# Chapter 4: Imputation

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## Motivating Example

- Basic Setup: Let (x, y)' be a vector of bivariate random variables. Assume that  $x_i$  are always observed and  $y_i$  are subject to missingness in the sample.
- In this case, an imputed estimator of  $\theta = E(Y)$  can be computed by

$$\hat{\theta}_{I} = \frac{1}{n} \sum_{i=1}^{n} \left\{ \delta_{i} y_{i} + (1 - \delta_{i}) y_{i}^{*} \right\}$$
 (1)

where  $y_i^*$  is an imputed value for  $y_i$ .

If y<sub>i</sub>\* satisfies

$$E(y_i^* \mid \delta_i = 0) = E(y_i \mid \delta_i = 0), \tag{2}$$

then the imputation estimator (1) is unbiased.

• A sufficient condition is to assume MAR and generate  $y_i^*$  from  $f(y_i \mid x_i, \delta_i = 1)$ .

### **Justification**

# Regression imputation (Example 4.1)

Imputation model (under MAR) is a linear regression model:

$$y_i \mid x_i \sim \left(\beta_0 + \beta_1 x_i, \sigma_e^2\right),$$

for some  $(\beta_0, \beta_1, \sigma_e^2)$ .

• Regression imputation: Use  $y_i^* = \hat{\beta}_0 + \hat{\beta}_1 x_i$  where

$$\left(\hat{\beta}_0,\hat{\beta}_1\right) = \left(\bar{y}_r - \hat{\beta}_1\bar{x}_r, S_{xxr}^{-1}S_{xyr}\right).$$

The regression imputation estimator can be written as

$$\hat{\theta}_{\mathrm{I,reg}} = \frac{1}{n} \sum_{i=1}^{n} \left\{ \delta_{i} y_{i} + (1 - \delta_{i}) \left( \hat{\beta}_{0} + \hat{\beta}_{1} x_{i} \right) \right\} = \frac{1}{n} \sum_{i=1}^{n} \left( \hat{\beta}_{0} + \hat{\beta}_{1} x_{i} \right)$$

• How to estimate the variance of  $\hat{\theta}_{I,reg}$ ?

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- **Y**: a vector of random variables with distribution  $F(\mathbf{y}; \boldsymbol{\theta})$ .
- $\mathbf{y}_1, \dots, \mathbf{y}_n$  are *n* independent realizations of  $\mathbf{Y}$ .
- We are interested in estimating  $\psi$  which is implicitly defined by  $E\{U(\psi; \mathbf{Y})\} = 0$ .
- Under complete observation, a consistent estimator  $\hat{\psi}_n$  of  $\psi$  can be obtained by solving estimating equation for  $\psi$ :

$$\sum_{i=1}^n U(\boldsymbol{\psi};\mathbf{y}_i) = 0.$$

- A special case of estimating function is the score function. In this case,  $\psi = \theta$ .
- How to find the asymptotic distribution of  $\hat{\psi}_n$ ?

## Asymptotically Linear Estimator

#### Definition

Let  $X_1, \dots, X_n$  be IID sample from  $f(x; \theta_0), \theta_0 \in \Theta$  and we are interested in estimating  $\gamma_0 = \gamma(\theta_0)$ , where  $\gamma(\cdot) : \Theta \to R^k$ . An estimator  $\hat{\gamma} = \hat{\gamma}_n$  is called asymptotically linear if there exist a random vector  $\mathbf{a}(x) = \mathbf{a}(x; \theta_0)$  such that

$$\sqrt{n}\left(\hat{\gamma}_n - \frac{\gamma_0}{\gamma_0}\right) = \frac{1}{\sqrt{n}} \sum_{i=1}^n \mathbf{a}(X_i) + o_p(1)$$
(3)

with  $E_{\theta_0}\{\mathbf{a}(X)\}=0$  and  $E_{\theta_0}\{\mathbf{a}(X)\mathbf{a}(X)'\}$  is finite. Here,  $Z_n=o_p(1)$  means that  $Z_n$  converges to zero in probability.

#### Remark

- The function  $\mathbf{a}(x)$  is referred to as the <u>influence function</u> for  $\hat{\gamma}$ . The phrase influence function was used by Hampel (1974) and is motivated by the fact that to the first order  $\mathbf{a}(x)$  is the influence of a single observation on the estimator  $\hat{\gamma} = \hat{\gamma}(X_1, \dots, X_n)$ .
- The asymptotic properties of an asymptotically linear estimator can be summarized by considering only its influence function.
- Since a(X) has zero mean, the CLT tells us that

$$\frac{1}{\sqrt{n}} \sum_{i=1}^{n} \mathbf{a}(X_i) \xrightarrow{\mathcal{L}} N\left[0, E_{\theta_0}\{\mathbf{a}(X)\mathbf{a}(X)'\}\right]. \tag{4}$$

Thus, combining (3) with (4) and applying Slutsky's theorem, we have

$$\sqrt{n} (\hat{\gamma}_n - \underline{\gamma_0}) \stackrel{\mathcal{L}}{\longrightarrow} N [0, E_{\theta_0} \{ \mathbf{a}(X) \mathbf{a}(X)' \}].$$



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### Example

- Let  $X_1, \ldots, X_n$  be IID from  $N(\mu, \sigma^2)$ .
- The MLE of  $\sigma^2$  is

$$\hat{\sigma}^2 = \frac{1}{n} \sum_{i=1}^n \left( X_i - \bar{X}_n \right)^2$$

• What is the influence function of  $\hat{\sigma}^2$ ?

### Lemma 4.1

Let  $\hat{\psi}$  be the solution to  $\hat{U}\left(\psi\right)=0$ , where

$$\hat{U}(\psi) = \frac{1}{n} \sum_{i=1}^{n} U(\psi; \mathbf{y}_i).$$

#### Lemma 4.1

Let  $\psi_0$  be the solution to  $E\{U(\psi; \mathbf{Y})\} = 0$ . Then, under some regularity conditions,

$$\sqrt{n}\left(\hat{\psi}-\boldsymbol{\psi_0}\right)=\frac{1}{\sqrt{n}}\sum_{i=1}^n \{\tau(\boldsymbol{\psi_0})\}^{-1}U(\boldsymbol{\psi_0};\mathbf{y}_i)+o_p(1),$$

where  $\tau(\psi) = -E\{\dot{U}(\psi; Y)\}\$ and  $\dot{U}(\psi; Y) = \partial U(\psi; Y)/\partial \psi'$ .

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### Sketched Proof

Its proof is based on Taylor linearization:

$$\hat{U}(\hat{\psi}) \cong \hat{U}(\psi_0) + \frac{\partial}{\partial \psi'} \hat{U}(\psi_0) \left(\hat{\psi} - \psi_0\right) 
\cong \hat{U}(\psi_0) + E\{\dot{U}(\psi_0)\} \left(\hat{\psi} - \psi_0\right),$$

where the second (approximate) equality follows by

$$\frac{\partial}{\partial \psi'}\hat{U}(\psi_0) = E\{\dot{U}(\psi_0)\} + o_p(1)$$

and  $\hat{\psi} = \psi_0 + o_p(1)$ .

- Need to assume that  $E\left\{\dot{U}(\psi_0)
  ight\}$  is nonsingular.
- Also, we need conditions for  $\hat{\psi} \stackrel{p}{\rightarrow} \psi_0$ .

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# Remark 1 (Sandwich formula)

• Lemma 4.1 can be used to obtain a consistent variance estimator of  $\hat{\psi}$ :

$$\hat{V}(\hat{\psi}) = \frac{1}{n} \hat{\tau}^{-1} \hat{V}(U) \left(\hat{\tau}^{-1}\right)'$$

where

$$\hat{\tau} = -n^{-1} \sum_{i=1}^{n} \dot{U}(\hat{\psi}; y_i)$$

$$\hat{V}(U) = n^{-1} \sum_{i=1}^{n} U(\hat{\psi}; y_i) U(\hat{\psi}; y_i)'$$

• The above formula is often called the sandwich formula.

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### Remark 2

• To solve a nonlinear equation  $\hat{U}(\psi)=0$ , one might use the Newton method

$$\hat{\psi}^{(t+1)} = \hat{\psi}^{(t)} - \left\{ \dot{U}(\hat{\psi}^{(t)}) \right\}^{-1} \hat{U}(\hat{\psi}^{(t)}), \tag{5}$$

where  $\dot{U}(\psi) = \partial \hat{U}(\psi)/\partial \psi'$ . However, the partial derivative  $\dot{U}(\psi)$  is not symmetric, and the iterative computation in (5) can have numerical problems.

To deal with the problem, we can use

$$\hat{\psi}^{(t+1)} = \hat{\psi}^{(t)} - \left\{ \dot{U}(\hat{\psi}^{(t)})' \dot{U}(\hat{\psi}^{(t)}) \right\}^{-1} \dot{U}(\hat{\psi}^{(t)})' \hat{U}(\hat{\psi}^{(t)}), \tag{6}$$

which is essentially equivalent to finding  $\hat{\psi}$  that minimizes  $Q(\psi) = \hat{U}(\psi)'\hat{U}(\psi)$ .



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### Remark 3

• Let  $\hat{ heta}_{\mathrm{MLE}}$  be the solution to

$$\hat{S}(\boldsymbol{\theta}) \equiv n^{-1} \sum_{i=1}^{n} S(\boldsymbol{\theta}; y_i) = 0,$$

where  $S(\theta; y) = \partial \log f(y; \theta) / \partial \theta$ .

• By Lemma 4.1, we can obtain

$$\sqrt{n}\left(\hat{\theta}_{MLE}-\frac{\theta_0}{0}\right)=\frac{1}{\sqrt{n}}\sum_{i=1}^n \{\mathcal{I}(\theta_0)\}^{-1}S(\theta_0;y_i)+o_p(1),$$

because

$$\mathcal{I}(\theta) = -E_{\theta} \left\{ \frac{\partial}{\partial \theta'} S(\theta; Y) \right\}.$$



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# Missing data setup

- Suppose that  $\mathbf{y}_i$  is not fully observed.
- $\mathbf{y}_i = (\mathbf{y}_{\mathrm{obs,i}}, \mathbf{y}_{\mathrm{mis,i}})$ : (observed, missing) part of  $\mathbf{y}_i$
- $\delta_i$ : response indicator functions for  $\mathbf{y}_i$ .
- Under the existence of missing data, we can use the following estimators:

$$\hat{\psi}$$
: solution to  $\sum_{i=1}^{n} E\left\{U\left(\psi; \mathbf{y}_{i}\right) \mid \mathbf{y}_{obs,i}, \boldsymbol{\delta}_{i}\right\} = 0.$  (7)

- The equation in (7) is often called the expected estimating equation.
- If  $U(\psi; Y)$  is a score function of  $\psi$ , then (7) reduces to the mean score equation of R.A. Fisher.

### Motivation (for imputation)

Computing the conditional expectation in (7) can be a challenging problem.

1 The conditional expectation depends on unknown parameter values. That is,

$$E\left\{U\left(\boldsymbol{\psi};\boldsymbol{y}_{i}\right)\mid\boldsymbol{y}_{obs,i},\boldsymbol{\delta}_{i}\right\}=E\left\{U\left(\boldsymbol{\psi};\boldsymbol{y}_{i}\right)\mid\boldsymbol{y}_{obs,i},\boldsymbol{\delta}_{i};\boldsymbol{\theta},\boldsymbol{\phi}\right\},$$

where  $\theta$  is the parameter in  $f(\mathbf{y}; \theta)$  and  $\phi$  is the parameter in  $p(\delta \mid \mathbf{y}; \phi)$ .

2 Even if we know  $\eta=(\theta,\phi)$ , computing the conditional expectation is numerically difficult.

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## What is imputation?

• Imputation: Monte Carlo approximation of the conditional expectation (given the observed data).

$$E\left\{U\left(\boldsymbol{\psi};\mathbf{y}_{i}\right)\mid\mathbf{y}_{obs,i},\boldsymbol{\delta}_{i}\right\}\cong\frac{1}{m}\sum_{i=1}^{m}U\left(\boldsymbol{\psi};\mathbf{y}_{obs,i},\mathbf{y}_{mis,i}^{*(i)}\right)$$

**1** Bayesian approach: generate  $\mathbf{y}_{mis,i}^*$  from

$$f(\mathbf{y}_{\textit{mis},i} \mid \mathbf{y}_{\textit{obs}}, \boldsymbol{\delta}) = \int f(\mathbf{y}_{\textit{mis},i} \mid \mathbf{y}_{\textit{obs}}, \boldsymbol{\delta}; \boldsymbol{\eta}) p(\boldsymbol{\eta} \mid \mathbf{y}_{\textit{obs}}, \boldsymbol{\delta}) d\boldsymbol{\eta}$$

**2** Frequentist approach: generate  $\mathbf{y}_{mis,i}^*$  from  $f\left(\mathbf{y}_{mis,i} \mid \mathbf{y}_{obs,i}, \boldsymbol{\delta}; \hat{\eta}\right)$ , where  $\hat{\eta}$  is a consistent estimator.

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# 2. Basic Theory (Frequentist approach)

- Parameter  $\psi$  defined by  $E\{U(\psi; \mathbf{y})\} = 0$ .
- Under complete response, a consistent estimator of  $\psi$  can be obtained by solving  $\hat{U}(\psi) = 0$ , where  $\hat{U}(\psi) = n^{-1} \sum_{i=1}^{n} U(\psi; \mathbf{y}_i)$ .
- Assume that some part of  $\mathbf{y}$ , denoted by  $\mathbf{y}_{\mathrm{mis}}$ , is not observed and m imputed values, say  $\mathbf{y}_{\mathrm{mis}}^{*(1)}, \cdots, \mathbf{y}_{\mathrm{mis}}^{*(m)}$ , are generated from  $f(\mathbf{y}_{\mathrm{mis}} \mid \mathbf{y}_{\mathrm{obs}}, \boldsymbol{\delta}; \hat{\eta}_{MLE})$ , where  $\hat{\eta}_{MLE}$  is the MLE of  $\eta_0 = (\theta_0, \phi_0)$ .
- The imputed estimating function using m imputed values is computed as

$$\bar{U}_{I,m}(\boldsymbol{\psi} \mid \hat{\eta}_{MLE}) = \frac{1}{m} \sum_{j=1}^{m} \hat{U}(\boldsymbol{\psi}; \mathbf{y}^{*(j)}), \tag{8}$$

where  $\mathbf{y}^{*(j)} = (\mathbf{y}_{\text{obs}}, \mathbf{y}_{\text{mis}}^{*(j)}).$ 

• If  $m \to \infty$ , the imputed estimating function converges to the expected estimating function  $\bar{U}_{I,\infty}\left(\psi\mid\hat{\eta}_{MLE}\right)=E\{\hat{U}(\psi)\mid\mathbf{y}_{\mathrm{obs}},\boldsymbol{\delta};\hat{\eta}_{MLE}\}$ 

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- Let  $\hat{\psi}_{I,m}$  be the solution to  $\bar{U}_{I,m}(\psi \mid \hat{\eta}_{MLE}) = 0$ . We are interested in the asymptotic properties of  $\hat{\psi}_{I,m}$ .
- Note that  $\hat{\psi}_{I,m} = \hat{\psi}_{I,m}(\hat{\eta}_{MLE})$ , which emphasize its dependence of  $\hat{\eta}_{MLE}$ , the MLE of  $\eta$ .
- Here,  $\eta$  is a nuisance parameter in the sense that we are not interested in estimating  $\psi$ , but we need an estimator of  $\eta$  in order to estimate  $\psi$ .
- Because of the sampling error of  $\hat{\eta}_{MLE}$ , the asymptotic distribution of  $\hat{\psi}_{I,m}(\hat{\eta}_{MLE}) \psi_0$  is different from that of  $\hat{\psi}_{I,m}(\eta_0) \psi_0$ .
- Our goal is to find an inflence function for  $\hat{\psi}_{I,m}$ .

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# Example 4.2

 Under the setup of Example 4.1, we are interested in estimating the asymptotic variance of the regression imputation estimator

$$\hat{\theta}_{\mathrm{I,reg}} = \frac{1}{n} \sum_{i=1}^{n} \left( \hat{\beta}_{0} + \hat{\beta}_{1} x_{i} \right),$$

where  $\hat{\boldsymbol{\beta}}=(\hat{\beta}_0,\hat{\beta}_1)'$  is the solution to

$$\hat{U}(\boldsymbol{\beta}) \equiv \frac{1}{n} \sum_{i=1}^{n} \delta_{i} (y_{i} - \beta_{0} - \beta_{1} x_{i}) \begin{pmatrix} 1 \\ x_{i} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

• How to find the influence function of  $\hat{ heta}_{\mathrm{I,reg}}$ ?

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### Linearization method

• Write  $\hat{\theta}_{I,reg} = \hat{\theta}_I(\hat{\boldsymbol{\beta}})$  and consider Taylor expansion of  $\hat{\theta}_I(\hat{\boldsymbol{\beta}})$  around  $\boldsymbol{\beta} = \boldsymbol{\beta}^*$ , where  $\boldsymbol{\beta}^* = p \lim \hat{\boldsymbol{\beta}}$ ,

$$\hat{\theta}_{I,reg}(\hat{\boldsymbol{\beta}}) = \hat{\theta}_{I}(\boldsymbol{\beta}^{*}) + E\left\{\nabla_{\boldsymbol{\beta}}\hat{\theta}_{I}(\boldsymbol{\beta}^{*})\right\} \left(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}^{*}\right) + o_{p}(n^{-1/2})$$

$$= \hat{\theta}_{I}(\boldsymbol{\beta}^{*}) + (1, E(X)) \left(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}^{*}\right) + o_{p}(n^{-1/2}) \tag{9}$$

• Also, Taylor expansion of  $\hat{U}(\hat{oldsymbol{eta}})=0$  around  $oldsymbol{eta}=oldsymbol{eta}^*$  to get

$$0 = \hat{U}(\beta^*) + E\left\{\nabla_{\beta}\hat{U}(\beta^*)\right\} \left(\hat{\beta} - \beta^*\right) + o_{\rho}(n^{-1/2})$$
$$= \hat{U}(\beta^*) - \begin{pmatrix} E(\delta) & E(\delta X) \\ E(\delta X) & E(\delta X^2) \end{pmatrix} \left(\hat{\beta} - \beta^*\right) + o_{\rho}(n^{-1/2})$$
(10)

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• Combining (9) with (10), we obtain

$$\begin{split} \hat{\theta}_{I,reg} &= \hat{\theta}_{I}(\beta^{*}) + (\kappa_{1}, \kappa_{2})\hat{U}(\beta^{*}) + o_{\rho}(n^{-1/2}) \\ &= \frac{1}{n} \sum_{i=1}^{n} \left\{ (\beta_{0} + \beta_{1}x_{i}) + \delta_{i}(y_{i} - \beta_{0} - \beta_{1}x_{i})(\kappa_{1} + \kappa_{2}x_{i}) \right\} + o_{\rho}(n^{-1/2}), \end{split}$$

where

$$\begin{pmatrix} \kappa_1 \\ \kappa_2 \end{pmatrix} = \begin{pmatrix} E(\delta) & E(\delta X) \\ E(\delta X) & E(\delta X^2) \end{pmatrix}^{-1} \begin{pmatrix} 1 \\ E(X) \end{pmatrix}.$$

• Therefore, the influence function of  $\hat{ heta}_{
m I,reg}$  is

$$a(x_i, y_i, \delta_i) = (\beta_0 + \beta_1 x_i) + \delta_i (y_i - \beta_0 - \beta_1 x_i) (\kappa_1 + \kappa_2 x_i) - \theta.$$

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### Remark

• If  $\hat{\theta} = \hat{\theta}(\hat{\beta})$  and  $\hat{\beta}$  is obtained by solving  $\hat{U}(\beta) = 0$ , then the linearization takes the following form:

$$\hat{ heta}(oldsymbol{eta},\mathbf{c})=\hat{ heta}(oldsymbol{eta})+\mathbf{c}'\hat{U}(oldsymbol{eta})$$

For  $\beta = \hat{\beta}$ , we have  $\hat{\theta}(\hat{\beta}, \mathbf{c}) = \hat{\theta}$  regardless of the choice of  $\mathbf{c}$ .

- Thus, we have only to find  $\mathbf{c}=\mathbf{c}^*$  such that no further Taylor expansion is necessary.
- We have only to solve

$$E\left\{
abla_{eta}\hat{ heta}(oldsymbol{eta}^*,\mathbf{c})
ight\}=0$$

to get  $\mathbf{c}^*$ , where  $\boldsymbol{\beta}^* = p \lim \hat{\boldsymbol{\beta}}$ .

• Originally considered by Randles (1982).



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