결측(缺測) 데이터와 그 대책

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Overview

1. Missing · Incomplete data
   - Types of Missing and Incomplete
   - Illustration of Missing Mechanism
   - Ad-hoc methods
   - Ad-hoc methods (deletion)
   - Ad-hoc methods (single imputation)
   - Which method can be used?

2. Multiple Imputation
   - MLE
   - EM algorithm
   - MI algorithm

Overview

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2. Multiple Imputation
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   - EM algorithm
   - MI algorithm

Types of Missing and Incomplete

- Missing data: no value is observed. (Little and Rubin, 2002)
  - Missing Completely AT Random (MCAR)
    if missingness does not depends on the data, $Y = (Y_{\text{obs}}, Y_{\text{mis}})$.
    $f_\theta(M|Y) = f_\theta(M)$, where M is a missing indicator.
  - Missing At Random (MAR)
    if missingness depends only on the observed data Y_{obs}.
    $f_\theta(M|Y) = f_\theta(M|Y_{\text{obs}})$.
  - Missing Not At Random (MNAR)
    if missingness depends on the data $Y = (Y_{\text{obs}}, Y_{\text{mis}})$.
    $f_\theta(M|Y) = \text{as it is}$
- Incomplete data: value is partially observed.
  - Truncation
  - Censoring
  - Grouping
  - Masking

Illustration of Missing Mechanism

Complete Data		**MCAR**		**MAR**		**MNAR**	
GPA	IQ	GPA	IQ	GPA	IQ	GPA	IQ
2.0	93	2.0	?	2.0	?	2.0	?
2.2	115	2.2	115	2.2	?	2.2	115
2.4	96	2.4	96	2.4	?	2.4	?
2.6	116	2.6	?	2.6	?	2.6	116
2.8	94	2.8	94	2.8	?	2.8	?
3.0	106	3.0	106	**3.0**	106	3.0	106
3.2	98	3.2	?	**3.2**	98	3.2	?
3.4	103	3.4	103	**3.4**	103	3.4	103
3.6	95	3.6	95	**3.6**	95	3.6	?
3.8	112	3.8	?	**3.8**	112	3.8	112
4.0	100	4.0	100	**4.0**	100	4.0	100
4.2	120	4.2	?	**4.2**	120	4.2	120

Ad-hoc methods

Deletion

- Complete-case analysis (listwise deletion, casewise deletion)
- Available-case analysis (pairwise deletion)

Single imputation

- Mean substitution
- Regression imputation
- Hot-deck, Cold-deck

Ad-hoc methods (deletion)

Original Data			**Complete case**			**Available case**		
GPA	IQ	Hours	GPA	IQ	Hours	GPA	IQ	Hours
2.0	93	NA	2.4	96	26	**2.4**	96	**26**
2.2	115	NA	2.6	116	28	**2.6**	116	**28**
2.4	96	26	3.8	112	40	**3.2**	NA	**34**
2.6	116	28	4.0	100	42	**3.8**	112	**40**
NA	NA	30	4.2	120	44	**4.0**	100	**42**
NA	NA	32				**4.2**	120	**44**
3.2	NA	34				2.0	93	NA
NA	103	36				2.2	115	NA
3.6	95	NA				NA	NA	30
3.8	112	40				NA	NA	32
4.0	100	42				NA	103	36
4.2	120	44				3.6	95	NA

Available case depends on an estimate. (Here, $\mathrm{Cov}(X_1, X_3)$ is assumed.)

Ad-hoc methods (deletion)

Complete case (listwise/casewise deletion)

- MCAR: unbiased.
- MAR: biased.
- Popular in regression data.
- Loss in power. (small sample size).

Available case (pairwise deletion)

- MCAR: biased.
- MAR: biased.
- Correlation estimate (small value case is OK).
  Refer to `Talk-R.r` at https://github.com/AppliedStat/seminar
  For the case of pairwise deletion, the correlation estimate is even greater than one.

Ad-hoc methods (Example: Available Case)

mean/sd GPA (X_1)	mean/sd Hours (X_3)	Covariance GPA (X_1)	Covariance Hours (X_3)
2.0	26	2.4	26
2.2	28	2.6	28
2.4	30	3.2	34
2.6	32	3.8	40
3.2	34	4.0	42
3.6	36	4.2	44
3.8	40	$\text{Cov}_{13} = 5.67$	
4.0	42		
4.2	44		
$\bar{X}_1 = 3.11$	$\bar{X}_3 = 34.67$		
$S_1 = 0.83$	$S_3 = 6.32$		

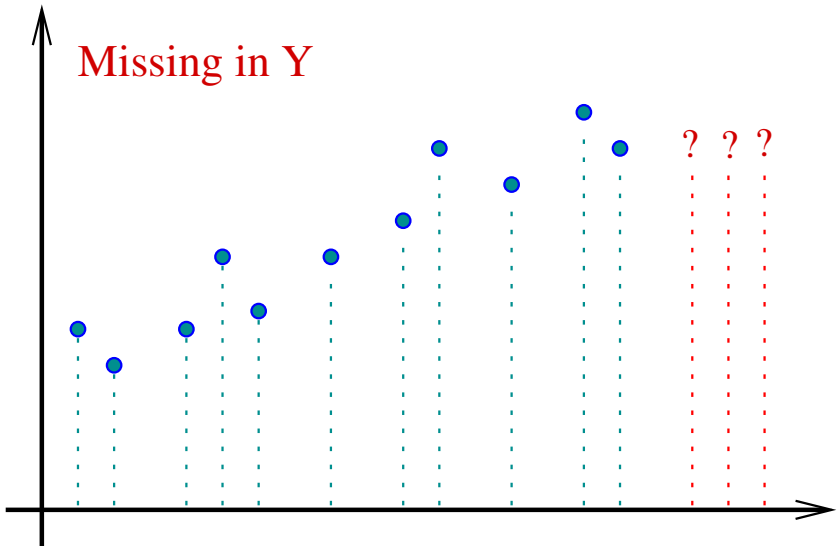
Thus, we have $r_{13} = \dfrac{\text{Cov}_{13}}{S_1 \cdot S_3} = \dfrac{5.67}{0.83 \times 6.32} = \mathbf{1.08 > 1}$, which does not make sense at all. Refer to `Talk-R.r` at ▸ Seminar

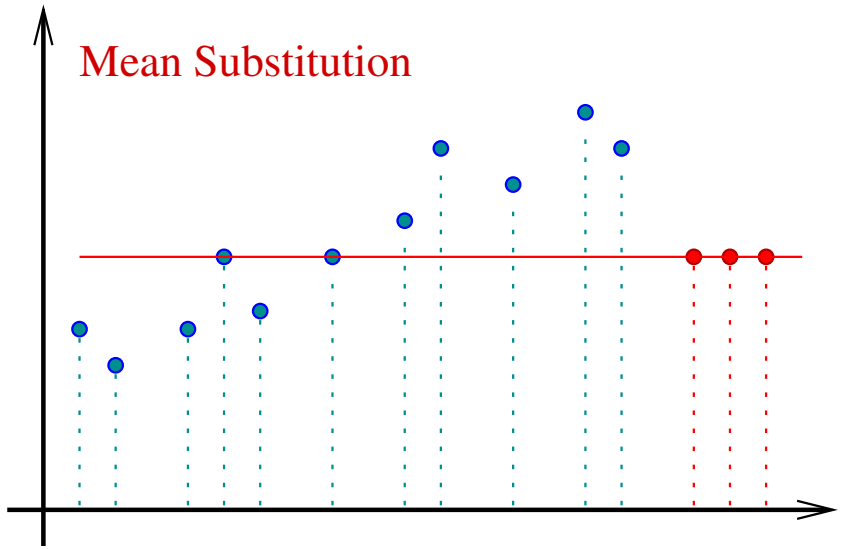
Ad-hoc methods (single imputation)

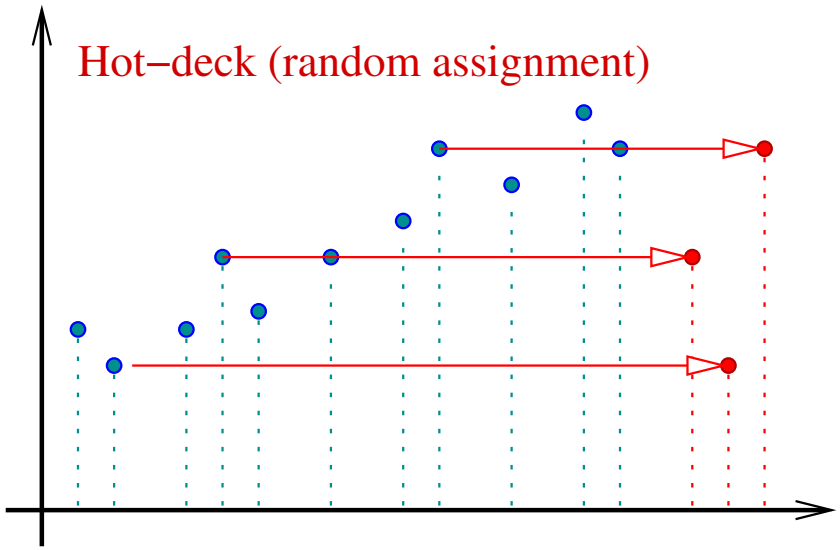
Single imputation

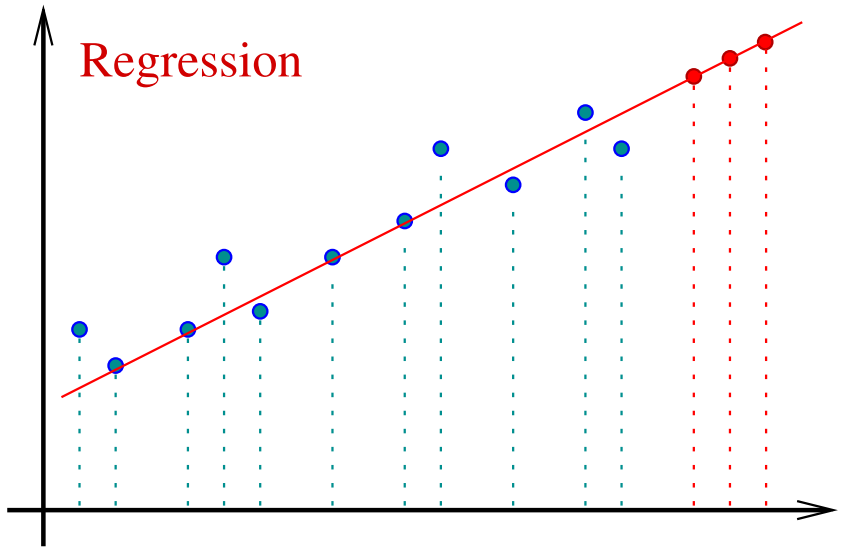
- **Mean substitution** (location estimate)
  Median, mode, HL, etc. are also OK instead of mean.
  Distorted variance/covariance. Easily biased.
- **Regression imputation**
  Distorted variance/covariance. can be unbiased.
  A random error can be added to avoid distortion of variance/covariance. Note: if a dummy variable is used for a predictor, it can include mean substitution.
- **Hot-deck / Cold-deck** (similar to bootstrap/jackknife).
  Hot-deck: random sample from **similar** hot responding values. (here, "hot" means current source.)
  Cold-deck: random sample from **similar** cold responding values. (here, "cold" means previous/external source.)
  Both can be easily biased.

Ad-hoc methods (single imputation)









Ad-hoc methods (Which method can be used?)

Recall "Complete case" versus "Available case"

Complete case (listwise/casewise deletion)

- MCAR: unbiased $\Longleftarrow$ It looks OK although wasteful with deletion.
- MAR: biased .

Available case (pairwise deletion)

- MCAR: biased .
- MAR: biased .

It is possible to test MCAR vs. MAR, but impossible to test MNAR.

> *Section 2.2.4 of van Buuren (2018) stated: several tests have been proposed to test MCAR vs. MAR. These tests are not widely used, and their practical value is unclear. ... It is not possible to test MAR versus MNAR since the information that is needed for such a test is missing.*

Ad-hoc methods (Which method can be used?)

Which method can be used?

- Listwise deletion is OK (in a sense of unbiasedness) under **MCAR** although it is wasteful .
  Note: listwise deletion is not robust to violations of the MCAR assumption. Also, the MCAR (too strong) is often unrealistic in practice.
- There are several specific methods under MAR,
  but these are not robust to violation of MAR assumption.
- We can think of imputation.
  However **single** imputation also has several drawbacks .

Multiple Imputation (MI) can handle both MAR and MNAR.
Some research papers show that listwise deletion method can outperform the MI method, but it is extremely rare in practice.

Multiple Imputation (MLE)

Multiple imputation have a very similar mechanism as EM algorithm. We look at MLE and EM and then multiple imputation.

Likelihood and log-likelihood

$$L(\boldsymbol{\theta}|\mathbf{x}) = \prod_{i=1}^{n} f(x_i) \quad \text{and} \quad \ell(\boldsymbol{\theta}|\mathbf{x}) = \log L(\boldsymbol{\theta}|\mathbf{x}) = \sum_{i=1}^{n} \log f(x_i),$$

where $\mathbf{x} = (x_1, x_2, \ldots, x_n)$ and $\boldsymbol{\theta} = (\theta_1, \theta_2, \ldots, \theta_p)$.

MLE (maximum likelihood estimate/estimator)

$$\hat{\boldsymbol{\theta}} = \arg\max_{\boldsymbol{\theta}} L(\boldsymbol{\theta}|\mathbf{x}) \quad \text{or} \quad \hat{\boldsymbol{\theta}} = \arg\max_{\boldsymbol{\theta}} \ell(\boldsymbol{\theta}|\mathbf{x}).$$

In many practical cases, the MLE is obtained in a closed form.

Multiple Imputation (EM algorithm)

What if $\mathbf{y} = (x_1, x_2, \ldots, x_m)$ are complete and $\mathbf{z} = (x_{m+1}, x_{m+2}, \ldots, x_n)$ are incomplete. Say, $a_j \leq x_j \leq b_j$, where $j = m+1, m+2, \ldots, n$. Then we have

$$L(\boldsymbol{\theta}|\mathbf{y}, \mathbf{z}) = \prod_{i=1}^{m} f(x_i) \prod_{j=m+1}^{n} \{F(b_j) - F(a_j)\}$$

$$\ell(\boldsymbol{\theta}|\mathbf{y}, \mathbf{z}) = \sum_{i=1}^{m} \log f(x_i) + \sum_{j=m+1}^{n} \log\{F(b_j) - F(a_j)\}.$$

In general, the MLE can not be obtained in a closed form.

Multiple Imputation (EM algorithm)

Treat incomplete part as random variable with an appropriate distribution. In this case, we can set up $\mathbf{z} = (z_{m+1}, z_{m+2}, \ldots, z_n)$ where z_j has the pdf $p(\mathbf{z}|\mathbf{y}, \boldsymbol{\theta})$. Then the complete likelihood is given by

$$L^c(\boldsymbol{\theta}|\mathbf{y}, \mathbf{z}) = \prod_{i=1}^{m} f(x_i) \prod_{j=m+1}^{n} f(z_j) \quad \text{and} \quad \ell^c(\boldsymbol{\theta}|\mathbf{y}, \mathbf{z}) = \log L^c(\boldsymbol{\theta}|\mathbf{y}, \mathbf{z}).$$

Start with an initial value (say, $t = 0$). Repeat E-step and M-step below.

- **E-step:** $Q(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)}) = \int \ell^c(\boldsymbol{\theta}|\mathbf{y}, \mathbf{z}) p(\mathbf{z}|\mathbf{y}, \boldsymbol{\theta}^{(t)}) d\mathbf{z}$
- **M-step:** $\boldsymbol{\theta}^{(t+1)} = \arg\max_{\boldsymbol{\theta}} Q(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)})$

This iterative method provides clear benefit over the Newton-Raphson method. (If the likelihood is unimodal, finding the MLE is guaranteed). The issue is how to obtain an explicit form after the integration in E-step. To relax this, **MC-EM** and **Q-EM** are developed.

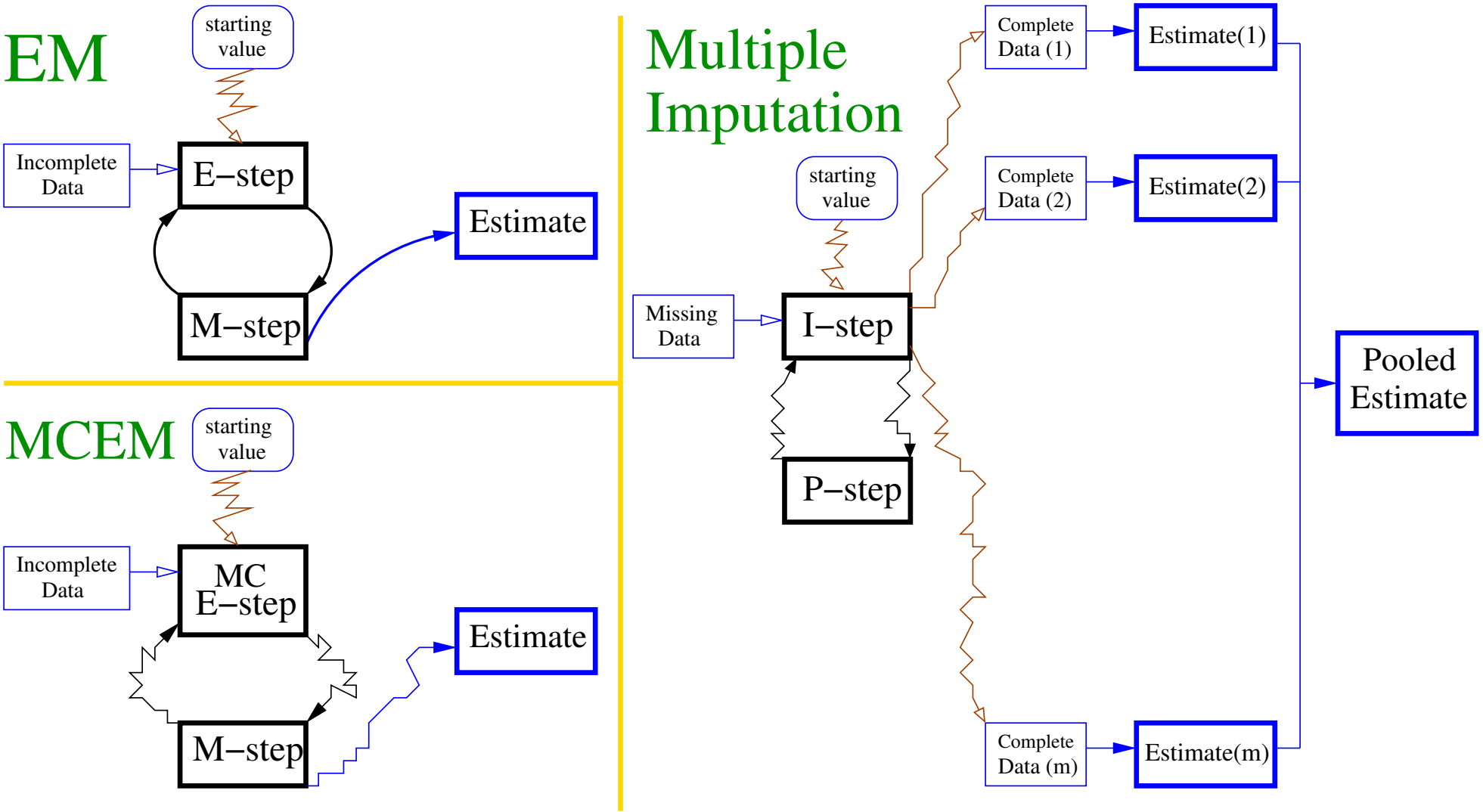
Multiple Imputation (MI algorithm)

MI is the similar line of EM algorithm which solves an incomplete-data problem by repeatedly solving the complete-data version. In MI, the unknown missing data Y_{mis} are replaced by simulated values $Y_{\text{mis}}^{(1)}, Y_{\text{mis}}^{(2)}, \ldots, Y_{\text{mis}}^{(m)}$.

- **I-step:** $Y_{\text{mis}}^{(t+1)} \sim p(Y_{\text{mis}} | Y_{\text{obs}}, \boldsymbol{\theta}^{(t)})$
- **P-step:** $\boldsymbol{\theta}^{(t+1)} \sim p(\boldsymbol{\theta} | Y_{\text{obs}}, Y_{\text{mis}}^{(t+1)})$

Thus, we obtain m completed data sets. With each of data sets, we analyze it by a **standard method** with a completed data set. We will have m different results. By pooling them (summarizing them), we can obtain a result along with the uncertainty due to missing.

Multiple Imputation (Algorithms)



Multiple Imputation (summary)

Recall

- MCAR: unbiased with listwise deletion (but, wasteful).
- MAR: biased.
- MNAR: biased. Impossible to test MNAR.

With MI, we can generate complete-data sets.

When MI works well

- MAR and Distinctness: unbiased.
  The parameters θ and ψ are distinct if $g(\theta, \psi) = g_1(\theta) \cdot g_2(\psi)$.
  See Definition 6.4 of Little and Rubin (2002).
- MI method is very robust to MNAR.
  See Section 6.2 of van Buuren (2018).

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