

# Sandwich estimator derivations for natural effect model parameters

Johan Steen

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## Weighting-based approach

### Stratum-specific effects

#### Models

natural effect model  $\mu_1(X, x^*, C; \beta)$ :

$$\text{e.g., } g[\mathbb{E}\{Y(X, M(x^*))|C\}] = \beta_0 + \beta_1 X + \beta_2 x^* + \beta_3 C$$

working model  $\mu_2(X, C; \theta)$ :

$$\text{e.g., } g[\mathbb{E}(M|X, C)] = \theta_0 + \theta_1 X + \theta_2 C$$

#### Estimating equations

$$U_1(X_i, x^*, C_i; \beta, \theta) = k^{-1} \sum_{j=1}^k \frac{\partial \mu_1(X_i, x_{ij}^*, C_i; \beta)}{\partial \beta} \Sigma_{\mu_1}^{-1} \frac{\Pr(M_i|x_{ij}^*, C_i; \theta)}{\Pr(M_i|X_i, C_i; \theta)} \cdot [Y_i - \mu_1(X_i, x_{ij}^*, C_i; \beta)]$$

$$U_2(X_i, C_i; \theta) = \frac{\partial \mu_2(X_i, C_i; \theta)}{\partial \theta} \Sigma_{\mu_2}^{-1} [M_i - \mu_2(X_i, C_i; \theta)]$$

with  $k$  the number of replications or hypothetical values  $x^*$  for each observation unit  $i$  and  $\Sigma_{\mu_i}$  the residual variance-covariance matrix for model  $\mu_i$ .

#### Sandwich estimator

Let  $\zeta = (\beta, \theta)$  and  $\tilde{U} = (U_1, U_2)$ . The sandwich estimator variance-covariance matrix can then be written as

$$n^{-1} \cdot \mathbb{E} \left( -\frac{\partial \tilde{U}}{\partial \zeta} \right)^{-1} \text{Var}(\tilde{U}) \cdot \mathbb{E} \left( -\frac{\partial \tilde{U}}{\partial \zeta} \right)^{-T}$$

with  $n$  the total sample size of the original dataset,

$$\mathbb{E} \left( -\frac{\partial \tilde{U}}{\partial \zeta} \right)^{-1} = \begin{bmatrix} \mathbb{E} \left( -\frac{\partial U_1}{\partial \beta} \right) & \mathbb{E} \left( -\frac{\partial U_1}{\partial \theta} \right) \\ 0 & \mathbb{E} \left( -\frac{\partial U_2}{\partial \theta} \right) \end{bmatrix}^{-1}$$

and

$$\begin{aligned} \frac{\partial U_1}{\partial \beta} &= -k^{-1} \sum_{j=1}^k \frac{\partial \mu_1(X_i, x_{ij}^*, C_i; \beta)}{\partial \beta} \Sigma_{\mu_1}^{-1} \frac{\Pr(M_i | x_{ij}^*, C_i; \theta)}{\Pr(M_i | X_i, C_i; \theta)} \frac{\partial \mu_1(X_i, x_{ij}^*, C_i; \beta)}{\partial \beta} \\ \frac{\partial U_1}{\partial \theta} &= k^{-1} \sum_{j=1}^k \frac{\partial \mu_1(X_i, x_{ij}^*, C_i; \beta)}{\partial \beta} \Sigma_{\mu_1}^{-1} \frac{\partial}{\partial \theta} \left( \frac{\Pr(M_i | x_{ij}^*, C_i; \theta)}{\Pr(M_i | X_i, C_i; \theta)} \right) [Y_i - \mu_1(X_i, x_{ij}^*, C_i; \beta)] \\ \frac{\partial U_2}{\partial \theta} &= -\frac{\partial \mu_2(X_i, C_i; \theta)}{\partial \theta} \Sigma_{\mu_2}^{-1} \frac{\partial \mu_2(X_i, C_i; \theta)}{\partial \theta} \end{aligned}$$

## Population-average effects

### Models

natural effect model  $\mu_1(X, x^*; \beta)$ :

$$\text{e.g., } g[\mathbb{E}\{Y(X, M(x^*))\}] = \beta_0 + \beta_1 X + \beta_2 x^*$$

working model  $\mu_2(X, C; \theta)$ :

$$\text{e.g., } g[\mathbb{E}(M|X, C)] = \theta_0 + \theta_1 X + \theta_2 C$$

working model  $\mu_3(C; \tau)$ :

$$\text{e.g., } g[\mathbb{E}(X|C)] = \tau_0 + \tau_1 C$$

### Estimating equations

$$U_1(X_i, x^*; \beta, \theta, \tau) = k^{-1} \sum_{j=1}^k \frac{\partial \mu_1(X_i, x_{ij}^*; \beta)}{\partial \beta} \Sigma_{\mu_1}^{-1} \Pr(X_i | C_i; \tau)^{-1} \cdot \frac{\Pr(M_i | x_{ij}^*, C_i; \theta)}{\Pr(M_i | X_i, C_i; \theta)} \cdot [Y_i - \mu_1(X_i, x_{ij}^*; \beta)]$$

$$U_2(X_i, C_i; \theta) = \frac{\partial \mu_2(X_i, C_i; \theta)}{\partial \theta} \Sigma_{\mu_2}^{-1} [M_i - \mu_2(X_i, C_i; \theta)]$$

$$U_3(C_i; \tau) = \frac{\partial \mu_3(C_i; \tau)}{\partial \tau} \Sigma_{\mu_3}^{-1} [X_i - \mu_3(C_i; \tau)]$$

### Sandwich estimator

Let  $\zeta = (\beta, \theta, \tau)$  and  $\tilde{U} = (U_1, U_2, U_3)$ . The sandwich estimator variance-covariance matrix can then be written as

$$n^{-1} \cdot \mathbb{E} \left( -\frac{\partial \tilde{U}}{\partial \zeta} \right)^{-1} \text{Var}(\tilde{U}) \cdot \mathbb{E} \left( -\frac{\partial \tilde{U}}{\partial \zeta} \right)^{-T}$$

with

$$\mathbb{E} \left( -\frac{\partial \tilde{U}}{\partial \zeta} \right)^{-1} = \begin{bmatrix} \mathbb{E} \left( -\frac{\partial U_1}{\partial \beta} \right) & \mathbb{E} \left( -\frac{\partial U_1}{\partial \theta} \right) & \mathbb{E} \left( -\frac{\partial U_1}{\partial \tau} \right) \\ 0 & \mathbb{E} \left( -\frac{\partial U_2}{\partial \theta} \right) & 0 \\ 0 & 0 & \mathbb{E} \left( -\frac{\partial U_3}{\partial \tau} \right) \end{bmatrix}^{-1}$$

and

$$\begin{aligned} \frac{\partial U_1}{\partial \beta} &= -k^{-1} \sum_{j=1}^k \frac{\partial \mu_1(X_i, x_{ij}^*; \beta)}{\partial \beta} \Sigma_{\mu_1}^{-1} \Pr(X_i | C_i; \tau)^{-1} \cdot \frac{\Pr(M_i | x_{ij}^*, C_i; \theta)}{\Pr(M_i | X_i, C_i; \theta)} \\ &\quad \cdot \frac{\partial \mu_1(X_i, x_{ij}^*; \beta)}{\partial \beta} \\ \frac{\partial U_1}{\partial \theta} &= k^{-1} \sum_{j=1}^k \frac{\partial \mu_1(X_i, x_{ij}^*; \beta)}{\partial \beta} \Sigma_{\mu_1}^{-1} \Pr(X_i | C_i; \tau)^{-1} \cdot \frac{\partial}{\partial \theta} \left( \frac{\Pr(M_i | x_{ij}^*, C_i; \theta)}{\Pr(M_i | X_i, C_i; \theta)} \right) \\ &\quad \cdot [Y_i - \mu_1(X_i, x_{ij}^*; \beta)] \\ \frac{\partial U_1}{\partial \tau} &= k^{-1} \sum_{j=1}^k \frac{\partial \mu_1(X_i, x_{ij}^*; \beta)}{\partial \beta} \Sigma_{\mu_1}^{-1} \frac{\partial \Pr(X_i | C_i; \tau)^{-1}}{\partial \tau} \cdot \frac{\Pr(M_i | x_{ij}^*, C_i; \theta)}{\Pr(M_i | X_i, C_i; \theta)} \\ &\quad \cdot [Y_i - \mu_1(X_i, x_{ij}^*; \beta)] \\ \frac{\partial U_2}{\partial \theta} &= -\frac{\partial \mu_2(X_i, C_i; \theta)}{\partial \theta} \Sigma_{\mu_2}^{-1} \frac{\partial \mu_2(X_i, C_i; \theta)}{\partial \theta} \\ \frac{\partial U_3}{\partial \tau} &= -\frac{\partial \mu_3(C_i; \tau)}{\partial \tau} \Sigma_{\mu_3}^{-1} \frac{\partial \mu_3(C_i; \tau)}{\partial \tau} \end{aligned}$$

## Imputation-based approach

### Stratum-specific effects

#### Models

natural effect model  $\mu_1(x, X, C; \beta)$ :

$$\text{e.g., } g[\mathbb{E}\{Y(x, M(X))|C\}] = \beta_0 + \beta_1 x + \beta_2 X + \beta_3 C$$

working model  $\mu_2(X, M, C; \gamma)$ :

$$\text{e.g., } g[\mathbb{E}(Y|X, M, C)] = \gamma_0 + \gamma_1 X + \gamma_2 M + \gamma_3 C$$

#### Estimating equations

$$U_1(x, X_i, C_i; \beta, \gamma) = k^{-1} \sum_{j=1}^k \frac{\partial \mu_1(x_{ij}, X_i, C_i; \beta)}{\partial \beta} \Sigma_{\mu_1}^{-1} \cdot [\mu_2(x_{ij}, M_i, C_i; \gamma) - \mu_1(x_{ij}, X_i, C_i; \beta)]$$

$$U_2(X_i, M_i, C_i; \gamma) = \frac{\partial \mu_2(X_i, M_i, C_i; \gamma)}{\partial \gamma} \Sigma_{\mu_2}^{-1} [Y_i - \mu_2(X_i, M_i, C_i; \gamma)]$$

#### Sandwich estimator

Let  $\zeta = (\beta, \gamma)$  and  $\tilde{U} = (U_1, U_2)$ . The sandwich estimator variance-covariance matrix can then be written as

$$n^{-1} \cdot \mathbb{E} \left( -\frac{\partial \tilde{U}}{\partial \zeta} \right)^{-1} \text{Var}(\tilde{U}) \cdot \mathbb{E} \left( -\frac{\partial \tilde{U}}{\partial \zeta} \right)^{-T}$$

with

$$\mathbb{E} \left( -\frac{\partial \tilde{U}}{\partial \zeta} \right)^{-1} = \begin{bmatrix} \mathbb{E} \left( -\frac{\partial U_1}{\partial \beta} \right) & \mathbb{E} \left( -\frac{\partial U_1}{\partial \gamma} \right) \\ 0 & \mathbb{E} \left( -\frac{\partial U_2}{\partial \gamma} \right) \end{bmatrix}^{-1}$$

and

$$\frac{\partial U_1}{\partial \beta} = -k^{-1} \sum_{j=1}^k \frac{\partial \mu_1(x_{ij}, X_i, C_i; \beta)}{\partial \beta} \Sigma_{\mu_1}^{-1} \frac{\partial \mu_1(x_{ij}, X_i, C_i; \beta)}{\partial \beta}$$

$$\frac{\partial U_1}{\partial \gamma} = k^{-1} \sum_{j=1}^k \frac{\partial \mu_1(x_{ij}, X_i, C_i; \beta)}{\partial \beta} \Sigma_{\mu_1}^{-1} \frac{\partial \mu_2(x_{ij}, M_i, C_i; \gamma)}{\partial \gamma}$$

$$\frac{\partial U_2}{\partial \gamma} = -\frac{\partial \mu_2(X_i, M_i, C_i; \beta)}{\partial \gamma} \Sigma_{\mu_2}^{-1} \frac{\partial \mu_2(X_i, M_i, C_i; \beta)}{\partial \gamma}$$

## Population-average effects

### Models

natural effect model  $\mu_1(x, X; \beta)$ :

$$\text{e.g., } g[\mathbb{E}\{Y(x, M(X))\}] = \beta_0 + \beta_1 x + \beta_2 X$$

working model  $\mu_2(X, M, C; \gamma)$ :

$$\text{e.g., } g[\mathbb{E}(Y|X, M, C)] = \gamma_0 + \gamma_1 X + \gamma_2 M + \gamma_3 C$$

working model  $\mu_3(C; \tau)$ :

$$\text{e.g., } g[\mathbb{E}(X|C)] = \tau_0 + \tau_1 C$$

### Estimating equations

$$U_1(x, X_i; \beta, \gamma, \tau) = k^{-1} \sum_{j=1}^k \frac{\partial \mu_1(x_{ij}, X_i; \beta)}{\partial \beta} \Sigma_{\mu_1}^{-1} \Pr(X_i | C_i; \tau)^{-1} \cdot [\mu_2(x_{ij}, M_i, C_i; \gamma) - \mu_1(x_{ij}, X_i; \beta)]$$

$$U_2(X_i, M_i, C_i; \gamma) = \frac{\partial \mu_2(X_i, M_i, C_i; \gamma)}{\partial \gamma} \Sigma_{\mu_2}^{-1} [Y_i - \mu_2(X_i, M_i, C_i; \gamma)]$$

$$U_3(C_i; \tau) = \frac{\partial \mu_3(C_i; \tau)}{\partial \tau} \Sigma_{\mu_3}^{-1} [X_i - \mu_3(C_i; \tau)]$$

### Sandwich estimator

Let  $\zeta = (\beta, \gamma, \tau)$  and  $\tilde{U} = (U_1, U_2, U_3)$ . The sandwich estimator variance-covariance matrix can then be written as

$$n^{-1} \cdot \mathbb{E} \left( -\frac{\partial \tilde{U}}{\partial \zeta} \right)^{-1} \text{Var}(\tilde{U}) \cdot \mathbb{E} \left( -\frac{\partial \tilde{U}}{\partial \zeta} \right)^{-T}$$

with

$$\mathbb{E} \left( -\frac{\partial \tilde{U}}{\partial \zeta} \right)^{-1} = \begin{bmatrix} \mathbb{E} \left( -\frac{\partial U_1}{\partial \beta} \right) & \mathbb{E} \left( -\frac{\partial U_1}{\partial \gamma} \right) & \mathbb{E} \left( -\frac{\partial U_1}{\partial \tau} \right) \\ 0 & \mathbb{E} \left( -\frac{\partial U_2}{\partial \gamma} \right) & 0 \\ 0 & 0 & \mathbb{E} \left( -\frac{\partial U_3}{\partial \tau} \right) \end{bmatrix}^{-1}$$

and

$$\begin{aligned}
\frac{\partial U_1}{\partial \beta} &= -k^{-1} \sum_{j=1}^k \frac{\partial \mu_1(x_{ij}, X_i; \beta)}{\partial \beta} \Sigma_{\mu_1}^{-1} \Pr(X_i|C_i)^{-1} \frac{\partial \mu_1(x_{ij}, X_i; \beta)}{\partial \beta} \\
\frac{\partial U_1}{\partial \gamma} &= k^{-1} \sum_{j=1}^k \frac{\partial \mu_1(x_{ij}, X_i; \beta)}{\partial \beta} \Sigma_{\mu_1}^{-1} \Pr(X_i|C_i)^{-1} \frac{\partial \mu_2(x_{ij}, M_i, C_i; \gamma)}{\partial \gamma} \\
\frac{\partial U_1}{\partial \tau} &= k^{-1} \sum_{j=1}^k \frac{\partial \mu_1(x_{ij}, X_i; \beta)}{\partial \beta} \Sigma_{\mu_1}^{-1} \frac{\partial \Pr(X_i|C_i; \tau)^{-1}}{\partial \tau} \\
&\quad \cdot [\mu_2(x_{ij}, M_i, C_i; \gamma) - \mu_1(x_{ij}, X_i; \beta)] \\
\frac{\partial U_2}{\partial \gamma} &= -\frac{\partial \mu_2(X_i, M_i, C_i; \beta)}{\partial \gamma} \Sigma_{\mu_2}^{-1} \frac{\partial \mu_2(X_i, M_i, C_i; \beta)}{\partial \gamma} \\
\frac{\partial U_3}{\partial \tau} &= -\frac{\partial \mu_3(C_i; \tau)}{\partial \tau} \Sigma_{\mu_3}^{-1} \frac{\partial \mu_3(C_i; \tau)}{\partial \tau}
\end{aligned}$$