# Notes: Flexible Imputation of Missing Data – Ch2 Multiple Imputation

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#### **Table of Contents**

Concepts in Incomplete Data

Why and When Multiple Imputation Works

More about Imputation Methods

# Notations

- m: number of multiple imputations
- Y: data of the sample
  - Includes both covariates and response
  - $\hspace{0.1 cm} \operatorname{Dimension} \hspace{0.1 cm} n \times p$
- R: observation indicator matrix, known
  - A  $n \times p$  0-1 matrix
  - $r_{ij} = 0$  for missing and 1 for observed
- Y<sub>obs</sub>: observed data
- Y<sub>mis</sub>: missing data
- $Y = (Y_{obs}, Y_{mis})$ : complete data
- $\psi$ : the parameter for the missing mechanism
- $\theta$ : the parameter for the full data Y

Concepts of MCAR, MAR, and MNAR, with notations

Missing completely at random (MCAR)

$$P(R = 0 \mid Y_{\text{obs}}, Y_{\text{mis}}, \psi) = P(R = 0 \mid \psi)$$

Missing at random (MAR)

$$P(R=0 \mid Y_{\text{obs}}, Y_{\text{mis}}, \psi) = P(R=0 \mid Y_{\text{obs}}, \psi)$$

Missing not at random (MNAR)

 $P(R = 0 \mid Y_{obs}, Y_{mis}, \psi)$  does not simplify

## Ignorable

- The missing data mechanism is ignorable for likelihood inference (on θ), if
  - 1. MAR, and
  - 2. Distinctness: the parameters  $\theta$  and  $\psi$  are independent (from a Bayesian's view)
- If the nonresponse if ignorable, then

$$P(Y_{\mathsf{mis}} \mid Y_{\mathsf{obs}}, R) = P(Y_{\mathsf{mis}} \mid Y_{\mathsf{obs}})$$

Thus, if the missing data model is ignorable, we can model  $\theta$  just using the observed data

## Goal of multiple imputation

- Note: for most multiple imputation practice, this goal is to train a (predictive) model with as small variances of the parameters as possible
- Q: estimand (the parameter to be estimated)
- - Unbias

 $E(\hat{Q} \mid Y) = Q$ 

Confidence valid:

$$E(U \mid Y) \ge V(\hat{Q} \mid Y)$$

where U is the estimated covariance matrix of  $\hat{Q}$ , the expectation is over all possible samples, and  $V(\hat{Q} \mid Y)$  is the variance caused by the sampling process

#### Within-variance and between-variance

$$\begin{split} E(Q \mid Y_{\text{obs}}) &= E_{Y_{\text{mis}} \mid Y_{\text{obs}}} \{ E(Q \mid Y_{\text{obs}}, Y_{\text{mis}}) \} \\ V(Q \mid Y_{\text{obs}}) &= \underbrace{E_{Y_{\text{mis}} \mid Y_{\text{obs}}} \{ V(Q \mid Y_{\text{obs}}, Y_{\text{mis}}) \}}_{\text{within-variance}} + \underbrace{V_{Y_{\text{mis}} \mid Y_{\text{obs}}} \{ E(Q \mid Y_{\text{obs}}, Y_{\text{mis}}) \}}_{\text{between variance}} \end{split}$$

• Within-variance: average of the repeated complete-data posterior variance of *Q*, estimated by

$$\bar{U} = \frac{1}{m} \sum_{l=1}^{m} \bar{U}_l,$$

where  $\bar{U}_l$  is the variance of  $\hat{Q}_l$  in the *l*th imputation

 Between-variance: variance between the complete-data posterior means of Q, estimated by

$$B = \frac{1}{m-1} \sum_{l=1}^{m} \left( \hat{Q}_{l} - \bar{Q} \right) \left( \hat{Q}_{l} - \bar{Q} \right)', \quad \bar{Q} = \frac{1}{m} \sum_{l=1}^{m} \hat{Q}_{l}$$

#### Decomposition of total variation

• Since  $\bar{Q}$  is estimated using finite m, the contribution to the variance is about B/m. Thus, the total posterior variance of Q can be decomposed into three parts:

$$T = \bar{U} + B + B/m = \bar{U} + \left(1 + \frac{1}{m}\right)B$$

- $\bar{U}$ : the conventional variance, due to sampling rather than getting the entire population.
- B: the extra variance due to missing values
- B/m: the extra simulation variance because  $\bar{Q}$  is estimated for finite m
  - Traditionally choices are m = 3, 5, 10, but the current advice is to use a larger m, e.g., m = 50

#### Properness of an imputation procedure

• An imputation procedure is confidence proper for complete-data statistics  $\hat{Q}, U$ , if it satisfies the following three conditions approximately at large m

$$E\left(\bar{Q} \mid Y\right) = \hat{Q}$$
$$E\left(\bar{U} \mid Y\right) = U$$
$$\left(1 + \frac{1}{m}\right)E(B \mid Y) \ge V(\bar{Q})$$

- Here  $\hat{Q}$  is the complete-sample estimator of Q, and U is its covariance
- $-\,$  If we replace the  $\geq$  by > in the third formula, then the procedure is said to be proper
- It is not always easy to check whether a procedure is proper.

## Scope of the imputation model

- Broad: one set of imputations to be used for all projects and analyses
- Intermediate: one set of imputations per project and use this for all analyses
- Narrow: a separate imputed dataset is created for each analysis
- Which one is better: depends on the use case

### Variance ratios

• Proportion of variation attributable to the missing data

$$\lambda = \frac{B + B/m}{T}$$

- -~ If  $\lambda>0.5,$  then the influence of the imputation model on the final result is larger than that of the complete-data model
- Relative increase in variance due to nonresponse

$$r = \frac{B + B/m}{\bar{U}} = \frac{\lambda}{1 - \lambda}$$

• Fraction of information about Q missing due to nonresponse

$$\gamma = \frac{r+2/(\nu+3)}{1+r} = \frac{\nu+1}{\nu+3}\lambda + \frac{2}{\nu+3}$$

- Here,  $\nu$  is the degrees of freedom (see next)
- When  $\nu$  is large,  $\gamma$  is very close to  $\lambda$

#### Degrees of freedom (df)

- The degrees of freedom is the number of observations after accounting for the number of parameters in the model.
- The "old" formula (as in Rubin 1987): may produce values larger than the sample size in the complete data

$$\nu_{\text{old}} = (m-1)\left(1 + \frac{1}{r^2}\right) = \frac{m-1}{\lambda^2}$$

• Let  $\nu_{\text{com}}$  be the conventional df in a complete-data inference problem. If the number of parameters in the model is k and the sample size is n, then  $\nu_{\text{com}} = n - k$ . The estimated observed data df that accounts for the missing information is

$$\nu_{\rm obs} = \frac{\nu_{\rm com} + 1}{\nu_{\rm com} + 3} \nu_{\rm com} (1 - \lambda)$$

 Barnard-Rubin correction: the adjusted df to be used for testing in multiple imputation is

$$\nu = \frac{\nu_{\text{old}}\nu_{\text{obs}}}{\nu_{\text{old}} + \nu_{\text{obs}}}$$
<sup>12</sup>

#### A numerical example

```
## Load the mice package
library(mice);
imp <- mice(nhanes, print = FALSE, m = 10, seed = 24415)
fit <- with(imp, lm(bmi ~ age))
est <- pool(fit); print(est, digits = 2)</pre>
```

##	C1	ass:	mipo	m	= 10							
##			term	m	estimate	ubar	b	t	dfcom	df	riv	1
##	1	(Inte	ercept)	10	30.8	3.4	2.52	6.2	23	9.2	0.82	
##	2		age	10	-2.3	0.9	0.39	1.3	23	12.3	0.48	

- Columns ubar, b, and t are the variances
- Column df com is ν<sub>com</sub>
- Column df is the Barnard-Rubin correction  $\nu$

#### **T-test for regression coefficients**

 Use the Barnard-Rubin correction of ν as the shape parameter of t-distribution.

print(summary(est, conf.int = TRUE), digits = 1)

##		term	estimate	std.error	statistic	df	p.value	2.5
##	1	(Intercept)	31	2	12	9	5e-07	
##	2	age	-2	1	-2	12	7e-02	

## Imputation evaluation criteria

- The following criteria are useful in simulation studies (when you know the true *Q*)
- 1. Raw bias (RB): upper limit 5%

$$\mathsf{RB} = \left| \frac{E\left(\bar{Q}\right) - Q}{Q} \right|$$

- 2. Coverage rate (CR): A CR below 90% for the nominal 95% interval is bad
- 3. Average width (AW) of confidence interval
- 4. Root mean squared error (RMSE): the smaller the better

$$\mathsf{RMSE} = \sqrt{\left(E\left(\bar{Q}\right) - Q\right)^2}$$

#### Imputation is not prediction

- Shall we evaluate an imputation method by examine how it can closely recover the missing values?
  - For example, using the RMSE to see if the imputed values  $\dot{y}_i$  are close to the true (removed) missing data  $y_i^{\text{mis}}$ ?

$$\mathsf{RMSE} = \sqrt{\frac{1}{n_{\mathsf{mis}}} \sum_{i=1}^{n_{\mathsf{mis}}} \left(y_i^{\mathsf{mis}} - \dot{y}_i\right)^2}$$

 NO! This will favor least squares estimates, and it will find the same values over and over; and thus it is single imputation. This ignores the inherent uncertainty of the missing values.

## When not to use multiple imputation

- For predictive modeling, if the missing values are in the target variable *Y*, then complete-case analysis and multiple imputation are equivalent.
- Two special cases where listwise deletion is better than multiple imputation
- 1. If the probability to be missing does not depend on Y
- 2. If the complete data model is logistic regression, and the missing data are confined to Y, not X

#### References

- Van Buuren, S. (2018). Flexible Imputation of Missing Data, 2nd Edition. CRC press.
  - https://stefvanbuuren.name/fimd/
- Rubin, D. (1987). Multiple Imputation for Nonresponse in Surveys. New York: John Wiley & Sons.