# Sandwich estimator derivations for natural effect model parameters

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# Weighting-based approach

## Stratum-specific effects

### Models

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

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

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

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

### **Estimating equations**

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

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

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

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

with n the total sample size of the original dataset,

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

and

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

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

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

## Population-average effects

### Models

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

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

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

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

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

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

## Estimating equations

$$U_{1}(X_{i}, x^{*}; \beta, \theta, \tau) = k^{-1} \sum_{j=1}^{k} \frac{\partial \mu_{1}(X_{i}, x_{ij}^{*}; \beta)}{\partial \beta} \Sigma_{\mu_{1}}^{-1} \Pr(X_{i} | C_{i}; \tau)^{-1} \cdot \frac{\Pr(M_{i} | x_{ij}^{*}, C_{i}; \theta)}{\Pr(M_{i} | X_{i}, C_{i}; \theta)} \cdot [Y_{i} - \mu_{1}(X_{i}, x_{ij}^{*}; \beta)]$$

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

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

### 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

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

with

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

and

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

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

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

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

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

# Imputation-based approach

# Stratum-specific effects

#### Models

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

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

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

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

### **Estimating equations**

$$U_{1}(x, X_{i}, C_{i}; \beta, \gamma) = k^{-1} \sum_{j=1}^{k} \frac{\partial \mu_{1}(x_{ij}, X_{i}, C_{i}; \beta)}{\partial \beta} \Sigma_{\mu_{1}}^{-1} \cdot \left[ \mu_{2}(x_{ij}, M_{i}, C_{i}; \gamma) - \mu_{1}(x_{ij}, X_{i}, C_{i}; \beta) \right]$$

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

#### Sandwich estimator

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

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

with

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

and

$$\begin{split} \frac{\partial U_1}{\partial \beta} &= -k^{-1} \sum_{j=1}^k \frac{\partial \mu_1(x_{ij}, X_i, C_i; \beta)}{\partial \beta} \Sigma_{\mu_1}^{-1} \frac{\partial \mu_1(x_{ij}, X_i, C_i; \beta)}{\partial \beta} \\ \frac{\partial U_1}{\partial \gamma} &= k^{-1} \sum_{j=1}^k \frac{\partial \mu_1(x_{ij}, X_i, C_i; \beta)}{\partial \beta} \Sigma_{\mu_1}^{-1} \frac{\partial \mu_2(x_{ij}, M_i, C_i; \gamma)}{\partial \gamma} \\ \frac{\partial U_2}{\partial \gamma} &= -\frac{\partial \mu_2(X_i, M_i, C_i; \beta)}{\partial \gamma} \Sigma_{\mu_2}^{-1} \frac{\partial \mu_2(X_i, M_i, C_i; \beta)}{\partial \gamma} \end{split}$$

## Population-average effects

### Models

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

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

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

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

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

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

### **Estimating equations**

$$U_{1}(x, X_{i}; \beta, \gamma, \tau) = k^{-1} \sum_{j=1}^{k} \frac{\partial \mu_{1}(x_{ij}, X_{i}; \beta)}{\partial \beta} \Sigma_{\mu_{1}}^{-1} \Pr(X_{i} | C_{i}; \tau)^{-1} \cdot \left[ \mu_{2}(x_{ij}, M_{i}, C_{i}; \gamma) - \mu_{1}(x_{ij}, X_{i}; \beta) \right]$$

$$U_{2}(X_{i}, M_{i}, C_{i}; \gamma) = \frac{\partial \mu_{2}(X_{i}, M_{i}, C_{i}; \gamma)}{\partial \gamma} \Sigma_{\mu_{2}}^{-1} \left[ Y_{i} - \mu_{2}(X_{i}, M_{i}, C_{i}; \gamma) \right]$$

$$U_{3}(C_{i}; \tau) = \frac{\partial \mu_{3}(C_{i}; \tau)}{\partial \tau} \Sigma_{\mu_{3}}^{-1} \left[ X_{i} - \mu_{3}(C_{i}; \tau) \right]$$

### 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

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

with

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

and

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

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

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

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

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