Introduction to missing values

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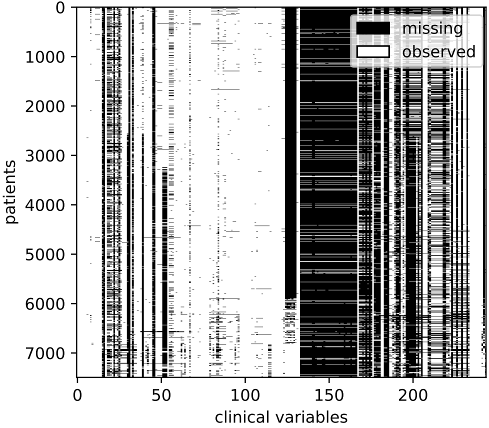
Incomplete data is ubiquitous in many fields



traumabase.eu

Statistical inference

Suppose we are given a data matrix $X \in \mathbb{R}^{n \times d}$ with n samples and d variables.

$$X = \begin{pmatrix} 1.2 & 0.7 & 0.2 & -0.4 \\ -0.3 & 0.1 & -0.1 & -0.9 \\ 1.5 & 0.4 & 2.3 & -0.5 \\ -2.8 & 1.9 & 1.6 & 2.2 \\ -0.4 & 1.7 & -2.4 & -1.5 \end{pmatrix}$$

We wish to make **inference** on some aspects of the distribution of X.

- Non-parametric inference: estimate the **mean**, the **covariance**, **variance**, ...
- Parametric inference: assume the data was drawn from a given probability distribution (e.g. Gaussian distribution) and estimate the parameters of the distribution.

Statistical inference

Suppose we are given a data matrix $X \in \mathbb{R}^{n \times d}$ with n samples and d variables.

$$X = \begin{pmatrix} 1.2 & \texttt{na} & 0.2 & -0.4 \\ -0.3 & \texttt{na} & \texttt{na} & -0.9 \\ \texttt{na} & 0.4 & \texttt{na} & \texttt{na} \\ -2.8 & 1.9 & 1.6 & 2.2 \\ \texttt{na} & 1.7 & -2.4 & \texttt{na} \end{pmatrix}$$

How to make valid inference using observed data only?

We wish to make **inference** on some aspects of the distribution of X.

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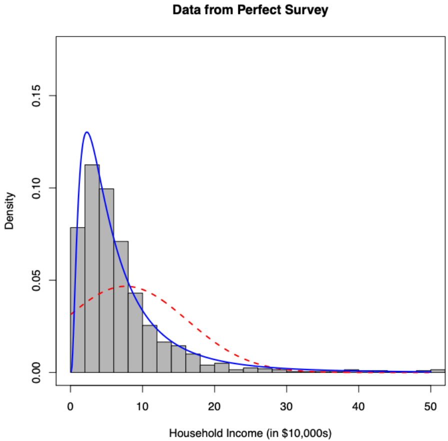
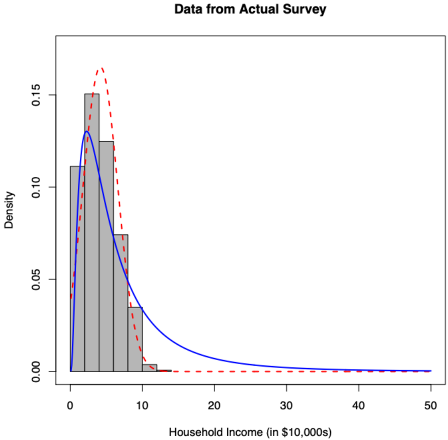
The importance of the missing data mechanism

Data from the US Census Bureau for 2012 indicate that median annual household income in the US is approximately 51,000$ (distribution represented by the blue curve).



100% of survey participants responded
Sample median: 50,556$



66% of survey participants responded
Sample median: 38,625$

The importance of the missing data mechanism

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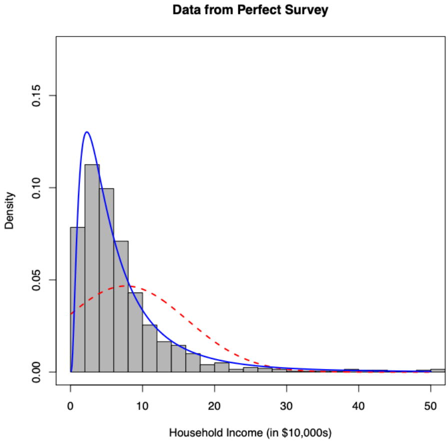
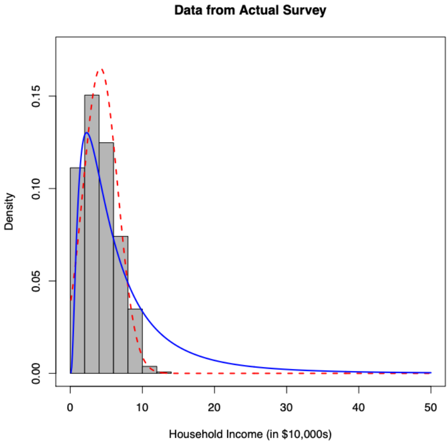


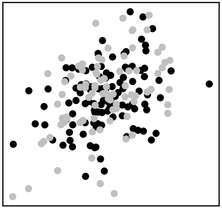


Different assumptions about the missing data mechanism leads to different inferences about the true distribution.

The missing data mechanisms: MCAR, MAR, and MNAR.

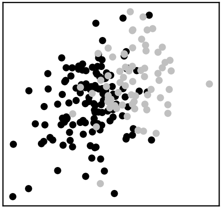
- In 1976, Rubin (1976) has formalized 3 missing data mechanisms:
  - Missing Completely at Random: $P(M = m|X) = P(M = m)$
  - Missing at Random: $P(M = m|X) = P(M = m|X_{obs(m)})$
  - Missing Non At Random: all other cases.

MCAR



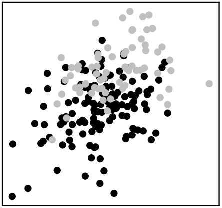
$P(M_2 = 1|X) = 0.5$

MAR



$P(M_2 = 1|X) = \sigma(X_1)$

MNAR



$P(M_2 = 1|X) = \sigma(X_2)$

The missing data mechanisms: MCAR, MAR, and MNAR.

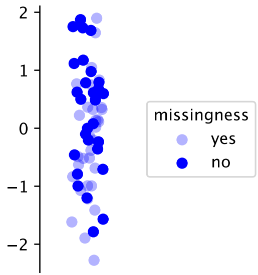
- The data analyst must make an assumption about the mechanism.
  - Difficulty for inference: MCAR $\leq$ MAR $\leq$ MNAR.
  - MCAR unrealistic in general.
  - Most developments for inference since the 70s require the MAR assumption to hold.
  - Fundamental challenge: the assumption cannot be verified from the observed data.
  - MAR can be justified using domain knowledge.
  - Guideline: collect rich additional variable, ideally always observed, to render MAR plausible.

The literature on missing values

Since the 70s, an abundant literature on missing data has flourished, mainly focused on **inference** and **imputation** tasks.

Inference

- e.g. estimating means and variances.



- Ad-hoc methods:
  - Complete-case analysis.
  - Single imputation.
- Principled methods:
  - Inverse Probability Weighting (IPW).
  - Likelihood-based inference on $P(M, X)$.
  - Multiple imputation.

Naive method 1: complete-case analysis

- **Complete-case analysis**: only keep the observations without missing values, and proceed with the complete subsample.

$$\begin{pmatrix} 1.2 & 3.2 & 0.2 & -0.4 \\ \texttt{na} & 0.4 & \texttt{na} & \texttt{na} \\ -2.8 & 1.9 & 1.6 & 2.2 \\ \texttt{na} & 1.7 & -2.4 & \texttt{na} \end{pmatrix} \implies \begin{pmatrix} 1.2 & 3.2 & 0.2 & -0.4 \\ -2.8 & 1.9 & 1.6 & 2.2 \end{pmatrix}$$

- **Example with inference of the mean**:

  Let $X \in \mathbb{R}^n$ be a variable with missing values.
  Let $M \in \{0,1\}^n$ be its missing indicator (1 means observed).

$$\hat{\mu}^{cc} = \frac{\sum_{i=1}^n M_i X_i}{\sum_{i=1}^n M_i}$$

- **Drawbacks:**
  - The loss of information can be considerable (d = 20, missing rate 10% $\implies$ proba of 0.13 to observe a complete case).
  - Dangerous when the data is not MCAR $\implies$ biased estimator.

Naive method 2: Single imputation methods

- **Single imputation analysis**: fill in the missing values and carry on with the completed dataset.
  - Unconditional imputation: use the mean of observed values.
  - Conditional imputation: learn a regressor to predict missing values from observed variables.

$$X = \begin{pmatrix} 1.2 & 3.2 & 0.2 & -0.4 \\ \texttt{na} & 0.4 & \texttt{na} & \texttt{na} \\ -2.8 & 1.9 & 1.6 & 2.2 \\ \texttt{na} & 1.7 & -2.4 & \texttt{na} \end{pmatrix} \implies \hat{X} = \begin{pmatrix} 1.2 & 3.2 & 0.2 & -0.4 \\ -0.8 & 0.4 & -0.2 & 0.9 \\ -2.8 & 1.9 & 1.6 & 2.2 \\ -0.8 & 1.7 & -2.4 & 0.9 \end{pmatrix}$$

- **Example with inference of the mean**:

  Let $X \in \mathbb{R}^n$ be a variable with missing values, and $\hat{X} \in \mathbb{R}^n$ its imputed version. Let $M \in \{0,1\}^n$ be its missing indicator (1 means observed).

$$\hat{\mu}^{imp} = \frac{1}{n}\sum_{i=1}^{n} M_i X_i + (1 - M_i)\hat{X}_i$$

Naive method 2: Single imputation methods

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  - Unconditional imputation: use the mean of observed values.
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- **Drawbacks**:
  - Biased inference unless MCAR in most cases.
  - Distorted measures of uncertainty in most cases (e.g. confidence intervals, variances, ...)

Inverse Probability Weighting - 1/2

- **Intuition**: Reweight samples so that those that are more likely to be missing are given larger weights to account for the similar samples that are missing.

- **Example with inference of the mean**:
  Let $X \in \mathbb{R}^n$ be a variable with missing values.
  Let $M \in \{0,1\}^n$ be its missing indicator (1 means observed).
  Let $V \in \mathbb{R}^n$ be a completely observed variable.
  Suppose that the proba of X_i being observed is given by $P(M_i = 1 | V_i) = \pi(V_i)$.

$$\hat{\mu}^{IPW} = \frac{1}{n} \sum_{i=1}^{n} \frac{X_i M_i}{\pi(V_i)}$$

- **Need to estimate** $\pi(V_i)$
  Usually estimated with a logistic regression where M_i are the labels, and V_i the features.

- Unbiased under MAR and if $\pi(V_i)$ is well specified.

Inverse Probability Weighting - 2/2

- **Drawbacks**:
  - Difficult to know whether $\pi(V_i)$ is well specified.
  - Instabilities when $\pi(V_i)$ is too small.
  - Data inefficiency because only complete cases are used.
- Subsequent works have focused on improving the IPW:
  - The Augmented IPW (AIPW) solves the inefficiency issue:

$$\hat{\mu}^{AIPW} = \frac{1}{n} \sum_{i=1}^{n} \left(\frac{X_i M_i}{\pi(V_i)} - \frac{M_i - \pi(V_i)}{\pi(V_i)} \mathbb{E}\left[X_i | V_i\right] \right)$$

  See how $\mathbb{E}\left[X_i | V_i\right]$ replaces X_i when X_i is missing.

Likelihood-based methods - 1/3

- Review of maximum likelihood estimation with complete data.

- We need to assume a **parametric model** for the probability density of X, with parameters θ:

$$X \sim p_\theta(X).$$

  For example, we can assume the data follows a Gaussian distribution with parameters $\theta = (\mu, \Sigma)$.

- The goal is to find the parameters $\hat{\theta}$ that maximize the **likelihood** $\mathcal{L}$ of the data:

$$\mathcal{L}(\theta) = \prod_{i=1}^{n} p_\theta(X_i)$$

  $\hat{\theta}$ is called a maximum likelihood estimator (MLE).

- Standard techniques for maximizing the likelihood cannot be applied when it is not fully observed.

Likelihood-based methods - 2/3

- We wish to estimate the parameter θ of the full data distribution $p_\theta(X)$ using only the observed data (M, X_{obs}).

$$\begin{aligned}
p_{\theta,\phi}(M, X_{obs}) &= \int p_{\theta,\phi}\left(M, X_{obs}, X_{mis}\right) dX_{mis} && \text{Marginalisation} \\
&= \int p_\phi\left(M|X_{obs}, X_{mis}\right) p_\theta\left(X_{obs}, X_{mis}\right) dX_{mis} && \text{Bayes rule} \\
&= \int p_\phi\left(M|X_{obs}\right) p_\theta\left(X_{obs}, X_{mis}\right) dX_{mis} && \textbf{MAR hyp.} \\
&= p_\phi\left(M|X_{obs}\right) \int p_\theta\left(X_{obs}, X_{mis}\right) dX_{mis} \\
&= p_\phi\left(M|X_{obs}\right) p_\theta\left(X_{obs}\right)
\end{aligned}$$

where $p_\phi(M|X)$ is called the missingness mechanism and $p_\theta(X_{obs})$ the observed data likelihood.

- **Ignorability**: The missingness mechanism can be ignored. It does not need to be modeled for the purpose of calculating the MLE $\hat{\theta}$.

$$\hat{\theta} = \underset{\theta}{\text{argmax}} \prod_{i=1}^{n} p_\theta(X_{i,obs})$$

Likelihood-based methods - 3/3

Question:How do we solve this optimization problem?

$$\hat{\theta} = \underset{\theta}{\text{argmax}} \prod_{i=1}^{n} p_\theta(X_{i,obs})$$

- Usually, we posit a model for the complete data distributuon: $p_\theta(X)$.
- It is not always analytically tractable to compute

$$p_\theta(X_{obs}) = \int p_\theta \left(X_{obs}, X_{mis}\right) dX_{mis}.$$

Answer: use the **Expectation-Maximization (EM)** algorithm.

- EM algorithm: maximizes objective functions in the presence of latent variables (in our case, the missing values).
- In practice, the `norm` package in R implements EM with missing values (assuming p_θ is multivariate Gaussian).

Multiple Imputation - 1/2

As for likelihood-based methods, we assume a parametric model $P_\theta(X)$, and the goal is inference on θ.

- Multiple Imputation involves 3 steps:
  1. **Impute** missing values R times to create R completed datasets:
  $$X^{(r)} = \left(X_{obs}, X_{mis}^{(r)}\right) \text{ for } r = 1, \ldots, R$$
  2. Carry out the **full data analysis**. For example, using the MLE:
  $$\hat{\theta}^{(r)} = \underset{\theta}{\operatorname{argmax}} \prod_{i=1}^{n} p_\theta(X_{i,obs}, X_{i,mis}^{(r)})$$
  3. **Combine** the M results into the final one by averaging:
  $$\hat{\theta} = \frac{1}{R} \sum_{r=1}^{R} \hat{\theta}^{(r)}$$
- Again, Multiple Imputation is only valid under **MAR** assumption.

Multiple Imputation - 2/2

Concerning the imputation (step 1):

- In theory, draw $X_{mis}^{(r)}$ from $p_{\theta^{(init)}}\left(X_{mis}|X_{obs}, M\right)$ (improper imputation).
- In practice, two widespread options to draw imputations:
  - Draw imputations assuming p_θ is a Gaussian distribution.
  - use the MICE imputation algorithm.
- Specialized packages in `R` (implement the 3 steps):
  - `norm`, `amelia` draw imputations from a multivariate Gaussian.
  - `mice` draw imputations based on the MICE algorithm.
- No specialized package in Python: use MICE + Maximum Likelihood estimation (MLE).
  - for MICE, `scikit-learn`'s `IterativeImputer`.
  - for MLE, `mvem` package, or define the likelihood yourself and use `scipy.optimize`.

Rubin, D. B. (1976). Inference and missing data. *Biometrika*, 63:581–590.