

SHARP BOUNDS AND COVARIATE ADJUSTMENT FOR ORDINAL OUTCOMES IN STRATIFIED RANDOMIZED EXPERIMENTS

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Supplementary Material

This supplementary material consists of five sections. Regarding the proofs of Propositions 1–4, Theorem 1–3, and one Corollary in the main text.

S1 Proposition 1, 2 and their proofs

We review some symbols and notations to facilitate understanding of the proof. The stratified relative effect under joint distribution $L_{[m]}$ is defined as follows

$$\begin{aligned}\gamma_{[m]} &= \Pr \{Y_i(1) > Y_i(0) | B_i = m\} - \Pr \{Y_i(1) < Y_i(0) | B_i = m\} \\ &= \sum_{k=0}^{J-1} \sum_{l=0}^{J-1} \text{sgn}(k - l) p_{kl}^{[m]},\end{aligned}$$

and the population relative treatment effect is

$$\gamma = \sum_{m=1}^M \sum_{k=0}^{J-1} \sum_{l=0}^{J-1} \pi_{[m]} \text{sgn}(k - l) p_{kl}^{[m]} = \sum_{m=1}^M \pi_{[m]} \gamma_{[m]}.$$

The stratified average treatment effect $\tau_{[m]}$ and population treatment effect τ are defined as

$$\tau_{[m]} = \left(n_{[m]}\right)^{-1} \sum_{i: B_i=m} Y_i(1) - Y_i(0) \text{ and } \tau = \sum_{m=1}^M \pi_{[m]} \tau_{[m]}.$$

Proof of Proposition 1. When $J = 2$, i.e., Y is binary, we expand $\gamma_{[m]}$ as follows:

$$\gamma_{[m]} = \sum_{k=0}^1 \sum_{l=0}^1 \text{sgn}(k-l) p_{kl}^{[m]} = p_{10}^{[m]} + (p_{11}^{[m]} - p_{01}^{[m]}) - p_{01}^{[m]} = p_{1+}^{[m]} - p_{+1}^{[m]},$$

and the marginal probabilities $p_{1+}^{[m]}, p_{+1}^{[m]}$ can be equivalently written as

$$p_{1+}^{[m]} - p_{+1}^{[m]} = E \{Y_i(1) - Y_i(0) | B_i = m\},$$

which is equivalent to average treatment effect $\tau_{[m]} = (n_{[m]})^{-1} \sum_{i: B_i=m} Y_i(1) - Y_i(0)$. According to the definitions of γ and τ , we have

$$\gamma = \sum_{m=1}^M \pi_{[m]} \gamma_{[m]} = \sum_{m=1}^M \pi_{[m]} \tau_{[m]} = \tau.$$

□

As discussed in Section 2, when the number of categories $J \geq 3$, $\gamma_{[m]}$ cannot be identified, so $\delta_{k'l'}^{[m]}$ is introduced as its loose upper bound. The proof is as follows.

Proof of Proposition 2. For each fixed $k' = 1, \dots, J-1$ and $l' = 1, \dots, J-k'$, define $\delta_{k'l'}^{[m]}$ as

$$\delta_{k'l'}^{[m]} = \sum_{k=k'}^{J-1} p_{k+}^{[m]} + \sum_{k=k'+l'}^{J-1} p_{k+}^{[m]} + \sum_{l=0}^{k'-2} p_{+l}^{[m]} - \sum_{l=k'+l'-1}^{J-1} p_{+l}^{[m]},$$

we consider $k' \in \{1, \dots, J-1\}$, the probability $\Pr\{Y_i(1) > Y_i(0) | B_i = m\}$ can be decomposed as follows:

$$\begin{aligned}
 & \Pr\{Y_i(1) > Y_i(0) | B_i = m\} \\
 &= \Pr\{Y_i(1) \geq k', Y_i(0) < Y_i(1) | B_i = m\} + \Pr\{Y_i(1) < k', Y_i(0) < Y_i(1) | B_i = m\} \\
 &= \Pr\{Y_i(1) \geq k', Y_i(0) \leq k' - 1, Y_i(0) < Y_i(1) | B_i = m\} \\
 &+ \Pr\{Y_i(1), Y_i(0) > k', Y_i(0) < Y_i(1) | B_i = m\} \\
 &+ \Pr\{Y_i(1) < k', Y_i(0) < Y_i(1) | B_i = m\} \\
 &= \underbrace{\Pr\{Y_i(1) \geq k', Y_i(0) \leq k' - 1 | B_i = m\}}_{T_1} + \underbrace{\Pr\{Y_i(1), Y_i(0) \geq k', Y_i(0) < Y_i(1) | B_i = m\}}_{T_2} \\
 &+ \underbrace{\Pr\{Y_i(1) < k', Y_i(0) < Y_i(1) | B_i = m\}}_{T_3},
 \end{aligned}$$

which is expanded into three terms, T_1 , T_2 , and T_3 . Similarly, by swapping the roles of treatment and control, we obtain

$$\begin{aligned}
 & \Pr\{Y_i(1) < Y_i(0) | B_i = m\} \\
 &= \underbrace{\Pr\{Y_i(0) \geq k', Y_i(1) \leq k' - 1 | B_i = m\}}_{T_4} + \underbrace{\Pr\{Y_i(0), Y_i(1) \geq k', Y_i(1) < Y_i(0) | B_i = m\}}_{T_5} \\
 &+ \underbrace{\Pr\{Y_i(0) < k', Y_i(1) < Y_i(0) | B_i = m\}}_{T_6}.
 \end{aligned}$$

Thus, the stratified treatment effect $\gamma_{[m]}$ can be written as

$$\begin{aligned}
 \gamma_{[m]} &= \Pr\{Y_i(1) > Y_i(0) | B_i = m\} - \Pr\{Y_i(1) < Y_i(0) | B_i = m\} \\
 &= (T_1 - T_4) + T_2 + T_3 - T_5 - T_6 \\
 &\leq T_1 - T_4 + T_2 + T_3,
 \end{aligned}$$

where the inequality holds since T_5 and T_6 are nonnegative. We now analyze the term $T_1 - T_4$,

that is

$$\begin{aligned}
 T_1 - T_4 &= \Pr\{Y_i(1) \geq k', Y_i(0) \leq k' - 1 | B_i = m\} - \Pr\{Y_i(0) \geq k', Y_i(1) \leq k' - 1 | B_i = m\} \\
 &= \Pr\{Y_i(1) \geq k' | B_i = m\} - \Pr\{Y_i(1) \geq k', Y_i(0) \geq k' | B_i = m\} - \Pr\{Y_i(0) \geq k' | B_i = m\} \\
 &\quad + \Pr\{Y_i(0) \geq k', Y_i(1) \geq k' | B_i = m\} \\
 &= \Pr\{Y_i(1) \geq k' | B_i = m\} - \Pr\{Y_i(0) \geq k' | B_i = m\} \\
 &= \sum_{k=k'}^{J-1} p_{k+}^{[m]} - \sum_{l=k'}^{J-1} p_{+l}^{[m]}.
 \end{aligned}$$

For a given $l' \in \{1, \dots, J - k'\}$, we proceed with the analysis of T_2 :

$$\begin{aligned}
 T_2 &= \Pr\{Y_i(1), Y_i(0) \geq k', Y_i(0) < Y_i(1) | B_i = m\} \\
 &= \Pr\{k' \leq Y_i(0) \leq k' + l' - 2, Y_i(0) < Y_i(1) | B_i = m\} + \Pr\{k' + l' - 1 \leq Y_i(0) \leq J - 2, \\
 &\quad Y_i(0) < Y_i(1) | B_i = m\} \\
 &= \sum_{l=k'}^{k'+l'-2} \sum_{k=l+1}^{J-1} p_{kl}^{[m]} + \sum_{l=k'+l'-1}^{J-2} \sum_{k=l+1}^{J-1} p_{kl}^{[m]} \\
 &= \sum_{l=k'}^{k'+l'-2} \sum_{k=l+1}^{J-1} p_{kl}^{[m]} + \sum_{k=k'+l'}^{J-1} \sum_{l=k'+l'-1}^{k-1} p_{kl}^{[m]} \\
 &\leq \sum_{l=k'}^{k'+l'-2} p_{+l}^{[m]} + \sum_{k=k'+l'}^{J-1} p_{k+}^{[m]}.
 \end{aligned}$$

Similarly, T_3 is transformed as:

$$\begin{aligned}
 T_3 &= \Pr\{Y_i(1) \leq k' - 1, Y_i(0) < Y_i(1) | B_i = m\} \\
 &= \sum_{k=1}^{k'-1} \sum_{l=0}^{k-1} p_{kl}^{[m]} = \sum_{l=0}^{k'-2} \sum_{k=l+1}^{k'-1} p_{kl}^{[m]} \leq \sum_{l=0}^{k'-2} p_{+l}^{[m]}.
 \end{aligned}$$

Therefore, combining $(T_1 - T_4), T_2, T_3$, we have

$$\begin{aligned}
 \gamma_{[m]} &\leq (T_1 - T_4) + T_2 + T_3 \\
 &\leq \sum_{k=k'}^{J-1} p_{k+}^{[m]} - \sum_{l=k'}^{J-1} p_{+l}^{[m]} + \sum_{l=k'}^{k'+l'-2} p_{+l}^{[m]} + \sum_{k=k'+l'}^{J-1} p_{k+}^{[m]} + \sum_{l=0}^{k'-2} p_{+l}^{[m]} \\
 &= \delta_{k'l'}^{[m]}
 \end{aligned}$$

completing the proof of Proposition 2. $\square$

S2 Proposition 3 and its proof

Proposition 2 above gives a loose upper bound for $\gamma_{[m]}$. By finding the matrix $L_{[m]} = \{p_{kl}^{[m]}\}$ through linear programming constraints, we can find sharp bounds $\gamma_{[m]}^L$ and $\gamma_{[m]}^U$. Prior to this, Proposition 3 provided a method for constructing matrices, which first requires two non-negative vectors $\mathbf{c}_1$ and $\mathbf{c}_2$ to be specified. Then, the tail sums $C_1^t(s) := \sum_{r=s}^{J-1} c_{1r}$, $C_2^t(s) := \sum_{r=s}^{J-1} c_{2r}$ and the prefix sums $C_1^p(s) := \sum_{r=0}^s c_{1r}$, $C_2^p(s) := \sum_{r=0}^s c_{2r}$ are defined. Under the tail capacity condition $C_1^t(s) \geq C_2^t(s)$, a lower triangular matrix $\mathbf{A}_J = (a_{kl})$ is constructed; similarly, under the prefix capacity condition $C_1^p(s) \leq C_2^p(s)$, matrix $\mathbf{B}_J = (b_{kl})$ is constructed. The detailed proof process is as follows.

Proof of Proposition 3. We prove Proposition 3(1) by induction.

(i) When $J = 1$, there are elements c_{10}, c_{20} , and the condition $C_1^t(0) = \sum_{r=0}^{J-1} c_{1r} \geq C_2^t(0) = \sum_{r=0}^{J-1} c_{2r}$ is satisfied, i.e., $c_{10} \geq c_{20}$. We set $\mathbf{A}_1 = (a_{00}) = (c_{20})$, and can verify that

$$\sum_{l=0}^{J-1} a_{kl} = c_{20} \leq c_{10}, \quad \sum_{k=0}^{J-1} a_{kl} = a_{00} = c_{20}.$$

(ii) When $J \geq 2$, suppose Proposition 3(1) holds for any $J - 1$. By the tail capacity condition $C_1^t(s) \geq C_2^t(s)$ for all $s = 1, \dots, J - 1$, the truncated vectors $(c_{11}, \dots, c_{1(J-1)})$ and

$(c_{21}, \dots, c_{2(J-1)})$ also satisfy the induction hypothesis; hence there exists a $(J-1) \times (J-1)$ lower triangular matrix $\mathbf{A}_{J-1}$ with

$$\sum_{l'=1}^{J-1} a_{kl'} \leq c_{1k}, \quad \sum_{k'=1}^{J-1} a_{k'l} = c_{2l} \quad (k, l = 1, \dots, J-1).$$

Construct $\mathbf{A}_J$ as

$$\mathbf{A}_J = \begin{pmatrix} a_{00} & \mathbf{0}^T \\ \mathbf{a} & \mathbf{A}_{J-1} \end{pmatrix},$$

where a_{00} is a scalar and $\mathbf{a} = (a_{10}, \dots, a_{J-1,0})^T$. We discuss two scenarios.

(ii-1) $c_{20} < c_{10}$. Let $a_{00} = c_{20}$ and $a_{k0} = 0$ for all $k \geq 1$. $\mathbf{A}_J$ has non-negative elements and

$$\sum_{l'=0}^{J-1} a_{kl'} \leq c_{1k}, \quad \sum_{k'=0}^{J-1} a_{k'l} = c_{2l}.$$

(ii-2) $c_{20} \geq c_{10}$. Let $a_{00} = c_{10}$. We need to construct $\mathbf{a} = (a_{10}, \dots, a_{J-1,0})^T$ such that the sum of the first column is c_{20} , i.e., $\sum_{k=1}^{J-1} a_{k0} = c_{20} - c_{10}$. If $c_{20} = c_{10}$, set $a_{k0} = 0$ for all $k \geq 1$. If $c_{20} > c_{10}$, define

$$a_{k0} = (c_{20} - c_{10}) \frac{c_{1k} - \sum_{l=1}^{J-1} a_{kl}}{\sum_{k'=1}^{J-1} \left(c_{1k'} - \sum_{l'=1}^{J-1} a_{k'l'} \right)}.$$

Note that, using the column-sum property of $\mathbf{A}_{J-1}$,

$$\begin{aligned} \sum_{k'=1}^{J-1} \left(c_{1k'} - \sum_{l'=1}^{J-1} a_{k'l'} \right) &= \sum_{k'=1}^{J-1} c_{1k'} - \sum_{l'=1}^{J-1} \sum_{k'=1}^{J-1} a_{k'l'} = \sum_{k'=1}^{J-1} c_{1k'} - \sum_{k'=1}^{J-1} c_{2k'} \\ &\geq c_{20} - c_{10} = c_{20} - a_{00} > 0, \end{aligned}$$

where the inequality follows from the tail capacity condition at $s = 0$, i.e., $\sum_{r=0}^{J-1} c_{1r} \geq \sum_{r=0}^{J-1} c_{2r}$. Hence the denominator is positive when $c_{20} > c_{10}$, and $a_{k0} \geq 0$. This construction guarantees

that the column sums of $\mathbf{A}_J$ are c_{2l} and that the row sums satisfy $\sum_{l'=0}^{J-1} a_{kl'} \leq c_{1k}$.

To prove Proposition 3(2), we directly apply $(c_{2(J-1)}, \dots, c_{20})$ and $(c_{1(J-1)}, \dots, c_{10})$ to (1), obtaining the matrix $\tilde{\mathbf{B}}_J = (\tilde{b}_{kl})$ such that

$$\sum_{k'=0}^{J-1} \tilde{b}_{k'l} = c_{1(J-l-1)}, \quad \sum_{l'=0}^{J-1} \tilde{b}_{kl'} \leq c_{2(J-k-1)} \quad (k, l = 0, \dots, J-1),$$

and let $\mathbf{B}_J = (\tilde{b}_{J-l-1, J-k-1})$. Then $\mathbf{B}_J$ is lower triangular and satisfies the desired inequalities, and the proof of the Proposition 3 is complete. $\square$

S3 Proposition 4 and its proof

The three cases for the values of k_0 and l_0 are given in Proposition 4, followed by three inequalities. Before that, we need to introduce Proposition 5, as shown below.

Proposition 5. *For a fixed $k' = 1, \dots, J-1$, $l' = 1, \dots, J-k'$ and $m = 1, \dots, M$ the distributional causal effect is defined as*

$$\Delta_{k'}^{[m]} = \Pr\{Y_i(1) \geq k' \mid B_i = m\} - \Pr\{Y_i(0) \geq k' \mid B_i = m\} = \sum_{k \geq k'} p_{k+}^{[m]} - \sum_{l \geq k'} p_{+l}^{[m]}.$$

Then we have

$$\delta_{k'l'}^{[m]} = \sum_{l=k'}^{k'+l'-2} p_{+l}^{[m]} + \sum_{k=k'+l'}^{J-1} p_{k+}^{[m]} + \sum_{l=0}^{k'-2} p_{+l}^{[m]} + \Delta_{k'}^{[m]}, \quad (\text{S3.1})$$

for any $l' \in \{1, \dots, J-k'\}$. Moreover, the following equalities hold for $\tilde{k} \in \{1, \dots, J-2\}$

and $\tilde{l} \in \{1, \dots, J-1-\tilde{k}\}$:

$$\delta_{\tilde{k}(\tilde{l}+1)}^{[m]} = \delta_{\tilde{k}\tilde{l}}^{[m]} + p_{+(\tilde{k}+\tilde{l}-1)}^{[m]} - p_{(\tilde{k}+\tilde{l})+}^{[m]}, \quad (\text{S3.2})$$

$$\delta_{\tilde{k}(\tilde{l}+1)}^{[m]} = \delta_{(\tilde{k}+1)\tilde{l}}^{[m]} + p_{\tilde{k}+}^{[m]} - p_{+(\tilde{k}-1)}^{[m]}, \quad (\text{S3.3})$$

$$\delta_{1\tilde{k}}^{[m]} = \delta_{(\tilde{k}+1)(J-1-\tilde{k})}^{[m]} + p_{+(J-1)}^{[m]} - p_{0+}^{[m]}. \quad (\text{S3.4})$$

Proof of Proposition 5. To prove (S3.1), from the definitions for $\delta_{k'l'}^{[m]}$ and $\Delta_{k'}^{[m]}$ we have

$$\begin{aligned} \delta_{k'l'}^{[m]} &= \sum_{k=k'+l'}^{J-1} p_{k+}^{[m]} + \sum_{l=0}^{k'-2} p_{+l}^{[m]} + \Delta_{k'}^{[m]} + \sum_{l=k'}^{k'+l'-2} p_{+l}^{[m]} \\ &= \sum_{k=k'+l'}^{J-1} p_{k+}^{[m]} + \sum_{l=0}^{k'-2} p_{+l}^{[m]} + \underbrace{\sum_{k \geq k'} p_{k+}^{[m]} - \sum_{l \geq k'} p_{+l}^{[m]}}_{\Delta_{k'}^{[m]}} + \sum_{l=k'}^{k'+l'-2} p_{+l}^{[m]} \\ &= \sum_{k=k'+l'}^{J-1} p_{k+}^{[m]} + \sum_{l=0}^{k'-2} p_{+l}^{[m]} + \sum_{k=k'}^{J-1} p_{k+}^{[m]} + \left(\sum_{l=k'}^{k'+l'-2} p_{+l}^{[m]} - \sum_{l=k'}^{J-1} p_{+l}^{[m]} \right) \\ &= \sum_{k=k'+l'}^{J-1} p_{k+}^{[m]} + \sum_{l=0}^{k'-2} p_{+l}^{[m]} + \sum_{k=k'}^{J-1} p_{k+}^{[m]} - \sum_{l=k'+l'-1}^{J-1} p_{+l}^{[m]} \end{aligned}$$

To prove (S3.2), we first present the following equalities,

$$\begin{aligned} \sum_{l=\tilde{k}}^{\tilde{k}+\tilde{l}-1} p_{+l}^{[m]} &= \sum_{l=\tilde{k}}^{\tilde{k}+\tilde{l}-2} p_{+l}^{[m]} + p_{+(\tilde{k}+\tilde{l}-1)}^{[m]}, \\ \sum_{k=\tilde{k}+\tilde{l}+1}^{J-1} p_{k+}^{[m]} &= \sum_{k=\tilde{k}+\tilde{l}}^{J-1} p_{k+}^{[m]} - p_{(\tilde{k}+\tilde{l})+}^{[m]}. \end{aligned}$$

Therefore we have

$$\begin{aligned}
 \delta_{\tilde{k}(\tilde{l}+1)}^{[m]} &= \Delta_{\tilde{k}}^{[m]} + \sum_{l=0}^{\tilde{k}-2} p_{+l}^{[m]} + \sum_{l=\tilde{k}}^{\tilde{k}+\tilde{l}-1} p_{+l}^{[m]} + \sum_{k=\tilde{k}+\tilde{l}+1}^{J-1} p_{k+}^{[m]} \\
 &= \Delta_{\tilde{k}}^{[m]} + \sum_{l=0}^{\tilde{k}-2} p_{+l}^{[m]} + \sum_{l=\tilde{k}}^{\tilde{k}+\tilde{l}-2} p_{+l}^{[m]} + p_{+(\tilde{k}+\tilde{l}-1)}^{[m]} + \sum_{k=\tilde{k}+\tilde{l}}^{J-1} p_{k+}^{[m]} - p_{(\tilde{k}+\tilde{l})+}^{[m]} \\
 &= \delta_{\tilde{k}\tilde{l}}^{[m]} + p_{+(\tilde{k}+\tilde{l}-1)}^{[m]} - p_{(\tilde{k}+\tilde{l})+}^{[m]}.
 \end{aligned}$$

To prove (S3.3), note that

$$\begin{aligned}
 \sum_{l=0}^{\tilde{k}-2} p_{+l}^{[m]} &= \sum_{l=0}^{\tilde{k}-1} p_{+l}^{[m]} - p_{+(\tilde{k}-1)}^{[m]}, \\
 \sum_{l=\tilde{k}}^{\tilde{k}+\tilde{l}-1} p_{+l}^{[m]} &= \sum_{l=\tilde{k}+1}^{\tilde{k}+\tilde{l}-1} p_{+l}^{[m]} + p_{+\tilde{k}}^{[m]}.
 \end{aligned}$$

We have

$$\begin{aligned}
 \delta_{\tilde{k}(\tilde{l}+1)}^{[m]} &= \Delta_{\tilde{k}}^{[m]} + \sum_{l=0}^{\tilde{k}-2} p_{+l}^{[m]} + \sum_{l=\tilde{k}}^{\tilde{k}+\tilde{l}-1} p_{+l}^{[m]} + \sum_{k=\tilde{k}+\tilde{l}+1}^{J-1} p_{k+}^{[m]} \\
 &= \Delta_{\tilde{k}+1}^{[m]} + p_{\tilde{k}+}^{[m]} + \sum_{l=0}^{\tilde{k}-1} p_{+l}^{[m]} - p_{+(\tilde{k}-1)}^{[m]} + \sum_{l=\tilde{k}+1}^{\tilde{k}+\tilde{l}-1} p_{+l}^{[m]} + \sum_{k=\tilde{k}+\tilde{l}+1}^{J-1} p_{k+}^{[m]} \\
 &= \delta_{(\tilde{k}+1)\tilde{l}}^{[m]} + p_{\tilde{k}+}^{[m]} - p_{+(\tilde{k}-1)}^{[m]}.
 \end{aligned}$$

To prove (S3.4), repeatedly applying (S3.2) and (S3.3), we obtain,

$$\begin{aligned}
 \delta_{(\tilde{k}+1)(J-1-\tilde{k})}^{[m]} &= \delta_{1\tilde{k}}^{[m]} + \left(1 - p_{+(J-1)}^{[m]}\right) - \left(1 - p_{0+}^{[m]}\right) \\
 &= \delta_{1\tilde{k}}^{[m]} + p_{0+}^{[m]} - p_{+(J-1)}^{[m]}.
 \end{aligned}$$

□

Proof of Proposition 4. We prove three cases sequentially.

(1) Consider the first case where $k_0 > 1$. Define $\Omega_1 = \{1, \dots, k_0 - 1\}$. For $k \in \Omega_1 \setminus \{k_0 - 1\}$, let $q_{k+}^{[m]}$ satisfy:

$$q_{k+}^{[m]} = p_{k+}^{[m]}, \text{ and } q_{(k_0-1)+}^{[m]} = p_{(k_0-1)+}^{[m]} + \min(0, \lambda_0^{[m]}).$$

Under this setup, we need to prove the inequality

$$\sum_{l=n-1}^{k_0-2} p_{+l}^{[m]} \leq \sum_{k=n}^{k_0-1} q_{k+}^{[m]}, \quad n = 1, \dots, k_0 - 1.$$

From the definition of $\delta_{k_0 l_0}^{[m]}$, we know that $\delta_{k_0 l_0}^{[m]} \leq \delta_{k' l'}^{[m]}$ for all $k' = 1, \dots, J-1$, $l' = 1, \dots, J-k'$.

Using (S3.3) of Proposition 5, we derive

$$\delta_{k_0 l_0}^{[m]} = \delta_{n(k_0+l_0-n)}^{[m]} + \sum_{s=n}^{k_0-1} (p_{+(s-1)}^{[m]} - p_{s+}^{[m]}), \quad n = 1, \dots, k_0 - 1.$$

Since $\delta_{k_0 l_0}^{[m]} \leq \delta_{n(k_0+l_0-n)}^{[m]}$, it follows that

$$\sum_{l=n-1}^{k_0-2} p_{+l}^{[m]} \leq \sum_{k=n}^{k_0-1} p_{k+}^{[m]}, \quad n = 1, \dots, k_0 - 1.$$

By further applying (S3.2) of Proposition 5, we obtain

$$\delta_{n(k_0+l_0-n)}^{[m]} = \delta_{n(k_0-n)}^{[m]} - \left(\sum_{k=k_0}^{k_0+l_0-1} p_{k+}^{[m]} - \sum_{l=k_0-1}^{k_0+l_0-2} p_{+l}^{[m]} \right) = \delta_{n(k_0-n)}^{[m]} - \lambda_0^{[m]}.$$

Combining with the previous display gives

$$\delta_{k_0 l_0}^{[m]} = \delta_{n(k_0-n)}^{[m]} + \left(-\lambda_0^{[m]} + \sum_{s=n}^{k_0-1} (p_{+(s-1)}^{[m]} - p_{s+}^{[m]}) \right).$$

Hence the term in parentheses is ≤ 0 , which implies

$$\sum_{l=n-1}^{k_0-2} p_{+l}^{[m]} \leq \lambda_0^{[m]} + \sum_{k=n}^{k_0-1} p_{k+}^{[m]}.$$

Recalling that $q_{k+}^{[m]} = p_{k+}^{[m]}$ for $k \neq k_0 - 1$ and $q_{(k_0-1)+}^{[m]} = p_{(k_0-1)+}^{[m]} + \min(0, \lambda_0^{[m]})$, the two bounds above yield, for all $n = 1, \dots, k_0 - 1$,

$$\sum_{l=n-1}^{k_0-2} p_{+l}^{[m]} \leq \sum_{k=n}^{k_0-1} q_{k+}^{[m]},$$

which concludes the proof of the first case.

(2) We consider the second case where $l_0 > 1$. Define $\Omega_2 = \{k_0 + 1, \dots, k_0 + l_0 - 1\}$. For $k \in \Omega_2 \setminus \{k_0 + l_0 - 1\}$, let

$$q_{k+}^{[m]} = p_{k+}^{[m]} \text{ and } q_{(k_0+l_0-1)+}^{[m]} = p_{(k_0+l_0-1)+}^{[m]} - \max(0, \lambda_0^{[m]}).$$

We need to prove the inequality:

$$\sum_{l=k_0+n-1}^{k_0+l_0-2} p_{+l}^{[m]} \leq \sum_{k=k_0+n}^{k_0+l_0-1} q_{k+}^{[m]}, \quad n = 1, \dots, l_0 - 1.$$

The proof for this case follows a similar structure to the first one. Based on (S3.1) of Proposition 5, we have

$$\delta_{k_0 l_0}^{[m]} = \delta_{k_0 n}^{[m]} + \sum_{s=n}^{l_0-1} \left(p_{+(k_0+s-1)}^{[m]} - p_{(k_0+s)+}^{[m]} \right), \quad n = 1, \dots, l_0 - 1,$$

Additionally, using (S3.3) of Proposition 5, we can derive another expression for $\delta_{k_0 l_0}^{[m]}$:

$$\delta_{k_0 l_0}^{[m]} = \delta_{n(k_0+l_0-n)}^{[m]} + \sum_{s=k_0}^{n-1} \left(p_{s+}^{[m]} - p_{+(s-1)}^{[m]} \right), \quad n = k_0 + 1, \dots, k_0 + l_0 - 1.$$

Since $\delta_{k_0 l_0}^{[m]} \leq \delta_{k_0 n}^{[m]}$, we obtain

$$\sum_{s=n}^{l_0-1} p_{+(k_0+s-1)}^{[m]} \leq \sum_{s=n}^{l_0-1} p_{(k_0+s)+}^{[m]} \text{ for } n = 1, \dots, l_0 - 1.$$

Rewriting this inequality, we have

$$\sum_{l=k_0+n-1}^{k_0+l_0-2} p_{+l}^{[m]} \leq \sum_{k=k_0+n}^{k_0+l_0-1} p_{k+}^{[m]}$$

Similarly, since $\delta_{k_0 l_0}^{[m]} \leq \delta_{n(k_0+l_0-n)}^{[m]}$, we have

$$\sum_{s=k_0}^{n-1} p_{s+}^{[m]} \leq \sum_{s=k_0}^{n-1} p_{+(s-1)}^{[m]}, \quad n = k_0 + 1, \dots, k_0 + l_0 - 1,$$

which can be rewritten as:

$$\sum_{k=k_0}^n p_{k+}^{[m]} \leq \sum_{l=k_0-1}^{n-1} p_{+l}^{[m]}, \quad n = k_0, \dots, k_0 + l_0 - 2.$$

By further expanding this inequality, we have

$$\sum_{k=k_0}^{k_0+l_0-1} p_{k+}^{[m]} - \sum_{k=n+1}^{k_0+l_0-1} p_{k+}^{[m]} \leq \sum_{l=k_0-1}^{k_0+l_0-2} p_{+l}^{[m]} - \sum_{l=n}^{k_0+l_0-2} p_{+l}^{[m]},$$

and thus,

$$\sum_{l=n}^{k_0+l_0-2} p_{+l}^{[m]} \leq \sum_{k=n+1}^{k_0+l_0-1} p_{k+}^{[m]} - \underbrace{\left(\sum_{k=k_0}^{k_0+l_0-1} p_{k+}^{[m]} - \sum_{l=k_0-1}^{k_0+l_0-2} p_{+l}^{[m]} \right)}_{\lambda_0^{[m]}}$$

which simplifies to:

$$\sum_{l=k_0+n-1}^{k_0+l_0-2} p_{+l}^{[m]} \leq \sum_{k=k_0+n}^{k_0+l_0-1} p_{k+}^{[m]} - \lambda_0^{[m]}, \quad n = 1, \dots, l_0 - 1.$$

Therefore, for $n = 1, \dots, l_0 - 1$,

$$\sum_{l=k_0+n-1}^{k_0+l_0-2} p_{+l}^{[m]} \leq \sum_{k=k_0+n}^{k_0+l_0-1} q_{k+}^{[m]},$$

because by definition $q_{k+}^{[m]} = p_{k+}^{[m]}$ ($k \neq k_0 + l_0 - 1$) and $q_{(k_0+l_0-1)+}^{[m]} = p_{(k_0+l_0-1)+}^{[m]} - \max\{0, \lambda_0^{[m]}\}$, so that

$$\sum_{k=k_0+n}^{k_0+l_0-1} q_{k+}^{[m]} = \sum_{k=k_0+n}^{k_0+l_0-1} p_{k+}^{[m]} - \max\{0, \lambda_0^{[m]}\}.$$

Combining the two displayed bounds (the one without $-\lambda_0^{[m]}$ when $\lambda_0^{[m]} < 0$, and the one with $-\lambda_0^{[m]}$ when $\lambda_0^{[m]} \geq 0$) yields the stated inequality with $q_{k+}^{[m]}$. The proof of the second case is complete.

(3) For the final case where $k_0 + l_0 < J$, let $\Omega_3 = \{k_0 + l_0 - 1, \dots, J - 2\}$. For $l \in \Omega_3 \setminus \{k_0 + l_0 - 1\}$, we define:

$$q_{+l}^{[m]} = p_{+l}^{[m]} \text{ and } q_{+(k_0+l_0-1)}^{[m]} = p_{+(k_0+l_0-1)}^{[m]} - \max(0, \lambda_0^{[m]}).$$

We need to prove that

$$\sum_{k=k_0+l_0}^{k_0+n-1} p_{k+}^{[m]} \leq \sum_{l=k_0+l_0-1}^{k_0+n-2} q_{+l}^{[m]}, \quad n = l_0 + 1, \dots, J - k_0.$$

The proof for the final case follows similar arguments as the earlier cases and leverages the relationship between the indices and summation bounds provided by Proposition 5. For $n = l_0 + 1, \dots, J - k_0$, we have the recursive formulation:

$$\delta_{k_0 l_0}^{[m]} = \delta_{k_0 n}^{[m]} + \sum_{s=l_0}^{n-1} p_{(k_0+s)+}^{[m]} - \sum_{s=l_0}^{n-1} p_{+(k_0+s-1)}^{[m]}.$$

Since $\delta_{k_0 l_0}^{[m]} \leq \delta_{k_0 n}^{[m]}$, this implies:

$$\sum_{s=l_0}^{n-1} p_{(k_0+s)+}^{[m]} \leq \sum_{s=l_0}^{n-1} p_{+(k_0+s-1)}^{[m]},$$

thus we have

$$\sum_{k=k_0+l_0}^{k_0+n-1} p_{k+}^{[m]} \leq \sum_{l=k_0+l_0-1}^{k_0+n-2} p_{+l}^{[m]}.$$

Based on the argument of the proof of the first case, the following equation can be established,

$$\delta_{k_0 l_0}^{[m]} = \delta_{n(k_0+l_0-n)}^{[m]} + \sum_{s=n}^{k_0-1} \left(p_{+(s-1)}^{[m]} - p_{s+}^{[m]} \right), n = 1, \dots, k_0 - 1.$$

Setting $n = 1$, the above equality becomes:

$$\begin{aligned} \delta_{k_0 l_0}^{[m]} &= \delta_{1(k_0+l_0-1)}^{[m]} + \sum_{s=1}^{k_0-1} \left(p_{+(s-1)}^{[m]} - p_{s+}^{[m]} \right) \\ &= \delta_{1(k_0+l_0-1)}^{[m]} + \sum_{l=0}^{k_0-2} p_{+l}^{[m]} - \sum_{k=1}^{k_0-1} p_{k+}^{[m]} \\ &= \delta_{1(k_0+l_0-1)}^{[m]} + \left(\sum_{l=0}^{J-1} p_{+l}^{[m]} - \sum_{l=k_0-1}^{J-1} p_{+l}^{[m]} \right) - \left(\sum_{k=0}^{J-1} p_{k+}^{[m]} - \sum_{k=k_0}^{J-1} p_{k+}^{[m]} - p_{0+}^{[m]} \right) \\ &= \delta_{1(k_0+l_0-1)}^{[m]} - \sum_{l=k_0-1}^{J-1} p_{+l}^{[m]} + \sum_{k=k_0}^{J-1} p_{k+}^{[m]} + p_{0+}^{[m]} \end{aligned}$$

Using (S3.4) of Proposition 5, we have

$$\delta_{1(k_0+l_0-1)}^{[m]} = \delta_{(k_0+l_0)(J-k_0-l_0)}^{[m]} + p_{+(J-1)}^{[m]} - p_{0+}^{[m]}.$$

Substituting this expression for $\delta_{1(k_0+l_0-1)}^{[m]}$ back into $\delta_{k_0 l_0}^{[m]}$, we obtain

$$\begin{aligned}\delta_{k_0 l_0}^{[m]} &= \delta_{(k_0+l_0)(J-k_0-l_0)}^{[m]} + \sum_{k=k_0}^{J-1} p_{k+}^{[m]} - \sum_{l=k_0-1}^{J-2} p_{+l}^{[m]} \\ &= \delta_{(k_0+l_0)n}^{[m]} + \sum_{k=k_0}^{k_0+l_0-1+n} p_{k+}^{[m]} - \sum_{l=k_0-1}^{k_0+l_0-2+n} p_{+l}^{[m]}.\end{aligned}$$

Following similar reasoning, it can be shown that $\delta_{k_0 l_0}^{[m]} \leq \delta_{(k_0+l_0)n}^{[m]}$. Consequently, we have, for $n = 1, \dots, J - k_0 - l_0$,

$$\sum_{k=k_0}^{k_0+l_0-1+n} p_{k+}^{[m]} \leq \sum_{l=k_0-1}^{k_0+l_0-2+n} p_{+l}^{[m]}. \quad (\text{S3.5})$$

From the definition of λ_0 ,

$$\lambda_0^{[m]} = \sum_{k=k_0}^{k_0+l_0-1} p_{k+}^{[m]} - \sum_{l=k_0-1}^{k_0+l_0-2} p_{+l}^{[m]},$$

adding $\lambda_0^{[m]}$ to (S3.5) gives,

$$\sum_{k=k_0+l_0}^{k_0+l_0-1+n} p_{k+}^{[m]} \leq \sum_{l=k_0+l_0-1}^{k_0+l_0-2+n} p_{+l}^{[m]} - \lambda_0^{[m]}.$$

Moreover, as shown above we also have the strengthened bound

$$\sum_{k=k_0+l_0}^{k_0+n-1} p_{k+}^{[m]} \leq \sum_{l=k_0+l_0-1}^{k_0+n-2} p_{+l}^{[m]} - \lambda_0^{[m]}.$$

By definition, $q_{+l}^{[m]} = p_{+l}^{[m]}$ for $l \neq k_0 + l_0 - 1$ and $q_{+(k_0+l_0-1)}^{[m]} = p_{+(k_0+l_0-1)}^{[m]} - \max\{0, \lambda_0^{[m]}\}$.

Hence

$$\sum_{l=k_0+l_0-1}^{k_0+n-2} q_{+l}^{[m]} = \sum_{l=k_0+l_0-1}^{k_0+n-2} p_{+l}^{[m]} - \max\{0, \lambda_0^{[m]}\}.$$

Combining the two displayed bounds shows that, for all $n = l_0 + 1, \dots, J - k_0$,

$$\sum_{k=k_0+l_0}^{k_0+n-1} p_{k+}^{[m]} \leq \sum_{l=k_0+l_0-1}^{k_0+n-2} q_{+l}^{[m]},$$

which is the desired inequality for Case (3). $\square$

S4 Proof of Theorem 1

To make the proof process clearer, we divide the proof of Theorem 1 into two parts. The first part derives the closed-form expressions in Theorem 1 given $L_{[m]}^*$. The second part verifies that the matrix $L_{[m]}^*$ constructed in Section 4 is feasible (i.e., satisfies the three linear constraints: nonnegativity, fixed row sums, and fixed column sums).

We first verify that the relative treatment effect γ can be maximized through $L_{[m]}^*$ and the sharp upper bound γ^U can be obtained. Note that $\gamma_{[m]}$ and $\gamma_{[m]}^U$ are defined as

$$\begin{aligned} \gamma_{[m]} &= \Pr \{Y_i(1) > Y_i(0) | B_i = m\} - \Pr \{Y_i(1) < Y_i(0) | B_i = m\} \\ &= \sum_{k=0}^{J-1} \sum_{l=0}^{J-1} \text{sgn}(k-l) p_{kl}^{[m]}, \end{aligned}$$

and

$$\begin{aligned} \gamma_{[m]}^U &= \max_{L_{[m]}} \sum_{k=0}^{J-1} \sum_{l=0}^{J-1} \text{sgn}(k-l) p_{kl}^{[m]}, \\ &\text{subject to } \sum_{l'=0}^{J-1} p_{kl'}^{[m]} = p_{k+}^{[m]}; \sum_{k'=0}^{J-1} p_{k'l}^{[m]} = p_{+l}^{[m]}; p_{kl}^{[m]} \geq 0. \\ &\text{for } k, l = 0, \dots, J-1, m = 1, \dots, M. \end{aligned}$$

Proposition 1 gives the upper bound $\delta_{k'l'}^{[m]}$. We only need to prove that under the probability distribution $L_{[m]}^*$, $\gamma_{[m]}$ takes the maximum value and equals $\min \delta_{k'l'}^{[m]}$, and $\delta_{k'l'}^{[m]}$ defined as

follows

$$\delta_{k'l'}^{[m]} = \sum_{k=k'}^{J-1} p_{k+}^{[m]} + \sum_{k=k'+l'}^{J-1} p_{k+}^{[m]} + \sum_{l=0}^{k'-2} p_{+l}^{[m]} - \sum_{l=k'+l'-1}^{J-1} p_{+l}^{[m]}.$$

Proof of Theorem 1. From the proof of Proposition 2, we know that $\gamma_{[m]} \leq \delta_{k'l'}^{[m]}$. From the definition of $\gamma_{[m]}$,

$$\gamma_{[m]} = \sum_{k=0}^{J-1} \sum_{l=0}^{J-1} \text{sgn}(k-l) p_{kl}^{[m]} = \sum_{k>l} \sum p_{kl}^{[m]} - \sum_{l>k} \sum p_{kl}^{[m]},$$

the first term $\sum_{k>l} \sum p_{kl}^{[m]}$ is divided into three terms (I, II, and III), according to the range of k , while the second term $\sum_{l>k} \sum p_{kl}^{[m]}$ corresponds to the chunking matrix $L_{[m]}^4$ under the condition $l > k$ (denoted as IV). These are expressed as follows:

$$\begin{aligned} \sum_{k>l} \sum p_{kl}^{[m]} &= \underbrace{\sum_{k=1}^{k_0-1} \sum_{l=0}^{k-1} p_{kl}^{[m]}}_{\text{I}} + \underbrace{\sum_{k=k_0}^{k_0+l_0-1} \sum_{l=k_0-1}^{k-1} p_{kl}^{[m]}}_{\text{II}} + \underbrace{\sum_{k=k_0+l_0}^{J-1} \sum_{l=k_0+l_0-1}^{k-1} p_{kl}^{[m]}}_{\text{III}}, \\ \sum_{l>k} \sum p_{kl}^{[m]} &= \underbrace{\sum_{k=0}^{k_0-1} \sum_{l=k_0+l_0-1}^{J-1} p_{kl}^{[m]}}_{\text{IV}}. \end{aligned}$$

By the definitions of $L_{[m]}^1$ and $L_{[m]}^3$, we obtain

$$\text{I} = \sum_{l=0}^{k_0-2} p_{+l}^{[m]}, \text{III} = \sum_{k=k_0+l_0}^{J-1} p_{k+}^{[m]}.$$

Similarly, based on the definitions of $L_{[m]}^2$, $L_{[m]}^5$, and $L_{[m]}^7$, with initialization from zero entries, term II can be expressed as:

$$\text{II} = \sum_{k=k_0}^{k_0+l_0-1} p_{k+}^{[m]} - p_{(k_0+l_0-1)(k_0+l_0-1)}^{[m]}.$$

The derivation of IV relies on matrix $L_{[m]}^6$ and we have

$$\begin{aligned}
\text{IV} &= \sum_{k=0}^{k_0-1} p_{k+}^{[m]} - \sum_{k=1}^{k_0-1} \sum_{l=0}^{k-1} p_{kl}^{[m]} - p_{(k_0-1)(k_0-1)}^{[m]} \\
&= \sum_{k=0}^{k_0-1} p_{k+}^{[m]} - \sum_{l=0}^{k_0-2} p_{+l}^{[m]} - \underbrace{\left(p_{+(k_0-1)}^{[m]} - \sum_{k=k_0}^{k_0+l_0-1} p_{k(k_0-1)}^{[m]} \right)}_{p_{(k_0-1)(k_0-1)}^{[m]}} \\
&= \sum_{k=k_0}^{k_0+l_0-1} p_{k(k_0-1)}^{[m]} + \sum_{k=0}^{k_0-1} p_{k+}^{[m]} - \sum_{l=0}^{k_0-1} p_{+l}^{[m]} \\
&= \sum_{k=k_0}^{k_0+l_0-1} p_{k(k_0-1)}^{[m]} - \sum_{k=k_0+1}^{k_0+l_0-1} \sum_{l=k_0}^{k_0+l_0-2} p_{kl}^{[m]} - p_{(k_0+l_0-1)(k_0+l_0-1)}^{[m]} \\
&\quad - \underbrace{\left(\sum_{k=k_0}^{J-1} p_{k+}^{[m]} - \sum_{l=k_0}^{J-1} p_{+l}^{[m]} \right)}_{\Delta_{k_0}^{[m]}} \\
&= \sum_{k=k_0}^{k_0+l_0-1} p_{k(k_0-1)}^{[m]} - \sum_{l=k_0}^{k_0+l_0-2} p_{+l}^{[m]} - p_{(k_0+l_0-1)(k_0+l_0-1)}^{[m]} - \Delta_{k_0}^{[m]}
\end{aligned}$$

By uniting terms I, II, III, and IV, we obtain:

$$\begin{aligned}
\gamma_{[m]} &= \underbrace{\sum_{l=0}^{k_0-2} p_{+l}^{[m]}}_{\text{I}} + \underbrace{\sum_{k=k_0}^{k_0+l_0-1} p_{k+}^{[m]} - p_{(k_0+l_0-1)(k_0+l_0-1)}^{[m]}}_{\text{II}} + \underbrace{\sum_{k=k_0+l_0}^{J-1} p_{k+}^{[m]}}_{\text{III}} \\
&\quad - \underbrace{\sum_{k=k_0}^{k_0+l_0-1} p_{k(k_0-1)}^{[m]} - \sum_{l=k_0}^{k_0+l_0-2} p_{+l}^{[m]} - p_{(k_0+l_0-1)(k_0+l_0-1)}^{[m]} - \Delta_{k_0}^{[m]}}_{\text{IV}} \\
&= \sum_{l=0}^{k_0-2} p_{+l}^{[m]} + \sum_{k=k_0+l_0}^{J-1} p_{k+}^{[m]} + \sum_{l=k_0}^{k_0+l_0-2} p_{+l}^{[m]} + \Delta_{k_0}^{[m]} \\
&= \delta_{k_0 l_0}^{[m]},
\end{aligned}$$

where the last equality holds based on (S3.1) of Proposition 5, thereby proving that $\gamma_{[m]}^U =$

$\min_{1 \leq k' \leq J-1} \min_{1 \leq l' \leq J-k'} \delta_{k' l'}^{[m]}$. As there exists matrix $L_{[m]}^*$ within block m that maximizes $\gamma_{[m]}$ to

$\gamma_{[m]}^U$, we define the population joint probability p_{kl} as

$$p_{kl} = \Pr \{Y_i(1) = k, Y_i(0) = l\} = \sum_{m=1}^M \pi_{[m]} p_{kl}^{[m]},$$

which satisfies $\sum_{k=0}^{J-1} \sum_{l=0}^{J-1} p_{kl} = 1$, $\sum_{l'=0}^{J-1} p_{kl'} = p_{k+}$, and $\sum_{k'=0}^{J-1} p_{k'l} = p_{+l}$. As the stratified randomized experiment ensures independence between strata, the upper sharp bound of the population treatment effect γ has

$$\gamma^U = \sum_{k=0}^{J-1} \sum_{l=0}^{J-1} \text{sgn}(k-l) p_{kl} = \sum_{k=0}^{J-1} \sum_{l=0}^{J-1} \sum_{m=1}^M \pi_{[m]} \text{sgn}(k-l) p_{kl}^{[m]} = \sum_{m=1}^M \pi_{[m]} \gamma_{[m]}^U.$$

To prove that $\gamma_{[m]}^U$ is the maximum value for any matrix $L_{[m]} \in \mathcal{F}_{[m]}$, we have the following analysis. Because the marginal probabilities $p_{k+}^{[m]}$ and $p_{+l}^{[m]}$ are truly computable, there exists at least one joint distribution $L_{[m]}$ that is compatible with them, and thus the set $\mathcal{F}_{[m]}$ is nonempty. All constraints in $\mathcal{F}_{[m]}$ are bounded, so it is a compact set.

From the definition of $\gamma_{[m]} = \sum_{k=0}^{J-1} \sum_{l=0}^{J-1} \text{sgn}(k-l) p_{kl}^{[m]}$, it is a continuous linear function. By the Weierstrass theorem, a continuous function $\gamma_{[m]}$ defined on a compact set $\mathcal{F}_{[m]}$ must attain its maximum value. Therefore, there exists a feasible matrix $L_{[m]}^*$ such that $\gamma(L_{[m]}^*) = \gamma_{[m]}^U$. Thus,

$$\gamma(L_{[m]}) \leq \gamma(L_{[m]}^*) = \gamma_{[m]}^U.$$

For a $J \times J$ joint distribution matrix with given marginals, the feasible set $\mathcal{F}_{[m]}$ has affine dimension $(J-1)^2$. When $J \geq 3$, this dimension is positive, meaning that $(J-1)^2$ entries of $L_{[m]}$ can be freely chosen, while the remaining $J^2 - (J-1)^2 = 2(J-1)$ entries are determined by the constraints. Within the polyhedron formed by the following constraints,

$$p_{kl}^{[m]} \geq 0, \quad \sum_{l=0}^{J-1} p_{kl}^{[m]} = p_{k+}^{[m]}, \quad \sum_{k=0}^{J-1} p_{kl}^{[m]} = p_{+l}^{[m]},$$

the optimal solution set is no longer a single point but entire edges or faces. Therefore, even

under identical marginal probabilities $p_{k+}^{[m]}$ and $p_{+l}^{[m]}$, there are still many optimal matrices $L_{[m]}^*$ satisfying $\gamma(L_{[m]}^*) = \gamma_{[m]}^U$. This complete the proof of Theorem 1. $\square$

S4.1 Verification of the Optimal Matrix L^*

The verification of matrix L^* is conducted from the following two aspects.

Proposition 6. *Let $L_{[m]}^* = \{p_{kl}^{[m]}\}_{k,l=0,\dots,J-1} \in \mathbb{R}^{J \times J}$ be the matrix constructed in Section 4. Then $p_{kl}^{[m]} \geq 0$ for all k, l , and*

$$\sum_{l=0}^{J-1} p_{kl}^{[m]} = p_{k+}^{[m]} \quad (k = 0, \dots, J-1), \quad \sum_{k=0}^{J-1} p_{kl}^{[m]} = p_{+l}^{[m]} \quad (l = 0, \dots, J-1).$$

Consequently, $L_{[m]}^* \in \mathcal{F}_{[m]}$ with the prescribed row and column marginals $p_{k+}^{[m]}$ and $p_{+l}^{[m]}$.

Proof of Proposition 6. We first establish nonnegativity. By construction in Section 4, all entries placed in $L_{[m]}^1$, $L_{[m]}^2$, and $L_{[m]}^3$ are nonnegative; the updates in $L_{[m]}^4$ use remaining (non-negative) row and column margins guaranteed by Propositions 3–4; the fill-ins in $L_{[m]}^5$ and $L_{[m]}^6$ are margins minus previously assigned nonnegatives; and $L_{[m]}^7$ sets a value $\max(0, \lambda_0^{[m]})$. Hence $p_{kl}^{[m]} \geq 0$ for all k, l .

We next verify the column sums. By construction, the only nonzero contributions to

$$l \in \{0, \dots, k_0 - 2\}, \quad l = k_0 - 1, \quad l \in \{k_0, \dots, k_0 + l_0 - 2\}, \quad l \in \{k_0 + l_0 - 1, \dots, J - 1\}$$

come from $L_{[m]}^1$, $L_{[m]}^5 \cup L_{[m]}^6$, $L_{[m]}^2$, and $L_{[m]}^3 \cup L_{[m]}^4$ respectively, with these blocks having disjoint support. In $L_{[m]}^1$ and $L_{[m]}^2$, the construction imposes

$$\sum_k p_{kl}^{[m]} = p_{+l}^{[m]} \quad (l = 0, \dots, k_0 - 2 \text{ and } l = k_0, \dots, k_0 + l_0 - 2).$$

For $l = k_0 - 1$, $L_{[m]}^5$ fills entries $p_{k(k_0-1)}^{[m]}$ for $k = k_0, \dots, k_0 + l_0 - 1$ and $L_{[m]}^6$ assigns $p_{(k_0-1)(k_0-1)}^{[m]}$

to match the residual, so that

$$\sum_k p_{k(k_0-1)}^{[m]} = p_{+(k_0-1)}^{[m]}.$$

For $l \geq k_0 + l_0 - 1$, $L_{[m]}^3$ contributes rows $k \geq k_0 + l_0$ (with column totals not exceeding the remaining margin) and $L_{[m]}^4$ allocates the remaining nonnegative column residuals across rows $k \leq k_0 - 1$, which together yield

$$\sum_k p_{kl}^{[m]} = p_{+l}^{[m]} \quad (l = k_0 + l_0 - 1, \dots, J - 1).$$

Hence $\sum_{k=0}^{J-1} p_{kl}^{[m]} = p_{+l}^{[m]}$ for all l .

A symmetric argument verifies the row sums. The only nonzero contributions to

$$k \in \{0, \dots, k_0 - 1\}, \quad k \in \{k_0, \dots, k_0 + l_0 - 1\}, \quad k \in \{k_0 + l_0, \dots, J - 1\}$$

come from $L_{[m]}^1 \cup L_{[m]}^4 \cup L_{[m]}^6$, $L_{[m]}^2 \cup L_{[m]}^5$, and $L_{[m]}^3$ respectively (again with disjoint support). In $L_{[m]}^3$ one imposes $\sum_l p_{kl}^{[m]} = p_{k+}^{[m]}$ for $k \geq k_0 + l_0$. For $k \in \{k_0, \dots, k_0 + l_0 - 1\}$, $L_{[m]}^2$ assigns mass up to the remaining row margin and $L_{[m]}^5$ places $p_{k(k_0-1)}^{[m]}$ to exhaust it, so $\sum_l p_{kl}^{[m]} = p_{k+}^{[m]}$. For $k \leq k_0 - 1$, $L_{[m]}^1$ assigns mass on columns $0, \dots, k_0 - 2$, $L_{[m]}^6$ fills $(k_0 - 1, k_0 - 1)$ if $k = k_0 - 1$, and $L_{[m]}^4$ allocates any remaining row residual across columns $l \geq k_0 + l_0 - 1$, giving

$$\sum_{l=0}^{J-1} p_{kl}^{[m]} = p_{k+}^{[m]} \quad (k = 0, \dots, k_0 - 1).$$

Therefore $\sum_{l=0}^{J-1} p_{kl}^{[m]} = p_{k+}^{[m]}$ for all k . Combining nonnegativity with the verified row and column equalities, we conclude $L_{[m]}^* \in \mathcal{F}_{[m]}$. This completes the proof. $\square$

Proposition 7. *For the probability matrix $L_{[m]}^* = \{p_{kl}^{[m]}\}_{k,l=0,\dots,J-1} \in \mathbb{R}^{J \times J}$, all elements satisfy the nonnegativity constraints.*

Proof of Proposition 7. The elements in sub-matrices $L_{[m]}^1$, $L_{[m]}^2$, $L_{[m]}^3$, and $L_{[m]}^7$ of the generating matrix $L_{[m]}^*$ satisfy the non-negativity requirement by definition. The next step is to

verify the remaining entries from sub-matrices $L_{[m]}^4$, $L_{[m]}^5$, and $L_{[m]}^6$. For sub-matrix $L_{[m]}^5$, we analyze two situations. First, if $l_0 = 1$, according to the definition of $L_{[m]}^7$,

$$p_{k_0 k_0}^{[m]} = \max(0, \lambda_0^{[m]}).$$

Using the definition of $\lambda_0^{[m]}$ and taking $l_0 = 1$, we have

$$\lambda_0^{[m]} = \sum_{k=k_0}^{k_0+l_0-1} p_{k+}^{[m]} - \sum_{l=k_0-1}^{k_0+l_0-2} p_{+l}^{[m]} = p_{k_0+}^{[m]} - p_{+(k_0-1)}^{[m]}.$$

Then

$$p_{k_0 k_0}^{[m]} = \max(0, \lambda_0^{[m]}) = \max(0, p_{k_0+}^{[m]} - p_{+(k_0-1)}^{[m]}) \leq p_{k_0+}^{[m]}.$$

Based on the definition from $L_{[m]}^5$,

$$p_{k_0(k_0-1)}^{[m]} = p_{k_0+}^{[m]} - \sum_{l=k_0}^{J-1} p_{k_0 l}^{[m]},$$

which implies that

$$p_{k_0, k_0-1}^{[m]} = p_{k_0+}^{[m]} - p_{k_0 k_0}^{[m]} - \sum_{l=k_0+1}^{J-1} p_{k_0 l}^{[m]} \geq 0.$$

For the second case, if $l_0 > 1$, for all $k = k_0, \dots, k_0 + l_0 - 2$, based on Proposition 4 and the definition of $L_{[m]}^2$, we have $p_{k(k_0-1)}^{[m]} \geq 0$. It remains to verify the case $k = k_0 + l_0 - 1$. We analyze the nonnegativity of $p_{(k_0+l_0-1)(k_0-1)}^{[m]}$:

$$p_{(k_0+l_0-1)(k_0-1)}^{[m]} = p_{(k_0+l_0-1)+}^{[m]} - \sum_{l=k_0}^{k_0+l_0-1} p_{(k_0+l_0-1)l}^{[m]} \geq 0.$$

By definition, $p_{(k_0+l_0-1)l}^{[m]}$ captures the probability contributions for the respective indices and $p_{(k_0+l_0-1)+}^{[m]}$ ensures consistency with the row sum constraints. Since all terms are either explicitly nonnegative or guaranteed by construction to satisfy row and column sum constraints, we conclude that $p_{(k_0+l_0-1)(k_0-1)}^{[m]} \geq 0$.

For sub-matrices $L_{[m]}^6$, we directly use its definition and the definition for $L_{[m]}^5$ to verify the nonnegativity condition. We have

$$\begin{aligned}
 p_{(k_0-1)(k_0-1)}^{[m]} &= p_{+(k_0-1)}^{[m]} - \sum_{k=k_0}^{k_0+l_0-1} p_{k(k_0-1)}^{[m]} \\
 &= p_{+(k_0-1)}^{[m]} - \sum_{k=k_0}^{k_0+l_0-1} \left(p_{k+}^{[m]} - \sum_{l=k_0}^{J-1} p_{kl}^{[m]} \right) \\
 &= p_{+(k_0-1)}^{[m]} - \sum_{k=k_0}^{k_0+l_0-1} p_{k+}^{[m]} + \sum_{l=k_0}^{k_0+l_0-2} p_{+l}^{[m]} + p_{(k_0+l_0-1)(k_0+l_0-1)}^{[m]}.
 \end{aligned}$$

Next, applying the definition for $L_{[m]}^4$ and $\lambda_0^{[m]}$,

$$\begin{aligned}
 &\left(p_{+(k_0-1)}^{[m]} + \sum_{l=k_0}^{k_0+l_0-2} p_{+l}^{[m]} \right) - \sum_{k=k_0}^{k_0+l_0-1} p_{k+}^{[m]} + \left(p_{(k_0+l_0-1)(k_0+l_0-1)}^{[m]} \right) \\
 &= \underbrace{\sum_{l=k_0-1}^{k_0+l_0-2} p_{+l}^{[m]} - \sum_{k=k_0}^{k_0+l_0-1} p_{k+}^{[m]}}_{-\lambda_0^{[m]}} + \max\left(0, \lambda_0^{[m]}\right) \\
 &= \max\left(0, -\lambda_0^{[m]}\right) \geq 0.
 \end{aligned}$$

Thus we conclude that the nonnegativity condition is satisfied for $L_{[m]}^6$. For the sub-matrices $L_{[m]}^4$, to show that it satisfies nonnegative condition equals to prove the following inequalities hold,

$$p_{k+}^{[m]} - \sum_{l=0}^{k_0+l_0-2} p_{kl}^{[m]} \geq 0 \quad \text{for } k = 0, \dots, k_0 - 1, \quad (\text{S4.6})$$

$$p_{+l}^{[m]} - \sum_{k=k_0}^{J-1} p_{kl}^{[m]} \geq 0 \quad \text{for } l = k_0 + l_0 - 1, \dots, J - 1. \quad (\text{S4.7})$$

To prove (S4.6), we analyze the case $k = 0, \dots, k_0 - 1$. For $l = 0, \dots, k_0 + l_0 - 2$, by construction $p_{0l}^{[m]} = 0$. For $k = 0, \dots, k_0 - 2$, it follows directly from the definition for $L_{[m]}^1$

and Proposition 4 that

$$p_{k+}^{[m]} - \sum_{l=0}^{k_0+l_0-2} p_{kl}^{[m]} \geq 0$$

If $k = k_0 - 1$, we verify

$$p_{(k_0-1)+}^{[m]} - \sum_{l=0}^{k_0-1} p_{(k_0-1)l}^{[m]} \geq 0.$$

We address this by considering three cases: (1) If $k_0 > 1$, From the definition of $L_{[m]}^1$,

$$\sum_{l=0}^{k_0-2} p_{(k_0-1)l}^{[m]} \leq q_{(k_0-1)+}^{[m]},$$

and from $L_{[m]}^6$,

$$p_{(k_0-1)(k_0-1)}^{[m]} \leq \max\{0, -\lambda_0^{[m]}\}.$$

(2) If $k_0 = 1$ and $l_0 = J - 1$, then

$$p_{0+}^{[m]} + \sum_{k=1}^{l_0} p_{k+}^{[m]} - \sum_{l=0}^{l_0-1} p_{+l}^{[m]} = p_{0+}^{[m]} + \lambda_0^{[m]} = \left(p_{0+}^{[m]} + \sum_{k=1}^{J-1} p_{k+}^{[m]} \right) - \sum_{l=0}^{J-2} p_{+l}^{[m]} \geq 0,$$

which implies

$$1 - \sum_{l=0}^{J-2} p_{+l}^{[m]} = p_{+(J-1)}^{[m]} \geq 0.$$

(3) If $k_0 = 1$ and $l_0 < J - 1$, then $\delta_{k_0 l_0}^{[m]} \leq \delta_{k_0 n}^{[m]}$ for all $n = l_0 + 1, \dots, J - k_0$. As in the proof of Proposition 4,

$$\delta_{k_0 l_0}^{[m]} = \delta_{k_0 n}^{[m]} + \left(\sum_{k=l_0+1}^{J-k_0-1} p_{k+}^{[m]} - \sum_{l=l_0}^{J-k_0-1} p_{+l}^{[m]} \right),$$

so

$$\sum_{k=l_0+1}^{J-1} p_{k+}^{[m]} \leq \sum_{l=l_0}^{J-1} p_{+l}^{[m]}.$$

Thus (S4.6) holds. The inequality (S4.7) follows similarly by considering the cases $k_0 + l_0 < J$

and $k_0 + l_0 = J$, using the first case of Proposition 4. This completes the proof of the nonnegativity condition for $L_{[m]}^4$. $\square$

S5 Proofs of other Theorems and Corollary

The proof of Theorem 2 follows directly from the proof of Theorem 1 by considering the reverse ordering of the treatment and control groups.

Proof of Theorem 2. We define the relative treatment effect when the roles of the treatment group (denoted as 1) and the control group (denoted as 0) are swapped:

$$\gamma_{[m]'} = \Pr\{Y_i(0) > Y_i(1) | B_i = m\} - \Pr\{Y_i(0) < Y_i(1) | B_i = m\} = -\gamma_{[m]},$$

which indicates that solving for the lower bound of $\gamma_{[m]}$ is equivalent to solving for the upper bound of $\gamma_{[m]}'$. Next, consider the differences in the cumulative distribution functions (CDFs) between the two groups, denoted as $\Delta_{k'}^{[m]}'$ for the swapped groups:

$$\Delta_{k'}^{[m]}' = \Pr\{Y_i(0) \geq k' | B_i = m\} - \Pr\{Y_i(1) \geq k' | B_i = m\} = -\Delta_{k'}^{[m]}, \quad k' = 1, \dots, J-1.$$

For the quantities $\delta_{k'l'}^{[m]}'$, which represent the partial sums used in the computation of the bounds, we have:

$$\delta_{k'l'}^{[m]}' = \sum_{k=k'}^{k'+l'-2} p_{k+}^{[m]} + \sum_{l=k'+l'}^{J-1} p_{+l}^{[m]} + \sum_{k=0}^{k'-2} p_{k+}^{[m]} + \Delta_{k'}^{[m]}' = -\xi_{k'l'}^{[m]}.$$

For brevity, we define quantity $-\xi_{k'l'}^{[m]} := \sum_{k=k'}^{k'+l'-2} p_{k+}^{[m]} + \sum_{l=k'+l'}^{J-1} p_{+l}^{[m]} + \sum_{k=0}^{k'-2} p_{k+}^{[m]} + \Delta_{k'}^{[m]}'$. Following the same arguments as the proof of Theorem 1, the sharp upper bound of the relative

treatment effect $\gamma_{[m]}'$ is expressed as

$$\gamma_{[m]}'^U = \min_{1 \leq k' \leq J-1} \min_{1 \leq l' \leq J-k'} (\delta_{k'l'}^{[m]'}),$$

which is equivalent to $\gamma_{[m]}'^U = \min_{1 \leq k' \leq J-1} \min_{1 \leq l' \leq J-k'} (-\xi_{k'l'}^{[m]})$. Thus, the lower bound of $\gamma_{[m]}$ is $\gamma_{[m]}^L = \max_{1 \leq k' \leq J-1} \max_{1 \leq l' \leq J-k'} (\xi_{k'l'}^{[m]})$, completing the proof of Theorem 2. $\square$

Proof of Corollary 1. Under the independence assumption of potential outcomes, the elements of the probability matrix $L_{[m]}$ are given by $p_{kl}^{[m]} = p_{k+}^{[m]} p_{+l}^{[m]}$ for $k, l = 0, 1, \dots, J-1$. Using this formulation, we directly compute $\gamma_{[m]}^{ind}$ based on the definition of $\gamma_{[m]}$:

$$\gamma_{[m]}^{ind} = \sum_{k>l} \sum p_{k+}^{[m]} p_{+l}^{[m]} - \sum_{l>k} \sum p_{k+}^{[m]} p_{+l}^{[m]}.$$

The lower bound of $\gamma_{[m]}$ is defined as follows

$$\gamma_{[m]}^L = \max_{1 \leq k' \leq J-1} \max_{1 \leq l' \leq J-k'} \xi_{k'l'}^{[m]},$$

which is derived under the assumption of extreme negative correlation between $Y(1)$ and $Y(0)$, and representing an overly conservative and unrealistic scenario that significantly underestimates the treatment effect $\gamma_{[m]}$. In contrast, imposing independence yields a lower bound $\gamma_{[m]}^{ind}$, and by feasibility it satisfies

$$\gamma_{[m]}^L \leq \gamma_{[m]}^{ind} \leq \gamma_{[m]}^U.$$

This ordering reflects the relative informativeness of the bounds under varying assumptions about the joint distribution of the potential outcomes, completing the proof. $\square$

Proof of Theorem 3. For 2-tuples (k', l') for $k' = 1, \dots, J-1$ and $l' = 1, \dots, J-k'$, the upper bound $\delta_{k'l'}^{[m]}(\cdot)$ of $\gamma_{[m]}$ is an affine function with respect to the marginal probability vector $\mathbf{p}$

within stratum m . We define $\phi^{[m]}(\mathbf{p})$ as follows

$$\phi^{[m]}(\mathbf{p}) := \min_{(k', l')} \delta_{k' l'}^{[m]}(\mathbf{p}),$$

denoting the minimum value of $\delta_{k' l'}^{[m]}(\mathbf{p})$. Then, for any value of $X = x$, we have

$$\gamma_{[m]}^U(x) = \phi^{[m]}(\mathbf{p}^{[m]}(x)),$$

where $\mathbf{p}^{[m]}(x)$ is the vector composed of marginal probabilities $p_{k+}^{[m]}$ and $p_{+l}^{[m]}$ within stratum m . Since function $\phi^{[m]}$ is the minimum of the affine functions $\delta_{k' l'}^{[m]}(\cdot)$, it is a concave function. By Jensen's inequality, we have

$$\phi^{[m]}(E[\mathbf{p}^{[m]}(x) \mid B_i = m]) \geq E[\phi^{[m]}(\mathbf{p}^{[m]}(x)) \mid B_i = m],$$

where since the left side of the inequality $E[\mathbf{p}^{[m]}(x) \mid B_i = m] = \mathbf{p}^{[m]}$, and $\mathbf{p}^{[m]}$ denotes marginal probability vector within stratum m , we have

$$\phi^{[m]}(E[\mathbf{p}^{[m]}(x) \mid B_i = m]) = \phi^{[m]}(\mathbf{p}^{[m]}) = \min_{(k', l')} \delta_{k' l'}^{[m]}(\mathbf{p}^{[m]}) = \gamma_{[m]}^U.$$

The right side of the inequality is expressed as

$$E[\phi^{[m]}(\mathbf{p}^{[m]}(x)) \mid B_i = m] = E\left[\min_{(k', l')} \delta_{k' l'}^{[m]}(\mathbf{p}^{[m]}(x))\right] = E[\gamma_{[m]}^U(x)] = \tilde{\gamma}_{[m]}^U,$$

Thus, we have

$$\gamma_{[m]}^U \geq \tilde{\gamma}_{[m]}^U.$$

Similarly, for the affine function $\xi_{kl}^{[m]}(\cdot)$, we define its maximum value as

$$\varphi^{[m]}(\mathbf{p}) := \max_{(k', l')} \xi_{k'l'}^{[m]}(\mathbf{p}).$$

As $\varphi^{[m]}$ is a convex function, by Jensen's inequality we have

$$\varphi^{[m]}(E[\mathbf{p}^{[m]}(x) | B_i = m]) \leq E[\varphi^{[m]}(\mathbf{p}^{[m]}(x)) | B_i = m],$$

where the left side of the inequality represents the unadjusted lower bound $\gamma_{[m]}^L$, while the right side denotes the adjusted lower bound $\tilde{\gamma}_{[m]}^L$. Therefore,

$$\gamma_{[m]}^L \leq \tilde{\gamma}_{[m]}^L.$$

In conclusion, the adjusted bounds are tighter than the unadjusted bounds, i.e.,

$$\gamma^L \leq \tilde{\gamma}^L \leq \tilde{\gamma}^U \leq \gamma^U.$$

Given the row sum probability vector $\mathbf{p}_{row}^{[m]}$ and column sum probability vector $\mathbf{p}_{col}^{[m]}$ within stratum m , denoted as $\mathbf{p}_{row}^{[m]}(x) = (p_{0+}^{[m]}(x), \dots, p_{J-1,+}^{[m]}(x))^T$, and $\mathbf{p}_{col}^{[m]}(x) = (p_{+0}^{[m]}(x), \dots, p_{+(J-1)}^{[m]}(x))^T$. We define the sign matrix $S = \{s_{kl}\}_{0 \leq k, l \leq J-1}$, and have

$$s_{kl} = \begin{cases} +1, & k > l \\ 0, & k = l \\ -1, & k < l \end{cases}$$

Therefore, the treatment effect on the independent potential outcomes $\gamma_{[m]}^{\text{ind}}(x)$ within stratum m under $X = x$ is $\gamma_{[m]}^{\text{ind}}(x) = (\mathbf{p}_{row}^{[m]}(x))^T \cdot S \cdot \mathbf{p}_{col}^{[m]}(x)$, the adjusted bound is

$$\tilde{\gamma}_{[m]}^{\text{ind}} = E\{\gamma_{[m]}^{\text{ind}}(X) | B_i = m\} = E\left\{(\mathbf{p}_{row}^{[m]}(X))^T \cdot S \cdot \mathbf{p}_{col}^{[m]}(X) | B_i = m\right\}.$$

The unadjusted bound is

$$\gamma_{[m]}^{\text{ind}} = (\mathbf{p}_{\text{row}}^{[m]})^T \cdot S \cdot \mathbf{p}_{\text{col}}^{[m]},$$

where $\mathbf{p}_{\text{row}}^{[m]} = E \left\{ \mathbf{p}_{\text{row}}^{[m]}(X) \mid B_i = m \right\}$ and $\mathbf{p}_{\text{col}}^{[m]} = E \left\{ \mathbf{p}_{\text{col}}^{[m]}(X) \mid B_i = m \right\}$ are the mean vectors within stratum m . To facilitate demonstrating the difference relationship between $\gamma_{[m]}^{\text{ind}}$ and $\tilde{\gamma}_{[m]}^{\text{ind}}$, we represent $\mathbf{p}_{\text{row}}^{[m]}(X)$ and $\mathbf{p}_{\text{col}}^{[m]}(X)$ in the following form:

$$\mathbf{p}_{\text{row}}^{[m]}(X) = \mathbf{p}_{\text{row}}^{[m]} + (\mathbf{p}_{\text{row}}^{[m]}(X) - \mathbf{p}_{\text{row}}^{[m]}), \quad \mathbf{p}_{\text{col}}^{[m]}(X) = \mathbf{p}_{\text{col}}^{[m]} + (\mathbf{p}_{\text{col}}^{[m]}(X) - \mathbf{p}_{\text{col}}^{[m]}),$$

where the residual vectors are defined as $\Delta \mathbf{p}_{\text{row}}^{[m]}(X) := \mathbf{p}_{\text{row}}^{[m]}(X) - \mathbf{p}_{\text{row}}^{[m]}$, and $\Delta \mathbf{p}_{\text{col}}^{[m]}(X) := \mathbf{p}_{\text{col}}^{[m]}(X) - \mathbf{p}_{\text{col}}^{[m]}$. We can express $\tilde{\gamma}_{[m]}^{\text{ind}}$ as

$$\begin{aligned} \tilde{\gamma}_{[m]}^{\text{ind}} &= (\mathbf{p}_{\text{row}}^{[m]})^T \cdot S \cdot \mathbf{p}_{\text{col}}^{[m]} + (\mathbf{p}_{\text{row}}^{[m]})^T \cdot S \cdot E \left[\Delta \mathbf{p}_{\text{col}}^{[m]}(X) \right] \\ &\quad + E \left[\Delta \mathbf{p}_{\text{row}}^{[m]}(X) \right]^T \cdot S \cdot \mathbf{p}_{\text{col}}^{[m]} + E \left[([\Delta \mathbf{p}_{\text{row}}^{[m]}(X)])^T \cdot S \cdot \Delta \mathbf{p}_{\text{col}}^{[m]}(X) \right], \end{aligned}$$

where the mean residual equals zero, that is, $E \left[\Delta \mathbf{p}_{\text{row}}^{[m]}(X) \right] = 0$ and $E \left[\Delta \mathbf{p}_{\text{col}}^{[m]}(X) \right] = 0$, so we can equivalently express the above equation as

$$\tilde{\gamma}_{[m]}^{\text{ind}} = \underbrace{(\mathbf{p}_{\text{row}}^{[m]})^T \cdot S \cdot \mathbf{p}_{\text{col}}^{[m]}}_{\gamma_{[m]}^{\text{ind}}} + E \left[([\Delta \mathbf{p}_{\text{row}}^{[m]}(X)])^T \cdot S \cdot \Delta \mathbf{p}_{\text{col}}^{[m]}(X) \right],$$

the first term in the above equation is denoted as the unadjusted bound $\gamma_{[m]}^{\text{ind}}$, and we have

$$\begin{aligned} \tilde{\gamma}_{[m]}^{\text{ind}} - \gamma_{[m]}^{\text{ind}} &= E \left[([\Delta \mathbf{p}_{\text{row}}^{[m]}(X)])^T \cdot S \cdot \Delta \mathbf{p}_{\text{col}}^{[m]}(X) \right] \\ &= \sum_{k=0}^{J-1} \sum_{l=0}^{J-1} s_{kl} \cdot E \left[\Delta p_{k+}^{[m]}(X) \cdot \Delta p_{+l}^{[m]}(X) \right] \\ &= \sum_{k=0}^{J-1} \sum_{l=0}^{J-1} s_{kl} \cdot \text{cov} \left(p_{k+}^{[m]}(X), p_{+l}^{[m]}(X) \right) \end{aligned}$$

where the last equality holds due to

$$\Delta p_{k+}^{[m]}(X) = p_{k+}^{[m]}(X) - E \left[p_{k+}^{[m]}(X) \right], \quad \Delta p_{+l}^{[m]}(X) = p_{+l}^{[m]}(X) - E \left[p_{+l}^{[m]}(X) \right],$$

where $\Delta p_{k+}^{[m]}(X)$ is the k th component of $\Delta \mathbf{p}_{row}^{[m]}(X)$, and $\Delta p_{+l}^{[m]}(X)$ is the l th component of $\Delta \mathbf{p}_{col}^{[m]}(X)$. For the population effects $\tilde{\gamma}^{\text{ind}}$ and γ^{ind} , the following equations hold:

$$\tilde{\gamma}^{\text{ind}} - \gamma^{\text{ind}} = \sum_{m=1}^M \sum_{k=0}^{J-1} \sum_{l=0}^{J-1} \pi_{[m]} \cdot s_{kl} \cdot \text{cov} \left(p_{k+}^{[m]}(X), p_{+l}^{[m]}(X) \right).$$

Thus, under the assumption of independent potential outcomes, the relationship between the adjusted bound $\tilde{\gamma}^{\text{ind}}$ and unadjusted bound γ^{ind} depends on the covariance of $\left(p_{k+}^{[m]}(X), p_{+l}^{[m]}(X) \right)$, completing the proof of Theorem 3. $\square$