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
   - MLE
   - 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 A: Missing Mechanism (IQ is asked)

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

1. Missing · Incomplete data: 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

Illustration B: Complete and Available cases (GPA, IQ, Hr are asked)

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.)

1. Missing · Incomplete data: 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 2020/Talk-R.
  For the case of pairwise deletion, the correlation estimate is even greater than one.

Illustration for available case continues on the next page.

mean/sd GPA (X_1)	mean/sd Hours (X_3)	Covariance between X_1 & X_3 GPA (X_1)	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	$\mathrm{Cov}(X_1, X_3) = 5.67$	
4.0	42		
4.2	44		
$\bar{X}_1 = 3.11$	$\bar{X}_3 = 34.67$		
$S_1 = 0.83$	$S_3 = 6.32$		

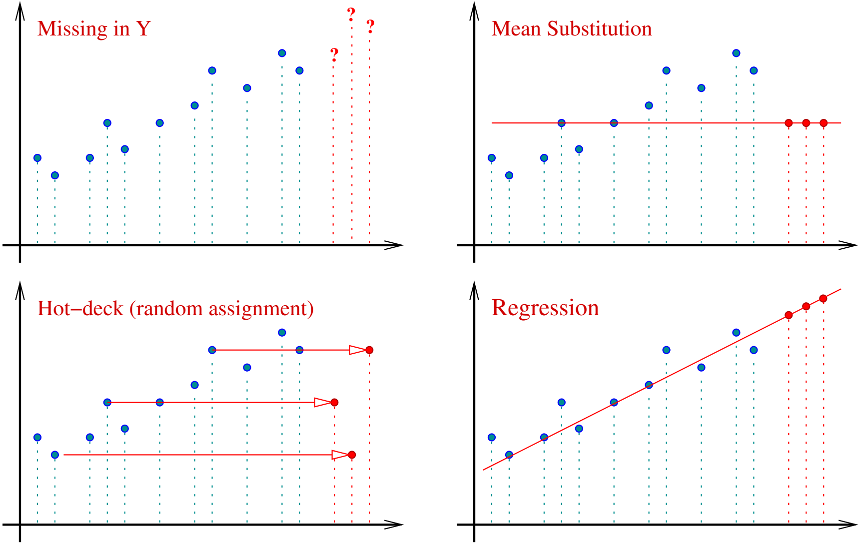
Thus, $\boxed{r_{13} = \frac{\mathrm{Cov}(X_1, X_3)}{S_1 \cdot S_3}} = \frac{5.67}{0.83 \times 6.32} = \mathbf{1.08 > 1}$, which does not make sense at all. Refer to `Talk-R.r` at 2020/Talk-R

1. Missing · Incomplete data: Ad-hoc (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.

1. Missing · Incomplete data: Ad-hoc (single imputation)



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.*

Which method can be used?

- Listwise deletion (complete case) 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 (very strong condition) is often unrealistic in practice.
- There are several *ad-hoc* 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.

2. Multiple Imputation: MLE

Multiple imputation has a very similar mechanism as EM algorithm. We look at MLE and EM first, and then multiple imputation later.

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.

2. 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, $a_j \le x_j \le b_j$, 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.

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

$$L^c(\boldsymbol{\theta}|\mathbf{y}, \mathbf{z}) = \prod_{i=1}^{m} f(x_i) \prod_{j=m+1}^{n} \boxed{f(z_j)},$$

where $\ell^c(\boldsymbol{\theta}|\mathbf{y}, \mathbf{z}) = \log L^c(\boldsymbol{\theta}|\mathbf{y}, \mathbf{z})$, z_j has a distribution whose value is between $a_j < z_j < b_j$ (we need to take an expectation w.r.t. z_j since z_j is like an random variable).

Compare the above complete likelihood with the previous original likelihood function:

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

2. Multiple Imputation: EM algorithm

Start with an initial value (say, $t = 0$). Repeat E-step and M-step below. (Note: we take an expectation w.r.t. z_j).

- **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:** $\boldsymbol{\theta}^{(t+1)} = \arg\max_{\boldsymbol{\theta}} Q(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)})$

- In the M-step, we need to obtain the closed-form maximizer.
- 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 the closed-form maximizer in the M-step. To relax this, **MC-EM** and **Q-EM** are developed.

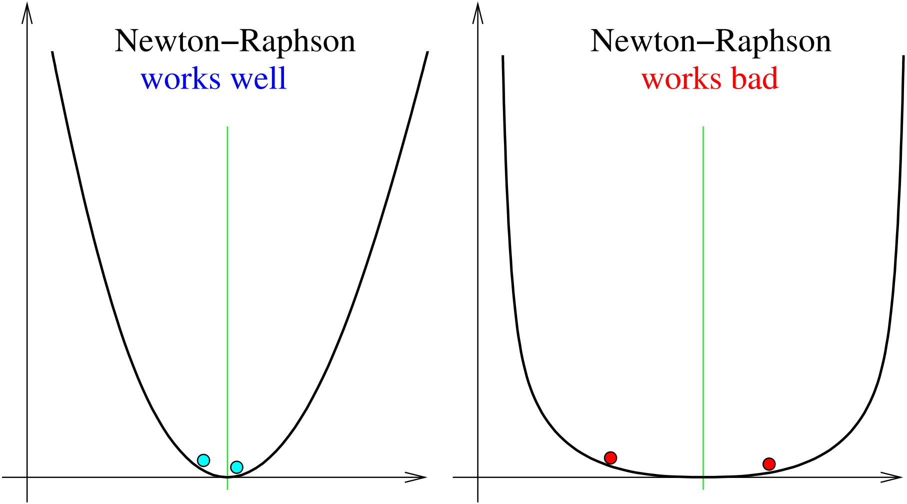
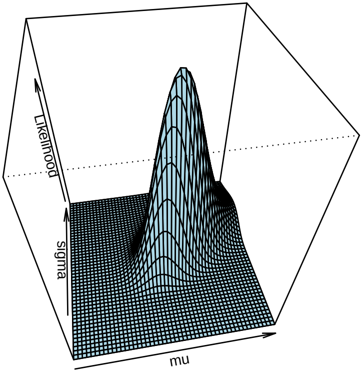

Newton–Raphson
works well
Newton–Raphson
works bad

Illustration: Likelihood function with two parameters. Lognormal example from (Park, 2013).



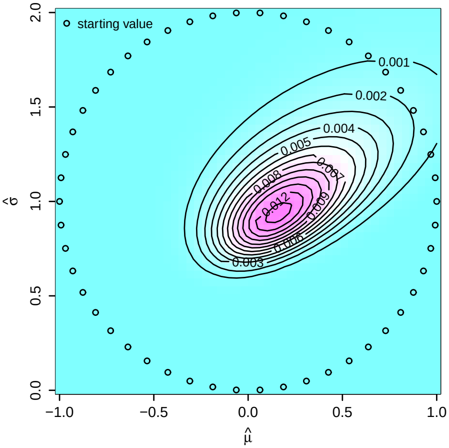
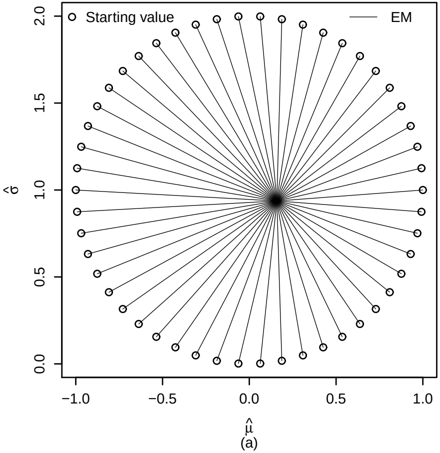
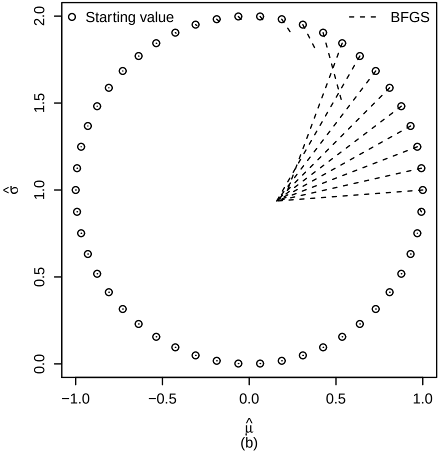


Illustration: Convergence of BFGS (improved Newton-Raphson) method (Park, 2013)





2. Multiple Imputation: MI algorithm

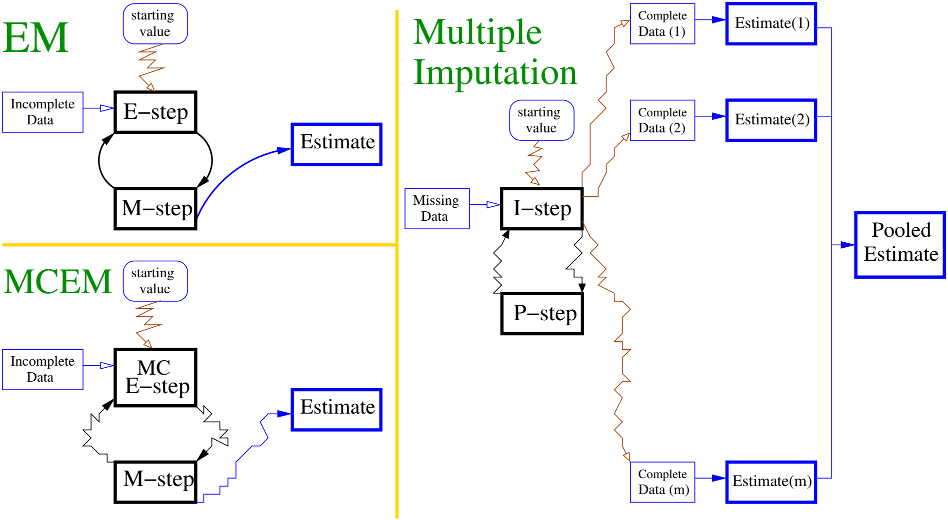
MI is the similar line of EM algorithm which solves an incomplete-data problem by repeatedly solving the complete-data version. In MI, the unknown missing data Y_{mis} are replaced by simulated values $Y_{\text{mis}}^{(1)}, Y_{\text{mis}}^{(2)}, \ldots, Y_{\text{mis}}^{(m)}$.

- **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.

R Packages for MI

- NORM: `https://cran.r-project.org/web/packages/norm/`
- MICE: `https://cran.r-project.org/web/packages/mice/`


EM
starting value
Incomplete Data
E–step
M–step
Estimate
MCEM
starting value
Incomplete Data
MC E–step
M–step
Estimate
Multiple Imputation
starting value
Missing Data
I–step
P–step
Complete Data (1)
Complete Data (2)
Complete Data (m)
Estimate(1)
Estimate(2)
Estimate(m)
Pooled Estimate

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).

References

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