Appendix

Proof of Theorems

First, we have the following Lemmas 4 and 5 from (Li and Pearl 2019).

Lemma 4. *The c-specific PNS $P(y_x, y'_{x'}|c)$ is bounded as follows:*

$$max \left\{ \begin{array}{c} 0, \\ P(y_x|c) - P(y_{x'}|c), \\ P(y|c) - P(y_{x'}|c), \\ P(y_x|c) - P(y|c) \end{array} \right\} \leq \textit{c-PNS},$$

$$min \left\{ \begin{array}{c} P(y_x|c), \\ P(y'_{x'}|c), \\ P(y,x|c) + P(y',x'|c), \\ P(y_x|c) - P(y_{x'}|c)+ \\ +P(y,x'|c) + P(y',x|c) \end{array} \right\} \geq \textit{c-PNS}.$$

Lemma 5.

$$\begin{aligned} & P(y_x, y'_{x'}|c) - P(y'_x, y_{x'}|c) \\ = \; & P(y_x|c) - P(y_{x'}|c). \end{aligned}$$

Lemma 6. *Given a causal diagram G and distribution compatible with G, let $Z \cup C$ be a set of variables that does not contain any descendant of X in G, then c-specific PNS $P(y_x, y'_{x'}|c)$ is bounded as follows:*

$$\sum_z \max \left\{ \begin{array}{c} 0, \\ P(y_x|z,c) - P(y_{x'}|z,c), \\ P(y|z,c) - P(y_{x'}|z,c), \\ P(y_x|z,c) - P(y|z,c) \end{array} \right\} \times P(z|c) \leq \textit{c-PNS}, \tag{3}$$

$$\sum_z \min \left\{ \begin{array}{c} P(y_x|z,c), \\ P(y'_{x'}|z,c), \\ P(y,x|z,c) + P(y',x'|z,c), \\ P(y_x|z,c) - P(y_{x'}|z,c)+ \\ +P(y,x'|z,c) + P(y',x|z,c) \end{array} \right\} \times P(z|c) \geq \textit{c-PNS}. \tag{4}$$

Proof.

$$\begin{aligned} c\text{-PNS} &= P(y_x, y'_{x'}|c) \\ &= \sum_z P(y_x, y'_{x'}|z,c) \times P(z|c). \end{aligned} \tag{5}$$

From Lemma 4, replace c with (z, c), we have the following:

$$\max \left\{ \begin{array}{c} 0, \\ P(y_x|z,c) - P(y_{x'}|z,c), \\ P(y|z,c) - P(y_{x'}|z,c), \\ P(y_x|z,c) - P(y|z,c) \end{array} \right\} \leq P(y_x, y'_{x'}|z,c), \tag{6}$$

$$\min \left\{ \begin{array}{c} P(y_x|z,c), \\ P(y'_{x'}|z,c), \\ P(y,x|z,c) + P(y',x'|z,c), \\ P(y_x|z,c) - P(y_{x'}|z,c)+ \\ +P(y,x'|z,c) + P(y',x|z,c) \end{array} \right\} \geq P(y_x, y'_{x'}|z,c). \tag{7}$$

Substituting Equations 6 and 7 into Equation 5, Lemma 6 holds.
Note that since we have,

$$\begin{aligned} & \sum_z \max\{0, \\ & P(y_x|z,c) - P(y_{x'}|z,c), \\ & P(y|z,c) - P(y_{x'}|z,c), \\ & P(y_x|z,c) - P(y|z,c)\} \times P(z|c) \\ \geq \; & \sum_z 0 \times P(z|c) \\ = \; & 0, \end{aligned}$$

$$\begin{aligned} & \sum_z \max\{0, \\ & P(y_x|z,c) - P(y_{x'}|z,c), \\ & P(y|z,c) - P(y_{x'}|z,c), \\ & P(y_x|z,c) - P(y|z,c)\} \times P(z|c) \\ \geq \; & \sum_z [P(y_x|z,c) - P(y_{x'}|z,c)] \times P(z|c) \\ = \; & P(y_x|c) - P(y_{x'}|c), \end{aligned}$$

$$\begin{aligned} & \sum_z \max\{0, \\ & P(y_x|z,c) - P(y_{x'}|z,c), \\ & P(y|z,c) - P(y_{x'}|z,c), \\ & P(y_x|z,c) - P(y|z,c)\} \times P(z|c) \\ \geq \; & \sum_z [P(y|z,c) - P(y_{x'}|z,c)] \times P(z|c) \\ = \; & P(y|c) - P(y_{x'}|c), \end{aligned}$$

$$\begin{aligned} & \sum_z \max\{0, \\ & P(y_x|z,c) - P(y_{x'}|z,c), \\ & P(y|z,c) - P(y_{x'}|z,c), \\ & P(y_x|z,c) - P(y|z,c)\} \times P(z|c) \\ \geq \; & \sum_z [P(y_x|z,c) - P(y|z,c)] \times P(z|c) \\ = \; & P(y_x|c) - P(y|c), \end{aligned}$$

then the lower bound in Lemma 6 is guaranteed to be no worse than the lower bound in Lemma 4. Similarly, the upper bound in Lemma 6 is guaranteed to be no worse than the upper bound in Lemma 4. Also note that, since $Z \cup C$ does not contain a descendant of X, the term $P(y_x|z,c)$ refers to experimental data under population z, c. □

Lemma 7.

$$\begin{aligned} f(c) &= \beta P(y_x, y'_{x'}|c) + \gamma P(y_x, y_{x'}|c) + \\ & \quad +\theta P(y'_x, y'_{x'}|c) + \delta P(y_{x'}, y'_x|c) \\ &= W + \sigma P(y_x, y'_{x'}|c). \end{aligned} \tag{8}$$

where,

$$W = (\gamma - \delta)P(y_x|c) + \delta P(y_{x'}|c) + \theta P(y'_{x'}|c),$$
$$\sigma = \beta - \gamma - \theta + \delta.$$

Proof.

$$\begin{aligned} & f(c) \\ = \quad & \beta P(y_x, y'_{x'}|c) + \gamma P(y_x, y_{x'}|c) + \\ & +\theta P(y'_x, y'_{x'}|c) + \delta P(y'_x, y_{x'}|c) \\ = \quad & \beta P(y_x, y'_{x'}|c) + \gamma[P(y_x|c) - P(y_x, y'_{x'}|c)] + \\ & +\theta[P(y'_{x'}) - P(y_x, y'_{x'}|c)] + \delta P(y'_x, y_{x'}|c) \\ = \quad & \gamma P(y_x|c) + \theta P(y'_{x'}|c) + \\ & +(\beta - \gamma - \theta)P(y_x, y'_{x'}|c) + \delta P(y'_x, y_{x'}|c). \end{aligned} \tag{9}$$

By Lemma 5, we have,

$$P(y'_x, y_{x'}|c) = P(y_x, y'_{x'}|c) - P(y_x|c) + P(y_{x'}|c). \tag{10}$$

Substituting Equation 10 into Equation 9, we have,

$$\begin{aligned} & f(c) \\ = \quad & \gamma P(y_x|c) + \theta P(y'_{x'}|c) + \\ & +(\beta - \gamma - \theta)P(y_x, y'_{x'}|c) + \delta P(y'_x, y_{x'}|c) \\ = \quad & \gamma P(y_x|c) + \theta P(y'_{x'}|c) + \\ & +(\beta - \gamma - \theta)P(y_x, y'_{x'}|c) + \\ & +\delta[P(y_x, y'_{x'}|c) - P(y_x|c) + P(y_{x'}|c)] \\ = \quad & (\gamma - \delta)P(y_x|c) + \delta P(y_{x'}|c) + \theta P(y'_{x'}|c) + \\ & +(\beta - \gamma - \theta + \delta)P(y_x, y'_{x'}|c). \end{aligned}$$

□

Theorem 1. *Given a causal diagram G and distribution compatible with G, let $Z \cup C$ be a set of variables that does not contain any descendant of X in G, then the benefit function $f(c) = \beta P(y_x, y'_{x'}|c) + \gamma P(y_x, y_{x'}|c) + \theta P(y'_x, y'_{x'}|c) + \delta P(y_{x'}, y'_x|c)$ is bounded as follows:*

$$W + \sigma U \le f \le W + \sigma L \qquad \textit{if } \sigma < 0,$$
$$W + \sigma L \le f \le W + \sigma U \qquad \textit{if } \sigma > 0,$$

where σ, W, L, U are given by,

$$\sigma = \beta - \gamma - \theta + \delta,$$
$$W = (\gamma - \delta)P(y_x|c) + \delta P(y_{x'}|c) + \theta P(y'_{x'}|c),$$
$$L = \sum_z \max \left\{ \begin{array}{c} 0, \\ P(y_x|z,c) - P(y_{x'}|z,c), \\ P(y|z,c) - P(y_{x'}|z,c), \\ P(y_x|z,c) - P(y|z,c) \end{array} \right\} \times P(z|c),$$
$$U = \sum_z \min \left\{ \begin{array}{c} P(y_x|z,c), \\ P(y'_{x'}|z,c), \\ P(y,x|z,c) + P(y',x'|z,c), \\ P(y_x|z,c) - P(y_{x'}|z,c) + \\ +P(y,x'|z,c) + P(y',x|z,c) \end{array} \right\} \times P(z|c).$$

Proof. By Lemmas 6 and 7,
substituting Equations 3 and 4 into Equation 8, Theorem 1 holds.

Note that, if we substituting Lemma 4 into Lemma 7, we have the same results as in Li-Pearl's Theorem. We showed that in Lemma 6 that the bounds in Lemma 6 is guaranteed to be no worse than the bounds in Lemma 4, therefore, the bounds in Theorem 1 is guaranteed to be no worse than the bounds in Li-Pearl's Theorem. □

Lemma 8. *Given a causal diagram G and distribution compatible with G, let $Z \cup C$ be a set of variables such that $\forall x, x' \in X : x \neq x', (Y_x \perp\!\!\!\perp X \cup Z_{x'} \mid Z_x, C)$ in G, then the c-PNS $P(y_x, y'_{x'}|c)$ is bounded as follows:*

$$\max \left\{ \begin{array}{c} 0, \\ P(y_x|c) - P(y_{x'}|c), \\ P(y|c) - P(y_{x'}|c), \\ P(y_x|c) - P(y|c) \end{array} \right\} \le \textit{c-PNS}, \tag{11}$$

$$\min \left\{ \begin{array}{c} P(y_x|c), \\ P(y'_{x'}|c), \\ P(y,x|c) + P(y',x'|c), \\ P(y_x|c) - P(y_{x'}|c) + \\ +P(y,x'|c) + P(y',x|c), \\ \sum_z \sum_{z'} \min\{P(y|z,x,c), \\ P(y'|z',x',c)\} \\ \times \min\{P(z_x|c), P(z'_{x'}|c)\} \end{array} \right\} \ge \textit{c-PNS}. \tag{12}$$

Proof.

$$\begin{aligned} & c\text{-PNS} \\ = \quad & P(y_x, y'_{x'}|c) \\ = \quad & \Sigma_z \Sigma_{z'} P(y_x, y'_{x'}, z_x, z'_{x'}|c) \\ = \quad & \Sigma_z \Sigma_{z'} P(y_x, y'_{x'}|z_x, z'_{x'}, c) \times P(z_x, z'_{x'}|c) \\ \le \quad & \Sigma_z \Sigma_{z'} \min\{P(y_x|z_x, z'_{x'}, c), P(y'_{x'}|z_x, z'_{x'}, c)\} \\ & \times \min\{P(z_x|c), P(z'_{x'}|c)\} \\ = \quad & \Sigma_z \Sigma_{z'} \min\{P(y_x|z_x, c), P(y'_{x'}|z'_{x'}, c)\} \\ & \times \min\{P(z_x|c), P(z'_{x'}|c)\} \qquad (13) \\ = \quad & \Sigma_z \Sigma_{z'} \min\{P(y|z_x, x, c), P(y'|z'_{x'}, x', c)\} \\ & \times \min\{P(z_x|c), P(z'_{x'}|c)\} \qquad (14) \\ = \quad & \Sigma_z \Sigma_{z'} \min\{P(y|z, x, c), P(y'|z', x', c)\} \\ & \times \min\{P(z_x|c), P(z'_{x'}|c)\}. \end{aligned}$$

Combined with the bounds in Lemma 4, Lemma 8 holds. Note that Equation 13 is due to $Y_x \perp\!\!\!\perp Z_{x'} \mid Z_x, C$ and $Y_{x'} \perp\!\!\!\perp Z_x \mid Z_{x'}, C$. Equation 14 is due to $\forall x \in X, Y_x \perp\!\!\!\perp X \mid Z_x, C$. □

Theorem 2. *Given a causal diagram G and distribution compatible with G, let Z be a set of variables such that $\forall x, x' \in X : x \neq x', (Y_x \perp\!\!\!\perp X \cup Z_{x'} \mid Z_x, C)$ in G, and C does not contain any descendant of X in G, then the benefit function $f(c) = \beta P(y_x, y'_{x'}|c) + \gamma P(y_x, y_{x'}|c) + \theta P(y'_x, y'_{x'}|c) + \delta P(y_{x'}, y'_x|c)$ is bounded as follows:*

$$W + \sigma U \le f \le W + \sigma L \qquad \textit{if } \sigma < 0,$$
$$W + \sigma L \le f \le W + \sigma U \qquad \textit{if } \sigma > 0,$$

where σ, W, L, U are given by,

$$\sigma = \beta - \gamma - \theta + \delta,$$
$$W = (\gamma - \delta)P(y_x|c) + \delta P(y_{x'}|c) + \theta P(y'_{x'}|c),$$
$$L = \max\left\{\begin{array}{c} 0, \\ P(y_x|c) - P(y_{x'}|c), \\ P(y|c) - P(y_{x'}|c), \\ P(y_x|c) - P(y|c) \end{array}\right\},$$
$$U = \min\left\{\begin{array}{c} P(y_x|c), \\ P(y'_{x'}|c), \\ P(y,x|c) + P(y',x'|c), \\ P(y_x|c) - P(y_{x'}|c)+ \\ +P(y,x'|c) + P(y',x|c), \\ \sum_z \sum_{z'} \min\{P(y|z,x,c), \\ P(y'|z',x',c)\} \\ \times \min\{P(z_x|c), P(z'_{x'}|c)\} \end{array}\right\}.$$

Proof. By Lemmas 8 and 7,
substituting Equations 11 and 12 into Equation 8, Theorem 2 holds.

Note that, if we substituting Lemma 4 into Lemma 7, we have the same results as in Li-Pearl's Theorem. From the proof of Lemma 8, we know that the lower bound in Lemma 8 is the same as in Lemma 4 and the upper bound in Lemma 8 is no worse than the upper bound in Lemma 4. Therefore, the lower bound in Theorem 2 is the same as in Li-Pearl's Theorem, and the upper bound in Theorem 2 is guaranteed to be no worse than the upper bound in Li-Pearl's Theorem. □

Lemma 9. *Given a causal diagram G in Figure 9 and distribution that compatible with G, and C is not a descendant of X, then c-PNS $P(y_x, y'_{x'}|c)$ is bounded as follow:*

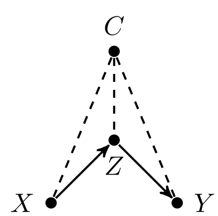

Figure 9: Mediator Z with no direct effects of X on Y.

$$\max\left\{\begin{array}{c} 0, \\ P(y_x|c) - P(y_{x'}|c), \\ P(y|c) - P(y_{x'}|c), \\ P(y_x|c) - P(y|c) \end{array}\right\} \le \textit{c-PNS}, \quad (15)$$

$$\min\left\{\begin{array}{c} P(y_x|c), \\ P(y'_{x'}|c), \\ P(y,x|c) + P(y',x'|c), \\ P(y_x|c) - P(y_{x'}|c)+ \\ +P(y,x'|c) + P(y',x|c), \\ \Sigma_z \Sigma_{z'\neq z} \min\{P(y|z,c), \\ P(y'|z',c)\} \\ \times \min\{P(z|x,c), P(z'|x',c)\} \end{array}\right\} \ge \textit{c-PNS}. \quad (16)$$

Proof. First we show that in graph G, if an individual is a c-complier from X to Y, then $Z_x|c$ and $Z_{x'}|c$ must have the different values. This is because the structural equations for Y and Z are $f_y(z, u_y, c)$ and $f_z(x, u_z, c)$, respectively. If an individual has the same $Z_x|c$ and $Z_{x'}|c$ value, then $f_z(x, u_z, c) = f_z(x', u_z, c)$. This means $f_y(f_z(x, u_z, c), u_y, c) = f_y(f_z(x', u_z, c), u_y, c)$, i.e., $Y_x|c$ and $Y_{x'}|c$ must have the same value. Thus this individual is not a c-complier. Therefore,

$$\begin{aligned} & c\text{-PNS} \\ = \; & P(y_x, y'_{x'}|c) \\ = \; & \Sigma_z \Sigma_{z'\neq z} P(y_z, y'_{z'}|c) \times P(z_x, z'_{x'}|c) \\ \le \; & \Sigma_z \Sigma_{z'\neq z} \min\{P(y_z|c), P(y'_{z'}|c)\} \\ & \times \min\{P(z_x|c), P(z'_{x'}|c)\} \\ = \; & \Sigma_z \Sigma_{z'\neq z} \min\{P(y|z,c), P(y'|z',c)\} \\ & \times \min\{P(z|x,c), P(z'|x',c)\}. \end{aligned}$$

Combined with the bounds in Lemma 4, Lemma 9 holds. □

Theorem 3. *Given a causal diagram G in Figure 9 and distribution compatible with G, and C does not contain any descendant of X, then the benefit function $f(c) = \beta P(y_x, y'_{x'}|c) + \gamma P(y_x, y_{x'}|c) + \theta P(y'_x, y'_{x'}|c) + \delta P(y_{x'}, y'_x|c)$ is bounded as follows:*

$$W + \sigma U \le f \le W + \sigma L \qquad \text{if } \sigma < 0,$$
$$W + \sigma L \le f \le W + \sigma U \qquad \text{if } \sigma > 0,$$

where σ, W, L, U are given by,

$$\sigma = \beta - \gamma - \theta + \delta,$$
$$W = (\gamma - \delta)P(y_x|c) + \delta P(y_{x'}|c) + \theta P(y'_{x'}|c),$$
$$L = \max\left\{\begin{array}{c} 0, \\ P(y_x|c) - P(y_{x'}|c), \\ P(y|c) - P(y_{x'}|c), \\ P(y_x|c) - P(y|c) \end{array}\right\},$$
$$U = \min\left\{\begin{array}{c} P(y_x|c), \\ P(y'_{x'}|c), \\ P(y,x|c) + P(y',x'|c), \\ P(y_x|c) - P(y_{x'}|c)+ \\ +P(y,x'|c) + P(y',x|c), \\ \Sigma_z \Sigma_{z'\neq z} \min\{P(y|z,c), \\ P(y'|z',c)\} \\ \times \min\{P(z|x,c), P(z'|x',c)\} \end{array}\right\}.$$

Proof. By Lemmas 9 and 7,
substituting Equations 15 and 16 into Equation 8, Theorem 3 holds.

Note that, if we substituting Lemma 4 into Lemma 7, we have the same results as in Li-Pearl's Theorem. From the proof of Lemma 9, we know that the lower bound in Lemma 9 is the same as in Lemma 4 and the upper bound in Lemma 9 is no worse than the upper bound in Lemma 4. Therefore, the lower bound in Theorem 3 is the same as in Li-Pearl's Theorem, and the upper bound in Theorem 3 is guaranteed to be no worse than the upper bound in Li-Pearl's Theorem. □

Calculation in the Examples

In order to clearly see the calculation steps, we list an equivalent form of Li-Pearl's Theorem as following (see the proof in the previous section for the equivalence):

Theorem 10. *Given a causal diagram G and distribution compatible with G, let C be a set of variables that does not contain any descendant of X in G, then the benefit function* $f(c) = \beta P(y_x, y'_{x'}|c) + \gamma P(y_x, y_{x'}|c) + \theta P(y'_x, y'_{x'}|c) + \delta P(y_{x'}, y'_x|c)$ *is bounded as follows:*

$$W + \sigma U \leq f(c) \leq W + \sigma L \qquad \text{if } \sigma < 0,$$
$$W + \sigma L \leq f(c) \leq W + \sigma U \qquad \text{if } \sigma > 0,$$

where σ, W, L, U are given by,

$$\sigma = \beta - \gamma - \theta + \delta,$$
$$W = (\gamma - \delta)P(y_x|c) + \delta P(y_{x'}|c) + \theta P(y'_{x'}|c),$$
$$L = \max\left\{\begin{array}{c} 0, \\ P(y_x|c) - P(y_{x'}|c), \\ P(y|c) - P(y_{x'}|c), \\ P(y_x|c) - P(y|c) \end{array}\right\},$$
$$U = \min\left\{\begin{array}{c} P(y_x|c), \\ P(y'_{x'}|c), \\ P(y, x|c) + P(y', x'|c), \\ P(y_x|c) - P(y_{x'}|c) + \\ +P(y, x'|c) + P(y', x|c) \end{array}\right\}.$$

Company Selection First, we apply Li-Pearl's Theorem (Theorem 10) to the data in Tables 1 and 2. The benefit vector is $(100, -60, 0, -140)$.
We have,

$$\begin{aligned} \sigma &= \beta - \gamma - \theta + \delta \\ &= 100 - (-60) - 0 + (-140) \\ &= 20 \end{aligned}$$

$$\begin{aligned} W &= (\gamma - \delta)P(r_a|c) + \delta P(r_{a'}|c) + \theta P(r'_{a'}|c) \\ &= (-60 - (-140)) \times 0.83729 + 0 \times 0.47405 + \\ &\quad +(-140) \times 0.52595 \\ &= -6.64980 \end{aligned}$$

$$\begin{aligned} L &= \max\left\{\begin{array}{c} 0, \\ P(r_a|c) - P(r_{a'}|c), \\ P(r|c) - P(r_{a'}|c), \\ P(r_a|c) - P(r|c) \end{array}\right\} \\ &= \max\left\{\begin{array}{c} 0, \\ 0.83729 - 0.52595, \\ 0.70714 - 0.52595, \\ 0.83729 - 0.70714 \end{array}\right\} \\ &= 0.31134 \end{aligned}$$

$$\begin{aligned} U &= \min\left\{\begin{array}{c} P(r_a|c), \\ P(r'_{a'}|c), \\ P(r, a|c) + P(r', a'|c), \\ P(r_a|c) - P(r_{a'}|c) + \\ +P(r, a'|c) + P(r', a|c) \end{array}\right\} \\ &= \min\left\{\begin{array}{c} 0.83729, \\ 1 - 0.52595, \\ 0.35286 + 0.20143, \\ 0.83729 - 0.52595 + \\ +0.35428 + 0.09143 \end{array}\right\} \\ &= 0.47405 \end{aligned}$$

Therefore,

$$\begin{aligned} & W + \sigma L \leq f(c) \leq W + \sigma U, \\ & -6.64980 + 20 \times 0.31134 \leq f(c) \\ & \leq -6.64980 + 20 \times 0.47405, \\ & -0.423 \leq f(c) \leq 2.832. \end{aligned}$$

Then, we apply Theorem 1 to the data in Tables 1 and 2. σ and W are the same as above.
And we have,

$$\begin{aligned} L &= \sum_z \max\left\{\begin{array}{c} 0, \\ P(r_a|z, c) - P(r_{a'}|z, c), \\ P(r|z, c) - P(r_{a'}|z, c), \\ P(r_a|z, c) - P(r|z, c) \end{array}\right\} \\ &\quad \times P(z|c) \\ &= \max\left\{\begin{array}{c} 0, \\ 0.44600 - 0.05000, \\ 0.49010 - 0.05000, \\ 0.44600 - 0.49010 \end{array}\right\} \times 0.28857 \\ &\quad + \max\left\{\begin{array}{c} 0, \\ 0.99600 - 0.71900, \\ 0.79518 - 0.71900, \\ 0.99600 - 0.79518 \end{array}\right\} \times 0.71143 \\ &= 0.44010 \times 0.28857 + 0.27700 \times 0.71143 \\ &= 0.32407 \end{aligned}$$

$$U = \sum_z \min\left\{\begin{array}{c} P(r_a|z,c), \\ P(r'_{a'}|z,c), \\ P(r,a|z,c)+P(r',a'|z,c), \\ P(r_a|z,c)-P(r_{a'}|z,c)+ \\ +P(r,a'|z,c)+P(r',a|z,c) \end{array}\right\} \times P(z|c)$$

$$= \min\left\{\begin{array}{c} 0.44600, \\ 1-0.05000, \\ 0.44555+0.20297, \\ 0.44600-0.05000+ \\ +0.04455+0.30693 \end{array}\right\} \times 0.28857 + \min\left\{\begin{array}{c} 0.99600, \\ 1-0.71900, \\ 0.31526+0.20080, \\ 0.99600-0.71900+ \\ +0.47992+0.00402 \end{array}\right\} \times 0.71143$$

$$= 0.44600 \times 0.28857 + 0.28100 \times 0.71143 = 0.32862$$

Therefore,

$$W+\sigma L \le f(c) \le W+\sigma U,$$
$$-6.64980 + 20 \times 0.32407 \le f(c) \le -6.64980 + 20 \times 0.32862,$$
$$-0.168 \le f(c) \le -0.077.$$

Effective Patients of a Drug First, the set $\{C\}$ satisfied the back-door criterion for both (A,Z) and (A,R). By Pearl's adjustment formula, the experimental data needed are:

$$P(r_a|c) = P(r|a,c) = 0.66666,$$
$$P(r_{a'}|c) = P(r|a',c) = 0.33265,$$
$$P(z_a|c) = P(z|a,c) = 0.68878,$$
$$P(z'_{a'}|c) = P(z'|a',c) = 0.01232.$$

Then, we apply Li-Pearl's Theorem (Theorem 10) to the data in Table 3 and the above experimental data. The benefit vector is $(1,-1,-1,-1)$.
We have,

$$\sigma = \beta-\gamma-\theta+\delta = 1-(-1)-(-1)+(-1) = 2$$

$$W = (\gamma-\delta)P(r_a|c)+\delta P(r_{a'}|c)+\theta P(r'_{a'}|c) = (-1+1)P(r_a|c)-P(r_{a'}|c)-P(r'_{a'}|c) = -1$$

$$L = \max\left\{\begin{array}{c} 0, \\ P(r_a|c)-P(r_{a'}|c), \\ P(r|c)-P(y_{a'}|c), \\ P(r_a|c)-P(r|c) \end{array}\right\} = \max\left\{\begin{array}{c} 0, \\ 0.66666-0.33265, \\ 0.51535-0.33265, \\ 0.66666-0.51535 \end{array}\right\} = 0.33401$$

$$U = \min\left\{\begin{array}{c} P(r_a|c), \\ P(r'_{a'}|c), \\ P(r,a|c)+P(r',a'|c), \\ P(r_a|c)-P(r_{a'}|c)+ \\ +P(r,a'|c)+P(r',a|c) \end{array}\right\} = \min\left\{\begin{array}{c} 0.66666, \\ 1-0.33265, \\ 0.36465+0.30233, \\ 0.66666-0.33265+ \\ +0.15070+0.18232 \end{array}\right\} = 0.66666$$

Therefore,

$$W+\sigma L \le f(c) \le W+\sigma U,$$
$$-1+2\times 0.33401 \le f(c) \le -1+2\times 0.66666,$$
$$-0.3320 \le f(c) \le 0.3333.$$

Then, we apply Theorem 2 to the data in Table 3 and the above experimental data. σ, W, and L are the same as above. And we have,

$$U = \min\left\{\begin{array}{c} P(r_a|c), \\ P(r'_{a'}|c), \\ P(r,a|c)+P(r',a'|c), \\ P(r_a|c)-P(r_{a'}|c)+ \\ +P(r,a'|c)+P(r',a|c), \\ \sum_z \sum_{z'} \min\{P(r|z,a,c), \\ P(r'|z',a',c)\} \\ \times \min\{P(z_a|c), P(z'_{a'}|c)\} \end{array}\right\}$$

$$= \min\left\{\begin{array}{c} 0.66666, \\ 1-0.33265, \\ 0.36465+0.30233, \\ 0.66666-0.33265+ \\ +0.15070+0.18232, \\ \min\{0.92593, 0.66944\}\times \\ \min\{0.68878, 0.98768\}+ \\ \min\{0.92593, 0.50000\}\times \\ \min\{0.68878, 0.01232\}+ \\ \min\{0.09290, 0.66944\}\times \\ \min\{0.31122, 0.98768\}+ \\ \min\{0.09290, 0.50000\}\times \\ \min\{0.31122, 0.01232\} \end{array}\right\} = 0.49731$$

Therefore,

$$W+\sigma L \le f(c) \le W+\sigma U,$$
$$-1+2\times 0.33401 \le f(c) \le -1+2\times 0.49731,$$
$$-0.3320 \le f(c) \le -0.0054.$$

Algorithm 1: Generate sample distributions for non-descendant covariates

Input: n, number of sample distributions needed.
Output: n sample distributions (observational data and experimental data).

for $i = 1$ to n **do**
  //$rand(0,1)$ is the function that random uniformly generate a number from 0 to 1.
  // t_1, t_2, t_3, and t_4 can be interpreted as the number of individuals such that $x \wedge z$, $x' \wedge z$, $x \wedge z'$, and $x' \wedge z'$ respectively.
  $t_1 = rand(0,1) \times 1000$;
  $t_2 = rand(0,1) \times (1000 - t_1)$;
  $t_3 = rand(0,1) \times (1000 - t_1 - t_2)$;
  $t_4 = 1000 - t_1 - t_2 - t_3$;
  // o_1, o_2, o_3, and o_4 can be interpreted as the number of individuals such that $x \wedge z \wedge y$, $x' \wedge z \wedge y$, $x \wedge z' \wedge y$, and $x' \wedge z' \wedge y$ respectively.
  $o_1 = rand(0,1) \times t_1$;
  $o_2 = rand(0,1) \times t_2$;
  $o_3 = rand(0,1) \times t_3$;
  $o_4 = rand(0,1) \times t_4$;
  // Each c_i corresponding to a sample distribution.
  // The following are experimental data that satisfied the general bounds provided by Tian and Pearl.
  $P(y|do(x), z, c_i) = rand(0,1) \times \frac{t_2}{t_1+t_2} + \frac{o_1}{t_1+t_2}$;
  $P(y|do(x'), z, c_i) = rand(0,1) \times \frac{t_1}{t_1+t_2} + \frac{o_2}{t_1+t_2}$;
  $P(y|do(x), z', c_i) = rand(0,1) \times \frac{t_4}{t_3+t_4} + \frac{o_3}{t_3+t_4}$;
  $P(y|do(x'), z', c_i) = rand(0,1) \times \frac{t_3}{t_3+t_4} + \frac{o_4}{t_3+t_4}$;
  // The following are observational data.
  $P(x, y, z|c_i) = o_1/1000$;
  $P(x, y, z'|c_i) = o_3/1000$;
  $P(x, y', z|c_i) = (t_1 - o_1)/1000$;
  $P(x, y', z'|c_i) = (t_3 - o_3)/1000$;
  $P(x', y, z|c_i) = o_2/1000$;
  $P(x', y, z'|c_i) = o_4/1000$;
  $P(x', y', z|c_i) = (t_2 - o_2)/1000$;
  $P(x', y', z'|c_i) = (t_4 - o_4)/1000$;
end for

Algorithm 2: Generate sample distributions for partial mediators

Input: n, number of sample distributions needed.
Output: n sample distributions (observational data in conditional probability tables).

for $i = 1$ to n **do**
  //$rand(0,1)$ is the function that random uniformly generate a number from 0 to 1.
  // Each c_i corresponding to a sample distribution.
  $P(x|c_i) = rand(0,1)$;
  $P(z|x, c_i) = rand(0,1)$;
  $P(z|x', c_i) = rand(0,1)$;
  $P(y|x, z, c_i) = rand(0,1)$;
  $P(y|x', z, c_i) = rand(0,1)$;
  $P(y|x, z', c_i) = rand(0,1)$;
  $P(y|x', z', c_i) = rand(0,1)$;
end for

Algorithm 3: Generate sample distributions for pure mediators

Input: n, number of sample distributions needed.
Output: n sample distributions (observational data in conditional probability tables).

for $i = 1$ to n **do**
  //$rand(0,1)$ is the function that random uniformly generate a number from 0 to 1.
  // Each c_i corresponding to a sample distribution.
  $P(x|c_i) = rand(0,1)$;
  $P(z|x, c_i) = rand(0,1)$;
  $P(z|x', c_i) = rand(0,1)$;
  $P(y|z, c_i) = rand(0,1)$;
  $P(y|z', c_i) = rand(0,1)$;
end for

Distribution Generating Algorithms

Here, the sample distribution generating algorithms in simulated studies are presented.

Non-descendant Covariates The Algorithm 1 is the sample distribution generating algorithm in the simulated study of non-descendant covariates case. It generated both experimental and observational data compatible with Figure 5 (X, Y, Z are binary) that satisfy the general relation provided by Tian and Pearl (i.e., the general relation between experimental and observational data).

Partial Mediators The observational data compatible with Figure 1 (X, Y, Z are binary) in the simulated study of partial mediators case was generated by Algorithm 2. The experimental data needed was computed via adjustment formula because the set $\{C\}$ satisfied the back-door criterion for both (X, Z) and (X, Y).

Pure Mediators The observational data compatible with Figure 2 (X, Y, Z are binary) in the simulated study of pure mediators case was generated by Algorithm 3. The experimental data needed was computed via adjustment formula because the set $\{C\}$ satisfied the back-door criterion for (X, Y).