

## Proposition (SM-MAR is equivalent to PMM-MAR)

<sup>18</sup>Heckman. Sample selection bias as a specification error. *Econometrica*. 1979

<sup>19</sup>Little. Pattern-mixture models for multivariate incomplete data. *JASA*. 1993

<sup>20</sup>Molenberghs et al. Every MNAR model has a MAR counterpart with equal fit. *JRSSB*. 2008

## MAR with shift in marginal distribution between patterns

- Gaussian PMM:  $X^* | M = m \sim N(\mu_m | \Sigma_m)$ . Ex: for two patterns  $m_1 = (0, 0)$  and  $m_2 = (1, 0)$  and a **shift**:

$$\mathbf{X} = \begin{pmatrix} x_{1,1} & x_{1,2} \\ NA & x_{2,2} \end{pmatrix}, \mathbf{M} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} m_1 \\ m_2 \end{pmatrix}.$$

## MAR with shift in marginal distribution between patterns

- Gaussian PMM:  $X^* | M = m \sim N(\mu_m | \Sigma_m)$ . Ex: for two patterns  $m_1 = (0, 0)$  and  $m_2 = (1, 0)$  and a **shift**:

$$(X_1, X_2) | M = m_1 \sim N \left( \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix} \right) \quad (X_1, X_2) | M = m_2 \sim N \left( \begin{pmatrix} 5 \\ 5 \end{pmatrix}, \begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix} \right).$$

## MAR with shift in marginal distribution between patterns

- Gaussian PMM:  $X^* | M = m \sim N(\mu_m | \Sigma_m)$ . Ex: for two patterns  $m_1 = (0, 0)$  and  $m_2 = (1, 0)$  and a **shift**:

$$(X_1, X_2) | M = m_1 \sim N \left( \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix} \right) \quad (X_1, X_2) | M = m_2 \sim N \left( \begin{pmatrix} 5 \\ 5 \end{pmatrix}, \begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix} \right).$$

- Not identifiable without restriction. How distributions can change?

$$= \underbrace{p^*(x_1 | x_2, M = m_2)}_{p^*(o^c(x, m_2) | o(x, m_2), M = m_2)} = N(x_2, 1)(x_1) = p^*(x_1 | x_2).$$

# MAR with shift in marginal distribution between patterns

- Gaussian PMM:  $X^* | M = m \sim N(\mu_m | \Sigma_m)$ . Ex: for two patterns  $m_1 = (0, 0)$  and  $m_2 = (1, 0)$  and a **shift**:

$$(X_1, X_2) | M = m_1 \sim N \left( \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix} \right) \quad (X_1, X_2) | M = m_2 \sim N \left( \begin{pmatrix} 5 \\ 5 \end{pmatrix}, \begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix} \right)$$

- Not identifiable without restriction. How distributions can change?

$$\underbrace{p^*(x_1 | x_2, M = m_1)}_{p^*(o^c(x, m_2) | o(x, m_2), M = m_1)} = \underbrace{p^*(x_1 | x_2, M = m_2)}_{p^*(o^c(x, m_2) | o(x, m_2), M = m_2)} = N(x_2, 1)(x_1) = p^*(x_1 | x_2).$$

## Definition (Conditional indep. MAR - CIMAR)

$$p^*(o^c(x, m) | o(x, m), M = m') = p^*(o^c(x, m) | o(x, m)).$$

for all  $m, m' \in \mathcal{M}, x \in \mathcal{X}$ . equivalent to  $o^c(X^*, m) | o(X^*, m) \perp\!\!\!\perp M$

# MAR with shifts in conditional distribution between patterns

$$\mathbf{X} = \begin{pmatrix} x_{1,1} & x_{1,2} & x_{1,3} \\ NA & x_{2,2} & x_{2,3} \\ NA & NA & x_{3,3} \end{pmatrix}, \mathbf{M} = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 1 & 0 \end{pmatrix} = \begin{pmatrix} m_1 \\ m_2 \\ m_3 \end{pmatrix}$$

## CIMAR

$$p^*(x_1, x_2 \mid x_3, M = m_1) = p^*(x_1, x_2 \mid x_3, M = m_2) = p^*(x_1, x_2 \mid x_3, M = m_3) = p^*(x_1, x_2 \mid x_3)$$

Distrib. of  $X_1, X_2 \mid X_3$  is not allowed to change from one pattern to another, though the marginal distrib. of  $X_3$  can change.

## PMM-MAR

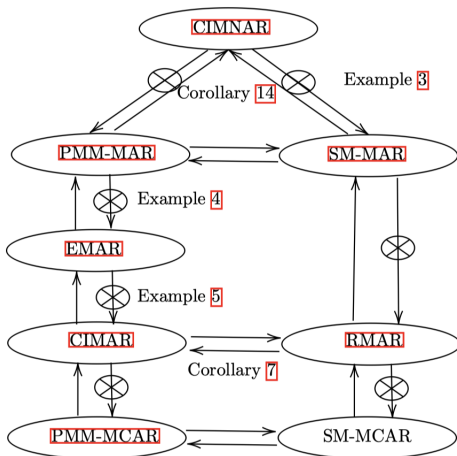
$$p^*(x_1, x_2 \mid x_3, M = m_3) = p^*(x_1, x_2 \mid x_3)$$

**Both distrib. of observed variables and conditional ones can change from pattern to pattern.**

**MCAR: No change allowed.**

$$m \in \mathcal{M}, m' \in \mathcal{M}, x \in \mathcal{X}, p^*(x) = p^*(x \mid M = m) = p^*(x \mid M = m')$$

# Relationships between the M(N)AR conditions





# (Non) Identifiability under non-parametric MAR

## Definition: Imputing with a mixture of distribution

$p^*(o^c(x, m) \mid o(x, m))$  is identifiable from  $\mathcal{M}_0 \subset \mathcal{M}$  if there exists some weights  $w_{m'}(o(x, m))$  (summing to 1) such that the mixture

$$h^*(o^c(x, m) \mid o(x, m)) = \sum_{m' \in \mathcal{M}_0} w_{m'}(o(x, m)) p^*(o^c(x, m) \mid o(x, m), M = m')$$

satisfies  $p^*(o^c(x, m) \mid o(x, m)) = h^*(o^c(x, m) \mid o(x, m))$ .

## Proposition: Identifiability under PMM-MAR is not trivial

Assume  $|\mathcal{M}| > 3$ . For any pattern  $m \in \mathcal{M}$ ,  $p^*(o^c(x, m) \mid o(x, m))$  is

- identifiable from any other pattern  $m' \neq m$  under CIMAR,
- is not identifiable from any single pattern  $m' \neq m$  under PMM-MAR.

If  $\left| \sum_{j=1}^d m_j \right| > 1$ ,  $p^*(o^c(x, m) \mid o(x, m))$  is not identifiable from  $L_m$ , the set of patterns for which  $o^c(x, m)$  is observed.

$L_m = \{m' \in \mathcal{M} : m'_j = 0 \text{ for all } j \text{ such that } m_j = 1\}$ .

# Identifiability under MAR considering one variable at a time

- Consider the following mixture of distribution

$$h^*(x_j | x_{-j}) = \sum_{m \in L_j} \frac{\mathbb{P}(M = m)}{\sum_{m \in L_j} p^*(x_{-j} | M = m) \mathbb{P}(M = m)} p^*(x | M = m),$$

with  $L_j = \{m \in \mathcal{M} : m_j = 0\}$ , the patterns where  $x_j$  is observed

## Theorem: Identifiability of the right conditional distribution

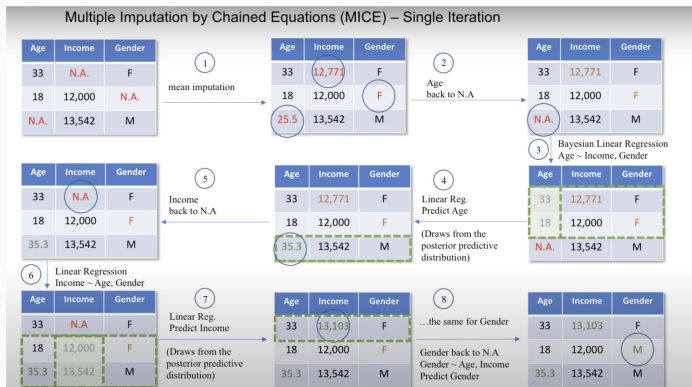
Assume **PMM-MAR** holds,

$$h^*(x_j | x_{-j}) = p^*(x_j | x_{-j}), \text{ for all } x_{-j} \text{ with } p^*(x_{-j}) > 0$$

At  $X_j$ , one can reduce the  $|\mathcal{M}|$  patterns to two, one where  $X_j$  is missing, and one where it is observed. Though these two aggregated patterns are mixtures of several patterns  $m \in \mathcal{M}$ , MAR implies that both aggregated patterns have the same conditional distribution  $X_j^* | X_{-j}^*$

# Fully conditional specification - FCS, (M)ICE

1. Fill NA with plausible values to get an initial completed dataset
2. For  $j \in \{1, \dots, d\}$ ,  $t \geq 1$  use a univariate imputation to sample new imputed values  $x_j^{(t+1)} \sim p^t(x_j | x_{-j}^{(t)})$ , where  $x_{-j}^{(t)} = \{x_l^{(t)}\}_{l \neq j}$  the imputed & observed values of other variables except  $j$  at the  $t$ th iteration.
3. Iterate until convergence



# Fully conditional specification - FCS, (M)ICE

1. Fill NA with plausible values to get an initial completed dataset
2. For  $j \in \{1, \dots, d\}$ ,  $t \geq 1$  use a univariate imputation to sample new imputed values  $x_j^{(t+1)} \sim p^t(x_j | x_{-j}^{(t)})$ , where  $x_{-j}^{(t)} = \{x_l^{(t)}\}_{l \neq j}$  the imputed & observed values of other variables except  $j$  at the  $t$ th iteration.
3. Iterate until convergence

**Theorem** shows that if we assume to have access to the true distribution  $p^*(x_{-j})$  (assume  $x_{-j}$  is well imputed), we can impute according to the true distribution  $p^*(x_j | x_{-j})$  by drawing from the conditional distrib. of  $X_j | X_{-j}$  **learned from all patterns in which  $x_j$  is observed**

**FCS approach can identify the right conditional distributions under PMM MAR**

# What is a good imputation method under MAR?

- ▷ both conditional and marginal **distribution shifts** can occur for different patterns under MAR.
- ▷ conditional shifts are handled with FCS

## An ideal imputation method should

- ▷ (1) be a distributional regression method,
- ▷ (2) be able to capture nonlinearities in the data,
- ▷ (3) be able to deal with distributional shifts in the observed variables,
- ▷ (4) be fast to fit,

1-3 are crucial for imputation under MAR

4 is only relevant to reduce the computational burden.

Rk: Block-wise FCS (multi-output methods to impute variables as blocks) should not be used: do not recover the correct distribution

# What is a good imputation method?

- (1) be a distributional regression method,
- (2) be able to capture nonlinearities in the data,
- (3) be able to deal with distributional shifts in the observed variables,

Method	(1)	(2)	(3)
missForest (Stekhoven & Bühlmann, 2011)		✓	
<a href="#">mice-cart</a> (Burgette & Reiter, 2010)	✓	✓	
<a href="#">mice-RF</a> (Doove et al., 2014)	✓	✓	
<a href="#">mice-DRF</a> (Näf et al., 2024)	✓	✓	
mice-norm.nob (Gaussian)	✓		✓
mice-norm.predict (Regression)			✓

# What is a good imputation method?

- (1) be a distributional regression method,
- (2) be able to capture nonlinearities in the data,
- (3) be able to deal with distributional shifts in the observed variables,

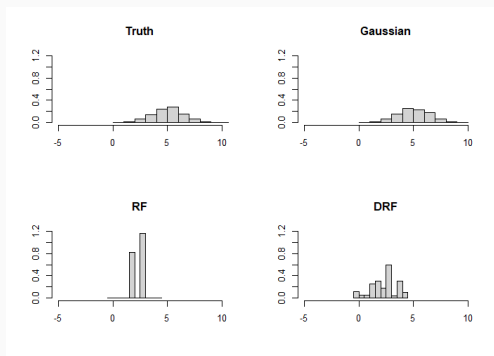
Method	(1)	(2)	(3)
missForest (Stekhoven & Bühlmann, 2011)		✓	
<a href="#">mice-cart</a> (Burgette & Reiter, 2010)	✓	✓	
<a href="#">mice-RF</a> (Doove et al., 2014)	✓	✓	
<a href="#">mice-DRF</a> (Näf et al., 2024)	✓	✓	
mice-norm.nob (Gaussian)	✓		✓
mice-norm.predict (Regression)			✓

- ▷ [mice-cart/RF](#) estimate a tree, a forest, on observed data and then draw imputations from the leaves (approx conditional distribution) whereas distributional forest<sup>21</sup> is a distributional method

<sup>21</sup>Cevid et al., Distributional Random Forests. *JMLR*. 2022

# Forests generalize poorly outside of the training set

Ex: Variables income & age with MAR missing values in income



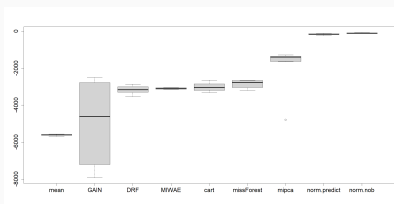
**Figure 1:** True distribution against a draw from different imputation methods.

DRF, a distributional method  $>$  mice-RF but fails to deal with the covariate shift (centering  $\approx 2$  instead of 5).

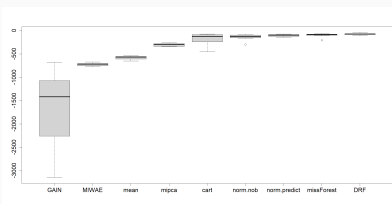
Finding an imputation method that meets (1) - (4) is still an open problem!



# Empirical study: ranking with energy scores and not RMSE



Gaussian relation with shifts



Non linear relation with shifts

Ex with  $d = 6$ ,  $n = 1500$ , 20% NA and CIMAR,  $X_{O^c} = \mathbf{B}f(X_O) + \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \end{pmatrix}$

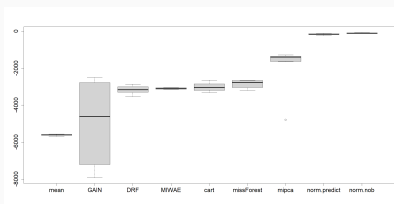
**Energy distance<sup>22</sup> between imputed & real data**

$$d(H, P^*) = 2\mathbb{E}[\|X - Y\|_{\mathbb{R}^d}] - \mathbb{E}[\|X - X'\|_{\mathbb{R}^d}] - \mathbb{E}[\|Y - Y'\|_{\mathbb{R}^d}],$$

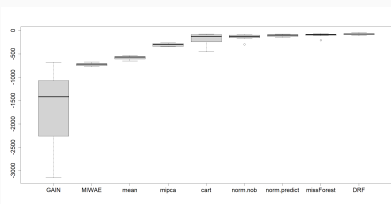
where  $\|\cdot\|_{\mathbb{R}^d}$  is the Euclidean metric on  $\mathbb{R}^d$ ,  $X \sim H$ ,  $Y \sim P^*$  and  $X'$ ,  $Y'$  are independent copies of  $X$  and  $Y$ .

<sup>22</sup>Székely & Rizzo. Energy statistics *Journal of stat. planning & inference*. 2013

# Empirical study: ranking with energy scores and not RMSE



Gaussian relation with shifts



Non linear relation with shifts

Ex with  $d = 6$ ,  $n = 1500$ , 20% NA and CIMAR,  $X_{0c} = \mathbf{B}f(X_0) + \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \end{pmatrix}$

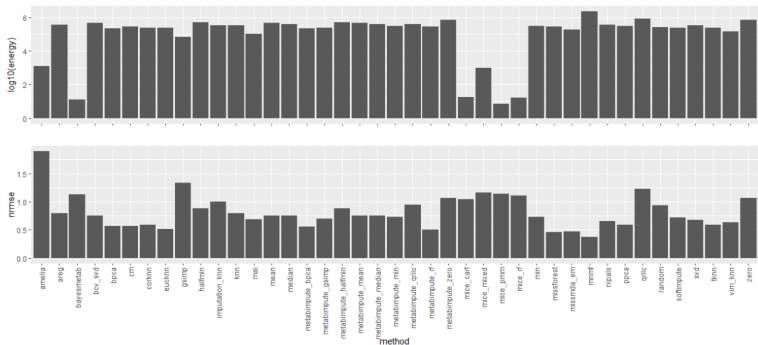
## Energy distance<sup>22</sup> between imputed & real data

$$d(H, P^*) = 2\mathbb{E}[\|X - Y\|_{\mathbb{R}^d}] - \mathbb{E}[\|X - X'\|_{\mathbb{R}^d}] - \mathbb{E}[\|Y - Y'\|_{\mathbb{R}^d}],$$

where  $\|\cdot\|_{\mathbb{R}^d}$  is the Euclidean metric on  $\mathbb{R}^d$ ,  $X \sim H$ ,  $Y \sim P^*$  and  $X'$ ,  $Y'$  are independent copies of  $X$  and  $Y$ .

<sup>22</sup>Székely & Rizzo. Energy statistics *Journal of stat. planning & inference*. 2013

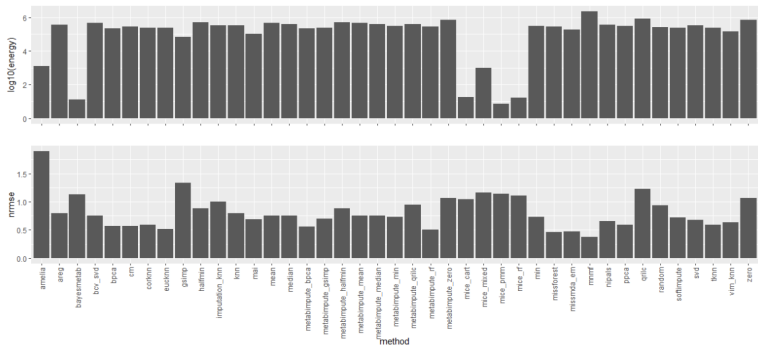
# Empirical study: ranking with energy scores and not RMSE



credit: Krystyna Grzesiak, Michal Burdukiewicz<sup>23</sup> 230 scenarios (10 missing values patterns 23 different-size datasets)

<sup>23</sup>imputomics: web server and R package for missing values imputation in metabolomics data. *Bioinformatics* 2024.

# Empirical study: ranking with energy scores and not RMSE



credit: Krystyna Grzesiak, Michal Burdukiewicz<sup>23</sup> 230 scenarios (10 missing values patterns 23 different-size datasets)

<sup>23</sup>imputomics: web server and R package for missing values imputation in metabolomics data. *Bioinformatics* 2024.

# Conclusion

- ▷ Non-parametric PMM view of missing (different environments) helps understand non-parametric imputation under MAR
- ▷ Identification result for FCS: the right conditional distributions are identifiable under MAR with no parametric assumption
- ▷ Identification under the weakest MAR assumption.<sup>24</sup> Beyond MAR.  $\forall j \in \{1, \dots, d\}, \forall x \in \mathcal{X}$ , CIMNAR:  $\mathbb{P}(M_j = 1|x) = \mathbb{P}(M_j = 1|x_{-j})$

<sup>24</sup>Deng et al., (2022) and Fang (2023) showed identifiability for GAN imputation under CIMAR

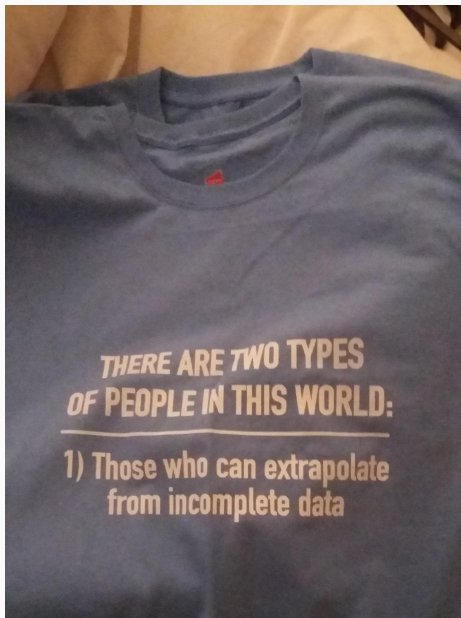
# Conclusion

- ▷ Non-parametric PMM view of missing (different environments) helps understand non-parametric imputation under MAR
- ▷ Identification result for FCS: the right conditional distributions are identifiable under MAR with no parametric assumption
- ▷ Identification under the weakest MAR assumption.<sup>24</sup> Beyond MAR.  $\forall j \in \{1, \dots, d\}, \forall x \in \mathcal{X}$ , CIMNAR:  $\mathbb{P}(M_j = 1|x) = \mathbb{P}(M_j = 1|x_{-j})$
- ▷ The quest for an FCS imputation method meeting all 3 points is open
- ▷ mice-DRF promising (code available)
- ▷ Imputation scores with missing values that are proper under MAR: ranking imputation methods
- ▷ Simulations MAR for benchmarks

---

<sup>24</sup>Deng et al., (2022) and Fang (2023) showed identifiability for GAN imputation under CIMAR

# Thank you



## Imputing with a mixture of patterns

$$\mathbf{X} = \begin{pmatrix} x_{1,1} & x_{1,2} & x_{1,3} \\ x_{2,1} & NA & x_{2,3} \\ NA & x_{3,2} & x_{3,3} \end{pmatrix}, \mathbf{M} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} = \begin{pmatrix} m_1 \\ m_2 \\ m_3 \end{pmatrix}.$$

whereby  $(X_1, X_2, X_3)$  are independently uniformly distributed on  $[0, 1]$ .

$$\mathbb{P}(M = m_1 | \mathbf{x}) = \mathbb{P}(M = m_1 | x_1) = x_1/3$$

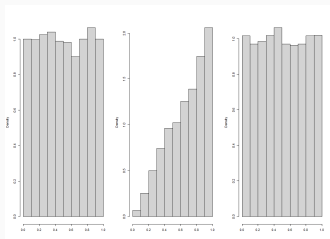
$$\mathbb{P}(M = m_2 | \mathbf{x}) = \mathbb{P}(M = m_2 | x_1) = 2/3 - x_1/3$$

$$\mathbb{P}(M = m_3 | \mathbf{x}) = \mathbb{P}(M = m_3) = 1/3.$$



# Imputing with a mixture of patterns

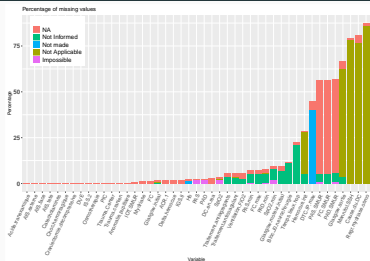
We want to impute  $X_1$  in the third pattern (with  $X_2$  and  $X_3$  observed)



**Figure 2:** Distrib. of  $X_1$  in different patterns. Left: Distrib. of  $X_1 \mid M = m_3$ . Middle:  $(X_1 \mid M = m_1)$ . Right: Distribution of all patterns for which  $X_1$  is observed (Mixture of the distribution of  $X_1$  in pattern 1 and 2).

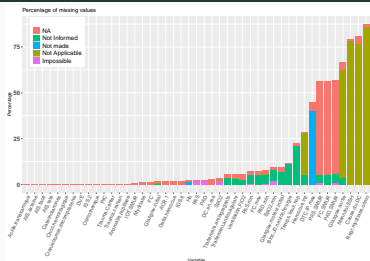
- As the distrib. of  $(X_2, X_3)$  in each patterns is the same, this shows the change of  $X_1 \mid X_2, X_3$  from  $m_3$  to  $m_1$ : PMM-MAR allows change in the conditional distrib. over patterns.
- Note that the distrib.  $X_1 \mid X_2, X_3$  in  $m_3$  corresponds to the mixture of distribution of  $X_1 \mid X_2, X_3$  in the patterns where  $X_1$  is observed.

# Missing data: important bottleneck in statistical practice



"One of the ironies of Big Data is that missing data play an ever more significant role"<sup>25</sup>

# Missing data: important bottleneck in statistical practice



*"One of the ironies of Big Data is that missing data play an ever more significant role"*<sup>25</sup>

Complete case analysis: delete incomplete samples

- **Bias:** Resulting sample not representative of the target population
- **Information loss:** Take a matrix with  $d$  features where each entry is missing with probability  $1/100$ , remove a row (of length  $d$ ) when one entry is missing

$$d = 5 \quad \implies \quad \approx 95\% \text{ of rows kept}$$

$$d = 300 \quad \implies \quad \approx 5\% \text{ of rows kept}$$

<sup>25</sup>Zhu, Wang, Samworth. High-dimensional PCA with heterogeneous missingness. *JRSSB*. 2022.