General Probabilities of Causation with Causal Knowledge

Xin Shu, Zhen Lei, Ang Li*

Department of Computer Science, Florida State University
xs24a@fsu.edu, zl24a@fsu.edu, angli@cs.fsu.edu

Abstract

Probabilities of causation (PoCs) characterize individual causal responses that cannot be directly observed and therefore generally require partial identification. Tian and Pearl first derived theoretically sharp bounds for binary PoCs, including the probability of necessity (PN), the probability of sufficiency (PS), and the probability of necessity and sufficiency (PNS). Mueller et al. subsequently tightened the bounds for binary PNS by incorporating causal information encoded in covariates and mediators. More recently, Li and Pearl, as well as Shu et al., extended PoCs to multivalued settings and derived corresponding theoretical bounds. These developments naturally raise the question of whether additional causal knowledge can further tighten the bounds in multivalued settings. This paper addresses this question by deriving tighter bounds for multivalued PoCs through the incorporation of causal information encoded in covariates and mediators. We illustrate the theoretical results with toy examples, while simulation studies further demonstrate that the proposed bounds are tighter than existing nonbinary bounds.

Introduction

The modern study of probabilities of causation (PoCs) began with Pearl (1999), who introduced three counterfactual measures of causation for binary treatments and outcomes within the Structural Causal Model (SCM) framework (Galles and Pearl 1998; Halpern 2000): PN, PS, and PNS. Tian and Pearl (2000) subsequently derived theoretically sharp bounds for these quantities by combining experimental and observational data using Balke's linear programming framework (Balke 1995). Li and Pearl (2019, 2022b) later applied them to unit-level utility analysis. Although the bounds derived by Tian and Pearl are sharp given the available distributional information, subsequent research has shown that incorporating covariates, mediators, and structural restrictions encoded by causal graphs can yield narrower bounds on probabilities of causation (Kuroki and Cai 2011; Dawid, Musio, and Murtas 2017; Mueller, Li, and Pearl 2021).

Recent research has extended probabilities of causation to settings with nonbinary treatments and outcomes. Zhang, Tian, and Bareinboim (2022) and Li and Pearl (2022a) developed numerical methods based on nonlinear programming for computing bounds on nonbinary probabilities of causation. Li and Pearl (2024) subsequently derived recursive theoretical bounds. More recently, Shu, Wang, and Li (2026) derived closed form bounds by combining experimental and observational data.

Despite these advances, whether causal graph information can further tighten the bounds of PoCs in nonbinary settings remains an open question. The answer does not follow immediately from the binary case, because a multivalued PoC involves a joint probability of several potential outcomes and therefore introduces a substantially more complex counterfactual structure. Moreover, the information contributed by an auxiliary variable depends on whether it is a pretreatment covariate, a partial mediator, or a pure mediator.

Consider a pharmaceutical company developing a new drug to prevent diabetes, which is increasingly common among younger populations. Its effectiveness can be evaluated using drug-use frequency and diabetes status, both of which may take multiple values. The probability of necessity and sufficiency (PNS) characterizes such individual response patterns by jointly considering the individual's potential diabetes outcomes under different frequencies of taking the drug. However, such bounds may remain wide (e.g., $[0.1, 0.9]$) and therefore be of limited use for decision making if they do not incorporate the causal structure underlying an individual's response. In practice, additional variables often encode information about this causal structure. For example, lifestyle regularity may influence both the frequency of taking the drug and diabetes status, appetite may partially mediate the effect of the drug, and blood glucose regulation may fully mediate this effect. A causal graph distinguishes these roles and imposes corresponding restrictions on feasible counterfactual response patterns. By incorporating these restrictions together with the available experimental and observational distributions, causal graph information can rule out response patterns that are mathematically possible but structurally incompatible, thereby yielding narrower and more informative PNS bounds.

Building on the nonbinary bounds of Shu, Wang, and Li (2026), this paper develops bounds with multivalued treatments and outcomes by incorporating causal graph information. We exploit causal graphs involving non-descendant

*Corresponding author.

covariates, including confounders and backdoor adjustment sets (Pearl 1993, 1995), as well as partial and pure mediators, to impose structural constraints on the feasible joint counterfactual distributions. For each causal structure, we derive bounds by integrating the available experimental and observational distributions with graph-based constraints on the feasible joint counterfactual distributions. These results extend the use of causal structure from binary to multivalued settings and show when auxiliary variables can exclude structurally incompatible response patterns, thereby tightening existing bounds on individual causal responses.

Key Contributions

- We extend existing bounds on PoCs that incorporate causal knowledge from the binary to the multivalued setting. Specifically, we derive bounds not only for PNS but also for PSub, PRep, and PN for general treatment and outcome settings. Unlike the binary case, the multivalued setting requires characterizing joint counterfactual probabilities across multiple treatment levels, introducing substantial new technical challenges while naturally including the binary setting as a special case.
- We derive results for the four representative forms of multivalued PoCs introduced by Shu, Wang, and Li (2026), which are sufficient to represent any discrete PoC. Consequently, the proposed framework immediately applies to a broad class of multivalued PoCs, substantially extending the scope and theoretical impact of incorporating causal knowledge.
- We consider multiple causal structures involving covariates that are not descendants of the treatment, covariates satisfying the back-door criterion, partial mediators, and pure mediators.

Preliminaries

In this section, we review the basic concepts of probabilities of causation (PoC) and the relevant notation used in Structural Causal Models (SCMs) (Galles and Pearl 1998; Halpern 2000). $Y_x = y$ denotes the counterfactual statement that "variable Y would have the value y had X been set to x." Here, X denotes the treatment variable, while Y denotes the outcome or effect. For simplicity, we use y_x as shorthand for $Y_x = y$. Since this paper considers nonbinary settings, we use $y_{j_{x_j}}$ to denote $Y_{x_j} = y_j$ throughout. In general, $P(y_{j_{x_j}})$ refers to a probability obtained from experimental data, whereas $P(x_j, y_j)$ refers to a probability obtained from observational data.

Let X and Y be binary variables in a causal model M. Let x and y denote the events $X = \text{true}$ and $Y = \text{true}$, respectively, and let x' and y' denote the events $X = \text{false}$ and $Y = \text{false}$, respectively. The three basic probabilities of causation are defined below (Pearl 1999):

Definition 1 (Probabilities of Causation)**.** *(Pearl 1999)*

$$PNS \triangleq P(y_x, y'_{x'}) PN \triangleq P(y'_{x'}|x, y), PS \triangleq P(y_x|y', x'),$$

In the multivalued setting, let the treatment variable X and the outcome variable Y each take n values. $PNS(k) = P(y_{1_{x_1}}, \ldots, y_{k_{x_k}})$, where $k \leq n$, was first introduced by Li and Pearl (2024), represents the probability that the same individual would exhibit outcome y_j if the treatment were set to x_j for every $j \in \{1, \ldots, k\}$. It therefore characterizes a joint individual causal response across multiple treatment levels.

Probability of necessity and sufficiency(k):
$\mathrm{PNS}(k) = P(y_{1_{x_1}}, ..., y_{k_{x_k}})$

Probability of substitute(k, p): $p \neq j$ for $1 \leq j \leq k$
$\mathrm{PSub}(k, p) = P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_p)$

Probability of replacement(k, q):
$\mathrm{PRep}(k, q) = P(y_{1_{x_1}}, ..., y_{k_{x_k}}, y_q)$

Probability of necessity(k, p, q): $p \neq j$ for $1 \leq j \leq k$
$\mathrm{PN}(k, p, q) = P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_p, y_q)$

Later, Shu, Wang, and Li (2026) derived closed-form bounds for nonbinary probabilities of causation. The four main theorems are presented above. Further details, together with the equivalence and replaceability theorems, are omitted here because of space limitations and can be found in Shu, Wang, and Li (2026).

In this paper, we derive narrower bounds for these four PoCs by incorporating information from causal graphs involving covariates and mediators. Under the specified graphical conditions, the proposed nonbinary bounds tighten existing bounds. We establish this improvement mathematically and use simulations to demonstrate and quantify the extent of the tightening.

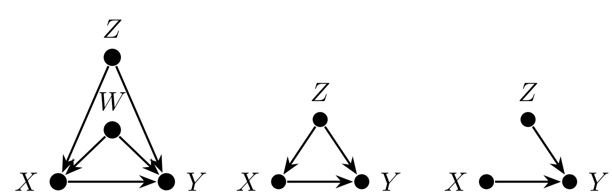
Bounds with Causal Diagram

In this section, we assume that variables X and Y each take n values, so that $|X| = |Y| = n$, with $k \leq n$. The generalization was formally established by Shu, Wang, and Li (2026). Proofs of the following theorems are provided in the appendix.

For each graphical structure, we derive improved versions of all four existing bounds for multivalued probabilities of causation ($\mathrm{PNS}(k)$, $\mathrm{PSub}(k, p)$, $\mathrm{PRep}(k, q)$, $\mathrm{PN}(k, p, q)$).

Non-descendant Covariates

Given a causal diagram G, we restrict Z to be a set of variables containing no descendants of X in G. Fig. 1 (a) illus-



(a) Covariates Z and W (b) Confounder Z (c) Outcome-affecting Z

Figure 1: In all three graphs, Z contains no descendants of X. In graphs (b) and (c), Z additionally satisfies the back-door criterion.

trates such a causal structure. This assumption ensures that Z is not affected by interventions on X and allows the conditional quantity $P(y_{j_{x_j}} \mid z)$ to be measured. Here, unless otherwise specified, $j \in \{1, \ldots, n\}$ throughout the rest of the paper.

Theorem 2.

$$\sum_z \max \left\{ \begin{array}{c} 0, \\ \\ \sum_{j=1}^{k} P(y_{j_{x_j}} \mid z) - k + 1, \\ \\ \textit{For } i \in \{1, ..., k\}: \\ \sum_{\substack{1 \le j \le k \\ j \ne i}} \Big[P(y_{j_{x_j}} \mid z) + \\ +P(x_j \mid z) - P(x_j, y_j \mid z)\Big] + \\ +P(x_i, y_i \mid z) - k + 1 \end{array} \right\} \times P(z) \le \mathrm{PNS}(k)$$

$$\sum_z \min \left\{ \begin{array}{c} \sum_{j=1}^{k} P(x_j, y_j \mid z) + \\ + \sum_{j=k+1}^{n} P(x_j \mid z), \\ \\ \textit{For } j \in \{1, ..., k\}: \\ P(y_{j_{x_j}} \mid z), \\ \\ \textit{For } m \in \{1, ..., k-1\}, \\ t_j \in \{1, ..., k\}: \\ \frac{1}{m}\Big[\sum_{j=0}^{m} P(y_{t_{j_{x_{t_j}}}} \mid z) - \\ -P(x_{t_j}, y_{t_j} \mid z)\Big] \end{array} \right\} \times P(z) \ge \mathrm{PNS}(k)$$

Here, we derive bounds on the conditional z-specific $\mathrm{PNS}(k)$ for each possible value z and then take a weighted sum of these stratum-specific bounds to obtain tighter bounds on the $\mathrm{PNS}(k)$. Bounds on $\mathrm{PSub}(k), \mathrm{PRep}(k), \mathrm{PN}(k)$ can be derived similarly.

Theorem 3. *$p \ne j$ for $1 \le j \le k$,*

$$\sum_z \max \left\{ \begin{array}{c} 0, \\ \\ \sum_{j=1}^{k} \Big[P(y_{j_{x_j}} \mid z) + P(x_j \mid z) - \\ -P(x_j, y_j \mid z)\Big] + P(x_p \mid z) - k \end{array} \right\} \times P(z) \le \mathrm{PSub}(k, p)$$

$$\sum_z \min \left\{ \begin{array}{c} P(x_p \mid z), \\ \\ \textit{For } j \in \{1, ..., k\}: \\ P(y_{j_{x_j}} \mid z) - P(x_j, y_j \mid z) \end{array} \right\} \times P(z) \ge \mathrm{PSub}(k, p)$$

Theorem 4.

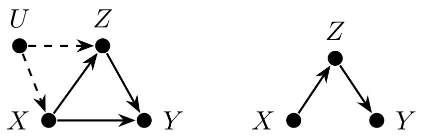
$$\sum_z \max \left\{ \begin{array}{c} 0, \\ \\ \sum_{j=1}^{k} \Big[P(y_{j_{x_j}} \mid z) + \\ +P(x_j \mid z) - P(x_j, y_j \mid z)\Big] + \\ + \sum_{\substack{k+1 \le j \le n \\ j \ne q}} P(x_j, y_q \mid z) + \\ +P(x_q, y_q \mid z) - k, \\ \\ \textit{If } q \in \{1, ..., k\}: \\ \sum_{\substack{1 \le j \le k \\ j \ne q}} \Big[P(y_{j_{x_j}} \mid z) + \\ +P(x_j \mid z) - P(x_j, y_j \mid z)\Big] + \\ +P(x_q, y_q \mid z) - (k-1) \end{array} \right\} \times P(z) \le \mathrm{PRep}(k, q)$$

$$\sum_z \min \left\{ \begin{array}{c} \textit{If } q \in \{1, ..., k\}: \\ P(y_{q_{x_q}} \mid z), \\ \\ P(x_q, y_q \mid z) + \\ + \sum_{\substack{k+1 \le j \le n \\ j \ne q}} P(x_j, y_q \mid z), \\ \\ \textit{For } j \in \{1, ..., k\}, \textit{ and } j \ne q \\ P(y_{j_{x_j}} \mid z) - P(x_j, y_j \mid z), \end{array} \right\} \times P(z) \ge \mathrm{PRep}(k, q)$$

Theorem 5. *$p \ne j$ for $1 \le j \le k$,*

$$\sum_z \max \left\{ \begin{array}{c} 0, \\ \\ \sum_{j=1}^{k} \Big[P(y_{j_{x_j}} \mid z) + \\ +P(x_j \mid z) - P(x_j, y_j \mid z)\Big] + \\ +P(x_p, y_q \mid z) - k \end{array} \right\} \times P(z) \le \mathrm{PN}(k, p, q)$$

$$\sum_z \min \left\{ \begin{array}{c} P(x_p, y_q \mid z), \\ \\ \textit{For } j \in \{1, ..., k\}: \\ P(y_{j_{x_j}} \mid z) - P(x_j, y_j \mid z) \end{array} \right\} \times P(z) \ge \mathrm{PN}(k, p, q)$$



(a) With direct effect (b) With no direct effect

Figure 2: In both graphs, Z is a mediator: (a) with a direct effect and (b) with no direct effect.

When Z not only contains no descendants of X in G but also satisfies the back-door criterion (Pearl 1993, 1995) (Figures 1(b) and 1(c) illustrate two examples of this setting), the back-door adjustment formula gives

$$P(y_{j_{x_j}} \mid z) = P(y_j \mid x_j, z).$$

Substituting this equality into Theorems 2–5 yields four new theorems that require only observational data, without the need for experimental data. For instance, the upper bound of PN(k,p,q) becomes

$$\sum_z \min \left\{ \begin{array}{c} P(x_p, y_q \mid z), \\ \\ \text{For } j \in \{1, ..., k\} : \\ P(y_j \mid x_j, z) - P(x_j, y_j \mid z) \end{array} \right\} \times P(z) \\ \geq \mathrm{PN}(k, p, q)$$

Mediation

When Z is a descendant of X, the previous results no longer apply. However, under certain mediation structures, information about Z can still tighten the upper bound.

Partial Mediator In Fig. 2(a), when Z is a mediator and X also has a direct effect on Y, let Z be a set of variables such that $\forall x_j, x_i \in X : \; x_j \neq x_i, \quad (Y_{x_j} \perp\!\!\!\perp X \cup Z_{x_i} \mid Z_{x_j})$, the lower bound remains unchanged from that of Shu, Wang, and Li (2026), while the upper bound includes an additional term. The proof of the additional term can be found in the appendix.

Theorem 6. *Let the bounds on* $\mathrm{PNS}(k)$ *given in Shu, Wang, and Li (2026) be denoted by*

$$PNS_{LB} \leq \mathrm{PNS}(k) \leq PNS_{UB}.$$

By treating Z *as a partial mediator, we can derive a new upper bound on* $\mathrm{PNS}(k)$ *as follows:*

$$\min \left\{ \begin{array}{c} PNS_{UB}, \\ \\ \textit{For } j \in \{1, \ldots, k\} : \\ \displaystyle\sum_{\substack{z_1, \ldots, z_k \\ \in \{1, \ldots, n\}^k}} \Big[\min_j \{ P(y_j \mid x_j, z_j) \} \times \\ \times \min_j \{ P(z_{j_{x_j}}) \} \Big] \end{array} \right\} \geq \mathrm{PNS}(k)$$

Theorem 7. *Given* $p \neq j$ *for* $1 \leq j \leq k$*. Let the bounds on* $\mathrm{PSub}(k, p)$ *given in Shu, Wang, and Li (2026) be denoted by*

$$PSub_{LB} \leq \mathrm{PSub}(k, p) \leq PSub_{UB}.$$

By treating Z *as a partial mediator, we can derive a new upper bound on* $\mathrm{PSub}(k, p)$ *as follows:*

$$\min \left\{ \begin{array}{c} PSub_{UB}, \\ \\ \textit{For } j \in \{1, ..., k\} : \\ \displaystyle\sum_{\substack{z_1, \ldots, z_k \\ \in \{1, \ldots, n\}^k}} \Big[\min_j \{ P(y_j \mid x_j, z_j) \} \times \\ \times \min_j \{ P(z_{j_{x_j}}), P(x_p) \} \Big] \end{array} \right\} \\ \geq \mathrm{PSub}(k, p)$$

Theorem 8. *Let the bounds on* $\mathrm{PRep}(k, q)$ *given in Shu, Wang, and Li (2026) be denoted by*

$$PRep_{LB} \leq \mathrm{PRep}(k, q) \leq PRep_{UB}.$$

By treating Z *as a partial mediator, we can derive a new upper bound on* $\mathrm{PRep}(k, q)$ *as follows:*

$$\min \left\{ \begin{array}{c} PRep_{UB}, \\ \\ \textit{For } j \in \{1, ..., k\} : \\ \displaystyle\sum_{\substack{z_1, \ldots, z_k \\ \in \{1, \ldots, n\}^k}} \Big[\min_j \{ P(y_j \mid x_j, z_j) \} \times \\ \times \min_j \{ P(z_{j_{x_j}}) \} \Big] \end{array} \right\} \\ \geq \mathrm{PRep}(k, q)$$

Theorem 9. *Given* $p \neq j$ *for* $1 \leq j \leq k$*. Let the bounds on* $\mathrm{PN}(k, p, q)$ *given in Shu, Wang, and Li (2026) be denoted by*

$$PN_{LB} \leq \mathrm{PN}(k, p, q) \leq PN_{UB}.$$

By treating Z *as a partial mediator, we can derive a new upper bound on* $\mathrm{PN}(k, p, q)$ *as follows:*

$$\min \left\{ \begin{array}{c} PN_{UB}, \\ \\ \textit{For } j \in \{1, ..., k\} : \\ \displaystyle\sum_{\substack{z_1, \ldots, z_k, z_p \\ \in \{1, \ldots, n\}^{k+1}}} \left[\min_j \left\{ \begin{array}{c} P(y_j \mid x_j, z_j), \\ P(y_q \mid x_p, z_p) \end{array} \right\} \times \right. \\ \left. \times \min_j \{ P(z_{j_{x_j}}), P(z_{p_{x_p}}), P(x_p) \} \right] \end{array} \right\} \\ \geq \mathrm{PN}(k, p, q)$$

Pure Mediator In Figure 2(b), X has no direct effect on Y and affects Y only through the mediator Z. The lower bound remains unchanged from that of Shu, Wang, and Li (2026), while the upper bound includes an additional term using observational quantities involving Z.

Theorem 10. *Let the bounds on* $\mathrm{PNS}(k)$ *given in Shu, Wang, and Li (2026) be denoted by*

$$PNS_{LB} \leq \mathrm{PNS}(k) \leq PNS_{UB}.$$

By treating Z as a pure mediator, we can derive a new upper bound on $\mathrm{PNS}(k)$ *as follows:*

$$\min\left\{\begin{array}{c} PNS_{UB}, \\ \\ \textit{For } j \in \{1,...,k\}: \\ \sum\limits_{\substack{z_1\neq\ldots\neq z_k \\ \in\{1,\ldots,n\}^k}} \Big[\min\limits_j\{P(y_j \mid z_j)\}\times \\ \times\min\limits_j\{P(z_j \mid x_j)\}\Big] \end{array}\right\} \geq \mathrm{PNS}(k)$$

Theorem 11. *Given $p \neq j$ for $1 \leq j \leq k$. Let the bounds on* $\mathrm{PSub}(k,p)$ *given in Shu, Wang, and Li (2026) be denoted by*

$$PSub_{LB} \leq \mathrm{PSub}(k,p) \leq PSub_{UB}.$$

By treating Z as a pure mediator, we can derive a new upper bound on $\mathrm{PSub}(k,p)$ *as follows:*

$$\min\left\{\begin{array}{c} PSub_{UB}, \\ \\ \textit{For } j \in \{1,...,k\}: \\ \sum\limits_{\substack{z_1\neq\ldots\neq z_k \\ \in\{1,\ldots,n\}^k}} \Big[\min\limits_j\{P(y_j \mid z_j)\}\times \\ \times\min\limits_j\{P(z_j \mid x_j)\}\Big] \times P(x_p) \end{array}\right\} \geq \mathrm{PSub}(k,p)$$

Theorem 12. *Let the bounds on* $\mathrm{PRep}(k,q)$ *given in Shu, Wang, and Li (2026) be denoted by*

$$PRep_{LB} \leq \mathrm{PRep}(k,q) \leq PRep_{UB}.$$

By treating Z as a pure mediator, we can derive a new upper bound on $\mathrm{PRep}(k,q)$ *as follows:*

$$\min\left\{\begin{array}{c} PRep_{UB}, \\ \\ \textit{For } j \in \{1,...,k\}: \\ \sum\limits_{\substack{z_1\neq\ldots\neq z_k \\ \in\{1,\ldots,n\}^k}} \Big[\min\limits_j\{P(y_j \mid z_j)\}\times \\ \times\min_j\{P(z_j \mid x_j)\}\Big] \end{array}\right\} \geq \mathrm{PRep}(k,q)$$

Theorem 13. *Given $p \neq j$ for $1 \leq j \leq k$. Let the bounds on* $\mathrm{PN}(k,p,q)$ *given in Shu, Wang, and Li (2026) be denoted by*

$$PN_{LB} \leq \mathrm{PN}(k,p,q) \leq PN_{UB}.$$

By treating Z as a pure mediator, we can derive a new upper bound on $\mathrm{PN}(k,p,q)$ *as follows:*

$$\min\left\{\begin{array}{c} PN_{UB}, \\ \\ \textit{For } j \in \{1,...,k\}: \\ \sum\limits_{\substack{z_1\neq\ldots\neq z_k\neq z_p \\ \in\{1,\ldots,n\}^{k+1}}} \Big[\min\limits_j\{P(y_j \mid z_j), P(y_q \mid z_p)\}\times \\ \times\min\limits_j\{P(z_j \mid x_j), P(z_p \mid x_p)\}\Big] \times P(x_p) \end{array}\right\} \geq \mathrm{PN}(k,p,q)$$

Examples

In this section, for simplicity, we illustrate only the proposed PNS bounds under different causal structures and focus on three-dimensional cases.

Returning to the motivating example introduced in the Introduction, consider the pharmaceutical company that has developed a new drug claimed to help prevent diabetes. To illustrate the proposed bounds under different causal structures, we construct synthetic studies based on this setting.

Let X denote how frequently an individual takes the drug, where x_1 indicates that the person takes the drug regularly and on time, x_2 indicates the person takes the drug occasionally, and x_3 indicates the person never takes the drug. Let Y denote the individual's diabetes status,where y_1, y_2, and y_3 correspond to the person not developing diabetes, developing prediabetes, and developing diabetes, respectively. The target quantity is $\mathrm{PNS}(3) = P\left(y_{1x_1}, y_{2x_2}, y_{3x_3}\right)$, which represents the proportion of individuals who would not develop diabetes if they took the drug regularly and on time, would develop prediabetes if they took it occasionally, and would develop diabetes if they never took it. This target quantity is chosen solely for ease of presentation; any joint counterfactual probability can be analyzed in the same manner using the proposed framework.

Family History as a Covariate

We now incorporate family history as an observed covariate in the diabetes example. Let Z denote an individual's family history of diabetes, where z_1, z_2, and z_3 correspond to no known family history of diabetes, diabetes only in a second-degree relative, and diabetes in a first-degree relative, respectively. Individuals with a family history of diabetes may be more likely to develop the disease and may also be more likely to take preventive medication regularly, giving $Z \to Y$ and $Z \to X$. The corresponding causal structure is shown in Figure 1(b). In this setting, Z also satisfies the back-door criterion. Therefore, in Theorem 2, all terms requiring experimental data can be replaced by their corresponding expressions based on observational data, yielding a modified version of the theorem that requires only observational data. The modified theorem is provided in the appendix.

To illustrate the calculation, we construct a synthetic study of 900 individuals. The sample was divided into three strata according to the levels of Z. The results are shown in Table 1.

Since Z also satisfies back-door criterion, for $j \in \{1,2,3\}$, we can compute $P(y_{j_{x_j}}) = \sum_z P(y_j \mid x_j, z) \times P(z)$. So we can derive $P(y_{1_{x_1}}) = 190/300, P(y_{2_{x_2}}) = 166/300, P(y_{3_{x_3}}) = 168/300$.

The company emphasizes that the three interventional probabilities appearing in the target probability of causation, $P(y_{1_{x_1}})$, $P(y_{2_{x_2}})$, and $P(y_{3_{x_3}})$, are all greater than 0.5. Based on these marginal probabilities, the company claims that the drug is effective.

Applying the bounds on $\mathrm{PNS}(3)$ derived by Shu, Wang, and Li (2026) gives

$$0 \leq \mathrm{PNS}(3) \leq 0.551.$$

This interval is too wide to determine whether the drug produces the target response pattern.

$Z = z_1$: No known family history			
$Y \backslash X$	Regular use	Occasional use	No use
Diabetes-free	46	4	54
Prediabetes	12	112	120
Diabetes	2	4	6

$Z = z_2$: Second-degree family history only			
$Y \backslash X$	Regular use	Occasional use	No use
Diabetes-free	3	3	2
Prediabetes	75	25	2
Diabetes	12	2	56

$Z = z_3$: First-degree family history			
$Y \backslash X$	Regular use	Occasional use	No use
Diabetes-free	192	44	4
Prediabetes	24	2	2
Diabetes	24	14	54

Table 1: Results of a drug study stratified by family history.

$Z = z_1$: normal blood glucose			
$Y \backslash X$	Regular use	Occasional use	No use
Diabetes-free	448	304	16
Prediabetes	364	247	13
Diabetes	28	19	1

$Z = z_2$: prediabetic blood glucose			
$Y \backslash X$	Regular use	Occasional use	No use
Diabetes-free	2	16	14
Prediabetes	27	216	189
Diabetes	1	8	7

$Z = z_3$: diabetic blood glucose			
$Y \backslash X$	Regular use	Occasional use	No use
Diabetes-free	6	18	132
Prediabetes	3	9	66
Diabetes	21	63	462

Table 2: Results of a drug study with blood glucose status.

By additionally incorporating information about family history, we obtain the tighter bounds (the detailed derivation is provided in the appendix):

$$0 \leq \text{PNS}(3) \leq 0.033.$$

The substantially smaller upper bound indicates that at most 3.3% of the population would exhibit the target response pattern. Thus, the company's marginal comparisons provide limited evidence that the drug has the claimed effect.

Blood glucose as a pure mediator

As in the previous example, let X and Y denote how frequently an individual takes the drug and the individual's diabetes status, respectively. A new investigation finds that the drug may affect an individual's blood glucose level and thereby help prevent the individual from developing diabetes. Accordingly, Let Z denote the individual's intermediate blood glucose status measured after treatment but before the final diabetes assessment, where z_1, z_2, and z_3 correspond to normal, prediabetic, and diabetic blood glucose levels, respectively. This setting corresponds to the causal structure shown in Figure 2(b).

To illustrate the calculation under the pure-mediator structure, we construct a synthetic study of $2{,}700$ individuals. The synthetic observations are grouped according to the three levels of Z, as shown in Table 2.

Applying the bounds on $\text{PNS}(3)$ given by Shu, Wang, and Li (2026), we obtain

$$0 \leq \text{PNS}(3) \leq 0.507.$$

This interval is too wide to provide informative conclusions about the target response pattern.

By additionally incorporating information on blood glucose, we obtain the following tighter upper bound using Thm. 10 (details are provided in the appendix):

$$0 \leq \text{PNS}(3) \ \leq 0.151.$$

The substantially smaller mediator-improved upper bound provides a substantially more informative characterization of the target response pattern.

Simulated Results

In this section, we empirically demonstrate that the proposed bounds, which incorporate information from the corresponding causal graphs, are tighter than the bounds derived by Shu, Wang, and Li (2026). In the figures and tables that follow, "Shu et al." refers to the bounds derived in that work. For simplicity, we focus on PNS to provide a clear visual illustration of the improvement achieved in practice.

To illustrate the improvement for individual instances, we consider representative settings with $n, k \in \{3, 4, 5\}$, chosen for ease of presentation. For each setting, we generate $100{,}000$ sample distributions compatible with the causal diagrams shown in Figures 1(a), 2(a), and 2(b), corresponding to Theorems 2, 6, and 10, respectively, and compute the

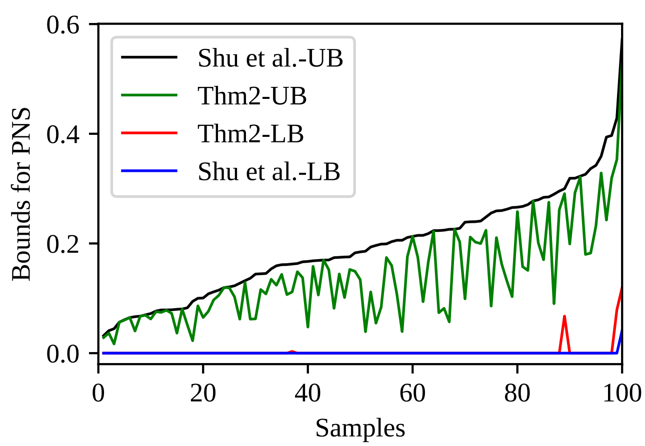


Figure 3: $\text{PNS}(3)$ bounds under the non-descendant structure shown in Fig. 1(a).

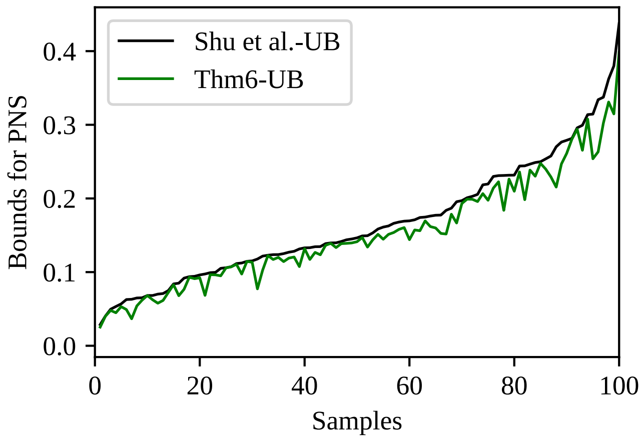


Figure 4: $\mathrm{PNS}(3)$ bounds under the partial mediator structure shown in Fig. 2(a).

bounds using both methods. For sample i, let $[a_i, b_i]$ denote the bounds obtained from our theorem and $[c_i, d_i]$ those obtained from Shu, Wang, and Li (2026). For each causal diagram, we summarize the following quantities:

- Average improvement in the lower bound: $\frac{\sum(a_i - c_i)}{100{,}000}$.
- Average improvement in the upper bound: $\frac{\sum(d_i - b_i)}{100{,}000}$.
- Average width of Shu et al. PNS bounds: $\frac{\sum(d_i - c_i)}{100{,}000}$.
- Average width of the Theorems 2, 6, and 10: $\frac{\sum(b_i - a_i)}{100{,}000}$.
- Count of sample distributions benefiting from tighter bounds: $\sum f_i$, where $f_i = 1$ if $a_i > c_i$ or $b_i < d_i$, and $f_i = 0$ otherwise.

Table 3 reports these summary statistics across different theorems and dimensions. The partial-mediator structure yields only a small improvement because, as the dimension increases, the proposed bound is tighter than the existing

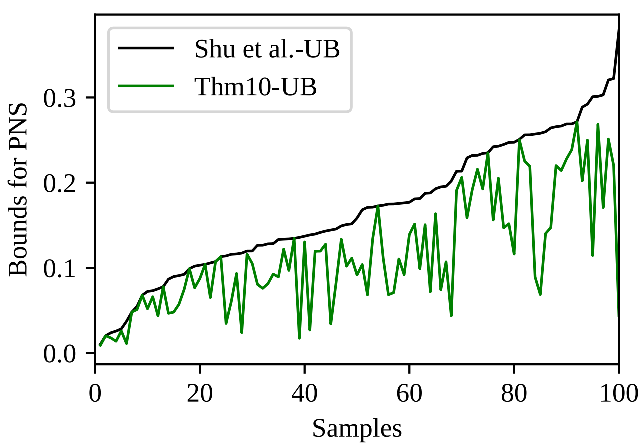


Figure 5: $\mathrm{PNS}(3)$ bounds under the pure mediator structure shown in Fig. 2(b).

	Avg. LB gain	Avg. UB gain	Shu et al. width	Thms width	Improved (%)
		$n = k = 3$			
Non-desc.	0.0014	0.0532	0.1953	0.1407	89.08%
Part. med.	0	6.52e-06	0.2038	0.2038	0.04%
Pure med.	0	0.0583	0.1776	0.1193	83.66%
		$n = k = 4$			
Non-desc.	3.78e-07	0.0577	0.1346	0.0769	98.44%
Part. med.	0	0	0.1406	0.1406	0%
Pure med.	0	0.0137	0.1245	0.1108	36.58%
		$n = k = 5$			
Non-desc.	0	0.0557	0.1033	0.0477	99.85%
Part. med.	0	0	0.1082	0.1082	0%
Pure med.	0	0.0003	0.0973	0.0970	1.26%

Table 3: Performance metrics for Theorems 2 (Non-desc.), 6 (Part. med.), and 10 (Pure med.). Here, LB and UB denote the lower and upper bounds, respectively.

bound in fewer and fewer simulation draws:

$$\begin{aligned}
n = 2,\ k = 2 :&\quad 8.2\% \text{ of the bounds are tightened,}\\
n = 3,\ k = 2 :&\quad 1.97\% \text{ of the bounds are tightened,}\\
n = 3,\ k = 3 :&\quad 0.035\% \text{ of the bounds are tightened,}\\
n = 4,\ k = 4 :&\quad 0 \text{ bounds are tightened in 20M draws.}
\end{aligned}$$

Thus, although the partial-mediator bound remains theoretically valid in higher-dimensional settings, it becomes increasingly unlikely to improve the existing bound in our simulations. Among the causal structures considered, the non-descendant covariate structure provides the most substantial tightening as the dimension increases.

In Figures 3 and 5, we randomly select 100 of the 100,000 sample distributions, plot the bounds obtained with and without incorporating causal graph information, and order the samples according to the upper bounds on $\mathrm{PNS}(3)$ given by Shu, Wang, and Li (2026). For Figure 4, because Table 3 shows that Theorem 6 yields narrower bounds less frequently, we continue generating samples until obtaining 100,000 instances for which the bounds are narrowed and then randomly select 100 of them for visualization.

Conclusion

In this paper, we extend bounds on probabilities of causation (PoCs) that incorporate causal graph information from binary to multivalued settings. Specifically, we derive new bounds under additional causal graph information for the four representative PoCs, PNS, PSub, PRep, and PN, which together could represent any discrete PoC. We consider several causal graph structures, including non-descendant covariates, backdoor adjustment sets, partial mediators, and pure mediators. Toy examples and simulation studies validate the proposed theorems and demonstrate that incorporating causal graph information consistently yields tighter bounds than approaches based solely on experimental and observational distributions.

References

Balke, A. A. 1995. *Probabilistic counterfactuals: semantics, computation, and applications*. University of California, Los Angeles.

Dawid, A. P.; Musio, M.; and Murtas, R. 2017. The probability of causation. *Law, Probability and Risk*, 16(4): 163–179.

Galles, D.; and Pearl, J. 1998. An axiomatic characterization of causal counterfactuals. *Foundations of Science*, 3(1): 151–182.

Halpern, J. Y. 2000. Axiomatizing causal reasoning. *Journal of Artificial Intelligence Research*, 12: 317–337.

Kuroki, M.; and Cai, Z. 2011. Statistical Analysis of 'Probabilities of Causation' Using Co-variate Information. *Scandinavian Journal of Statistics*, 38(3): 564–577.

Li, A.; and Pearl, J. 2019. Unit selection based on counterfactual logic. In *Proceedings of the twenty-eighth international joint conference on artificial intelligence*.

Li, A.; and Pearl, J. 2022a. Bounds on causal effects and application to high dimensional data. In *Proceedings of the AAAI conference on artificial intelligence*, volume 36, 5773–5780.

Li, A.; and Pearl, J. 2022b. Unit selection with causal diagram. In *Proceedings of the AAAI conference on artificial intelligence*, volume 36, 5765–5772.

Li, A.; and Pearl, J. 2024. Probabilities of causation with nonbinary treatment and effect. In *Proceedings of the AAAI conference on artificial intelligence*, volume 38, 20465–20472.

Mueller, S.; Li, A.; and Pearl, J. 2021. Causes of Effects: Learning individual responses from population data. arXiv:2104.13730.

Pearl, J. 1993. Aspects of Graphical Models Connected With Causality. *Proceedings of the 49th Session of the International Statistical Institute, Italy*, 399–401.

Pearl, J. 1995. Causal Diagrams for Empirical Research. *Biometrika*, 669–688.

Pearl, J. 1999. Probabilities Of Causation: Three Counterfactual Interpretations And Their Identification. *Synthese*, 121(1-2): 93.

Shu, X.; Wang, S.; and Li, A. 2026. Identification of Probabilities of Causation: from Recursive to Closed-Form Bounds. arXiv:2505.15274.

Tian, J.; and Pearl, J. 2000. Probabilities of causation: Bounds and identification. *Annals of Mathematics and Artificial Intelligence*, 28(1): 287–313.

Zhang, J.; Tian, J.; and Bareinboim, E. 2022. Partial counterfactual identification from observational and experimental data. In *International conference on machine learning*, 26548–26558. PMLR.

Technical appendices and supplementary material

Theorem proofs

Proof of Theorem 2

Proof.

$$\begin{aligned} PNS(k) &= P(y_{1_{x_1}}, ..., y_{k_{x_k}}) \\ &= \sum_z P(y_{1_{x_1}}, ..., y_{k_{x_k}} \mid z) \times P(z) \end{aligned} \quad (1)$$

First, we need to prove:

$$\max \left\{ \begin{array}{c} 0, \\ \\ \sum_{j=1}^{k} P(y_{j_{x_j}} \mid z) - k + 1, \\ \\ \text{For } i \in \{1, ..., k\} : \\ \sum_{\substack{1 \le j \le k \\ j \ne i}} \Big[P(y_{j_{x_j}} \mid z) + P(x_j \mid z) - \\ -P(x_j, y_j \mid z) \Big] + P(x_i, y_i \mid z) - k + 1 \end{array} \right\} \le P(y_{1_{x_1}}, ..., y_{k_{x_k}} \mid z)$$

$$\min \left\{ \begin{array}{c} \sum_{j=1}^{k} P(x_j, y_j \mid z) + \sum_{j=k+1}^{n} P(x_j \mid z), \\ \\ \text{For } j \in \{1, ..., k\} : \\ P(y_{j_{x_j}} \mid z), \\ \\ \text{For } m \in \{1, ..., k-1\}, \\ t_j \in \{1, ..., k\} : \\ \frac{1}{m} \Big[\sum_{j=0}^{m} P(y_{t_{j_{x_{t_j}}}} \mid z) - P(x_{t_j}, y_{t_j} \mid z) \Big] \end{array} \right\} \ge P(y_{1_{x_1}}, ..., y_{k_{x_k}} \mid z)$$

By the Fréchet Inequalities, for any z with $P(z) > 0$, we have

$$\begin{aligned} & P(y_{1_{x_1}}, ..., y_{k_{x_k}} \mid z) \\ & \ge \max \left\{ 0, \sum_{j=1}^{k} P(y_{j_{x_j}} \mid z) - k + 1 \right\} \\ & P(y_{1_{x_1}}, ..., y_{k_{x_k}} \mid z) \le \min_{1 \le j \le k} \left\{ P(y_{j_{x_j}} \mid z) \right\} \end{aligned}$$

The equality of the first lower bound holds when $\exists j \in [1, k]$, that $P(y_{j_{x_j}} \mid z) = 0$.

The equality of the second lower bound holds when $\exists i \in [1, k]$, $P(y_{j_{x_j}} \mid z) = 1$ for $\forall j \in [1, k], j \ne i$.

The equality of the second upper bound holds when $\exists j \in [1, k]$, $P(y_{i_{x_i}} \mid z) = 1$ for $\forall i \in [1, k]$, $i \ne j$.

Also,

$$\begin{aligned} & P(y_{1_{x_1}}, ..., y_{k_{x_k}} \mid z) \\ = & \sum_{j=1}^{n} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j \mid z) \\ \ge & \sum_{j=1}^{k} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j \mid z) \end{aligned}$$

here, the equal sign holds when $\forall x_j = 0$ for $j \in [k+1, n]$.

For $\forall i$, s.t., $i \in \{1, ..., k\}$,

$$\begin{aligned} & \sum_{j=1}^{k} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j \mid z) \\ \ge & P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_i \mid z) \end{aligned}$$

here, the equal sign holds when $\forall x_j = 0$ for $j \in [1, k]$ and $j \ne i$.

Thus, we have

$$\begin{aligned} & P(y_{1_{x_1}}, ..., y_{k_{x_k}} \mid z) \\ \ge & P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_i \mid z) \\ = & P(y_{1_{x_1}}, ..., y_{i-1_{x_{i-1}}}, y_{i+1_{x_{i+1}}}, ..., y_{k_{x_k}}, x_i, y_i \mid z) \\ = & P(y_{1_{x_1}}, ..., y_{i-1_{x_{i-1}}}, y_{i+1_{x_{i+1}}}, ..., y_{k_{x_k}}, x_i, y_i \mid z) \\ & + \sum_{j=1}^{n} P(x_j \mid z) - 1 \\ & + \sum_{j=1}^{n} \sum_{q=1}^{n} P(y_{1_{x_1}}, ..., y_{i-1_{x_{i-1}}}, y_{i+1_{x_{i+1}}}, ..., y_{k_{x_k}}, \\ & x_j, y_q \mid z) \\ & - \sum_{j=1}^{n} \sum_{q=1}^{n} P(y_{1_{x_1}}, ..., y_{i-1_{x_{i-1}}}, y_{i+1_{x_{i+1}}}, ..., y_{k_{x_k}}, \\ & x_j, y_q \mid z) \\ = & P(y_{1_{x_1}}, ..., y_{i-1_{x_{i-1}}}, y_{i+1_{x_{i+1}}}, ..., y_{k_{x_k}}, x_i, y_i \mid z) \\ & + \sum_{\substack{1 \le j \le k \\ j \ne i}} P(x_j \mid z) + P(x_i \mid z) + \sum_{j=k+1}^{n} P(x_j \mid z) \\ & -1 + P(y_{1_{x_1}}, ..., y_{i-1_{x_{i-1}}}, y_{i+1_{x_{i+1}}}, ..., y_{k_{x_k}} \mid z) \\ & - \sum_{\substack{1 \le j \le k \\ j \ne i}} P(y_{1_{x_1}}, ..., y_{i-1_{x_{i-1}}}, y_{i+1_{x_{i+1}}}, ..., y_{k_{x_k}}, \\ & x_j, y_j \mid z) \\ & - \sum_{q=1}^{n} P(y_{1_{x_1}}, ..., y_{i-1_{x_{i-1}}}, y_{i+1_{x_{i+1}}}, ..., y_{k_{x_k}}, x_i, \\ & y_q \mid z) \end{aligned}$$

$$
\begin{aligned}
& - \sum_{j=k+1}^{n} \sum_{q=1}^{n} P(y_{1_{x_1}}, ..., y_{i-1_{x_{i-1}}}, y_{i+1_{x_{i+1}}}, ..., \\
& y_{k_{x_k}}, x_j, y_q \mid z) \\
= \; & P(y_{1_{x_1}}, ..., y_{i-1_{x_{i-1}}}, y_{i+1_{x_{i+1}}}, ..., y_{k_{x_k}} \mid z) - 1 \\
& + \sum_{\substack{1 \leq j \leq k \\ j \neq i}} P(x_j \mid z) \\
& - \sum_{\substack{1 \leq j \leq k \\ j \neq i}} P(y_{1_{x_1}}, ..., y_{i-1_{x_{i-1}}}, y_{i+1_{x_{i+1}}}, ..., y_{k_{x_k}}, \\
& x_j, y_j \mid z) \\
& + P(x_i \mid z) \\
& - \sum_{q=1}^{n} P(y_{1_{x_1}}, ..., y_{i-1_{x_{i-1}}}, y_{i+1_{x_{i+1}}}, ..., y_{k_{x_k}}, \\
& x_i, y_q \mid z) \\
& + P(y_{1_{x_1}}, ..., y_{i-1_{x_{i-1}}}, y_{i+1_{x_{i+1}}}, ..., y_{k_{x_k}}, x_i, \\
& y_i \mid z) \\
& + \sum_{j=k+1}^{n} P(x_j \mid z) \\
& - \sum_{j=k+1}^{n} \sum_{q=1}^{n} P(y_{1_{x_1}}, ..., y_{i-1_{x_{i-1}}}, y_{i+1_{x_{i+1}}}, ..., \\
& y_{k_{x_k}}, x_j, y_q \mid z) \\
= \; & P(y_{1_{x_1}}, ..., y_{i-1_{x_{i-1}}}, y_{i+1_{x_{i+1}}}, ..., y_{k_{x_k}} \mid z) - 1 \\
& + \sum_{\substack{1 \leq j \leq k \\ j \neq i}} P(x_j \mid z) \\
& - \sum_{\substack{1 \leq j \leq k \\ j \neq i}} P(y_{1_{x_1}}, ..., y_{i-1_{x_{i-1}}}, y_{i+1_{x_{i+1}}}, ..., y_{k_{x_k}}, \\
& x_j, y_j \mid z) \\
& + P(x_i \mid z) \\
& - \sum_{\substack{1 \leq q \leq n \\ q \neq i}} P(y_{1_{x_1}}, ..., y_{i-1_{x_{i-1}}}, y_{i+1_{x_{i+1}}}, ..., y_{k_{x_k}}, \\
& x_i, y_q \mid z) \\
& + \sum_{j=k+1}^{n} P(x_j \mid z) \\
& - \sum_{j=k+1}^{n} P(y_{1_{x_1}}, ..., y_{i-1_{x_{i-1}}}, y_{i+1_{x_{i+1}}}, ..., y_{k_{x_k}}, \\
& x_j \mid z)
\end{aligned}
$$

By applying the Frechet inequalities, for any z with $P(z) > 0$, we have

$$
\begin{aligned}
& P(y_{1_{x_1}}, ..., y_{k_{x_k}} \mid z) \\
\geq \; & \sum_{\substack{1 \leq j \leq k \\ i \neq j}} P(y_{j_{x_j}} \mid z) - (k-2) - 1 \\
& + \sum_{\substack{1 \leq j \leq k \\ j \neq i}} P(x_j \mid z) - \sum_{\substack{1 \leq j \leq k \\ j \neq i}} P(x_j, y_j \mid z) \\
& + P(x_i \mid z) - \sum_{\substack{1 \leq q \leq n \\ q \neq i}} P(x_i, y_q \mid z) \\
& + \sum_{j=k+1}^{n} P(x_j \mid z) - \sum_{j=k+1}^{n} P(x_j \mid z)
\end{aligned}
$$

here, the equal sign holds when $\exists i \in [1, k]$, and $P(y_{j_{x_j}} \mid z) = 1$ for $\forall j \in [1, k], j \neq i$.

$$
\begin{aligned}
= \; & \sum_{\substack{1 \leq j \leq k \\ i \neq j}} \Big[P(y_{j_{x_j}} \mid z) + P(x_j \mid z) - P(x_j, y_j \mid z) \Big] \\
& + P(x_i, y_i \mid z) - k + 1
\end{aligned}
$$

To proof the first upper bound,

$$
\begin{aligned}
& P(y_{1_{x_1}}, ..., y_{k_{x_k}} \mid z) \\
= \; & \sum_{j=1}^{n} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j \mid z) \\
= \; & \sum_{j=1}^{k} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j \mid z) \\
& + \sum_{j=k+1}^{n} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j \mid z) \\
\leq \; & \sum_{j=1}^{k} P(x_j, y_j \mid z) + \sum_{j=k+1}^{n} P(x_j \mid z)
\end{aligned}
$$

The equality of the first upper bound holds when $P(y_{j_{x_j}} \mid z) = 1$ for $\forall j \in [1, k]$.

To proof the remaining upper bound, for $m \in \{1, ..., k-1\}$, $t_j \in \{1, ..., k\}$, we can first write

$$
\begin{aligned}
& P(y_{1_{x_1}}, ..., y_{k_{x_k}} \mid z) \\
= \; & \sum_{j=1}^{n} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j \mid z) \\
= \; & \frac{1}{m} \times \left[(m) \sum_{j=1}^{n} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j \mid z) \right] \qquad (2)
\end{aligned}
$$

For $m = 1$,

$$\begin{aligned}
&\frac{1}{m}\left[\sum_{j=0}^{m} P(y_{t_j\, x_{t_j}} \mid z) - P(x_{t_j}, y_{t_j} \mid z)\right] \\
= &\sum_{j=0}^{1} P(y_{t_j\, x_{t_j}} \mid z) - P(x_{t_j}, y_{t_j} \mid z) \\
= &P(y_{t_0\, x_{t_0}} \mid z) + P(y_{t_1\, x_{t_1}} \mid z) - P(x_{t_0}, y_{t_0} \mid z) \\
&-P(x_{t_1}, y_{t_1} \mid z)
\end{aligned}$$

W.L.O.G., let $1 \le t_0 < t_1 \le k$:

$$\begin{aligned}
&P(y_{1_{x_1}}, ..., y_{k_{x_k}} \mid z) \\
= &\sum_{j=1}^{n} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j \mid z) \\
= &\sum_{j=1}^{k} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j \mid z) \\
&+ \sum_{j=k+1}^{n} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j \mid z) \\
\le &\sum_{j=1}^{t_0} P(y_{t_0\, x_{t_0}}, x_j, y_{j+t_1-t_0\, x_{j+t_1-t_0}} \mid z) \\
&+ \sum_{j=t_0+1}^{k-t_1+t_0} P(y_{t_0\, x_{t_0}}, x_j, y_{j+t_1-t_0\, x_{j+t_1-t_0}} \mid z) \\
&+ \sum_{j=1}^{t_1-t_0} P(y_{t_0\, x_{t_0}}, x_{k-t_1+t_0+j}, y_{j\, x_j} \mid z) \\
&+ \sum_{j=k+1}^{n} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j \mid z)
\end{aligned}$$

here, the equal sign holds when $\exists 1 \le t_0 < t_1 \le k$, and $P(y_{i_{x_i}} \mid z) = 1$ for $\forall i \in [1, k], i \ne t_0$, $i \ne j + t_1 - t_0$ for $j \in [1, k - t_1 + t_0]$.

$$\begin{aligned}
= &\sum_{j=1}^{t_0} P(y_{t_0\, x_{t_0}}, x_j, y_{j+t_1-t_0\, x_{j+t_1-t_0}} \mid z) \\
&+ \sum_{j=t_0+1}^{k-t_1+t_0} P(y_{t_0\, x_{t_0}}, x_j, y_{j+t_1-t_0\, x_{j+t_1-t_0}} \mid z) \\
&+ \sum_{j=1}^{t_1-t_0} P(y_{t_0\, x_{t_0}}, x_{k-t_1+t_0+j}, y_{j\, x_j} \mid z) \\
&+ \sum_{j=k+1}^{n} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j \mid z) \\
&+P(y_{t_0\, x_{t_0}} \mid z) + P(y_{t_1\, x_{t_1}} \mid z) - P(x_{t_0}, y_{t_0} \mid z) \\
&-P(x_{t_1}, y_{t_1} \mid z) \\
&- \sum_{\substack{\{i_1,...,i_{t_0-1}, i_{t_0+1},...,i_{k+2}\} \\ \in \{1,...,n\}^{k+1}}} P(y_{i_1\, x_1}, ..., y_{i_{t_0-1}\, x_{t_0-1}}, \\
&y_{t_0\, x_{t_0}}, y_{i_{t_0+1}\, x_{t_0+1}}, ..., y_{i_k\, x_k}, x_{i_{k+1}}, y_{i_{k+2}} \mid z) \\
&- \sum_{\substack{\{i_1,...,i_{t_1-1}, i_{t_1+1},...,i_{k+2}\} \\ \in \{1,...,n\}^{k+1}}} P(y_{i_1\, x_1}, ..., y_{i_{t_1-1}\, x_{t_1-1}}, \\
&y_{t_1\, x_{t_1}}, y_{i_{t_1+1}\, x_{t_1+1}}, ..., y_{i_k\, x_k}, x_{i_{k+1}}, y_{i_{k+2}} \mid z) \\
&+ \sum_{\substack{\{i_1,...,i_{t_0-1}, i_{t_0+1},...,i_k\} \\ \in \{1,...,n\}^{k-1}}} P(y_{i_1\, x_1}, ..., y_{i_{t_0-1}\, x_{t_0-1}}, \\
&y_{t_0\, x_{t_0}}, y_{i_{t_0+1}\, x_{t_0+1}}, ..., y_{i_k\, x_k}, x_{t_0}, y_{t_0} \mid z) \\
&+ \sum_{\substack{\{i_1,...,i_{t_1-1}, i_{t_1+1},...,i_k\} \\ \in \{1,...,n\}^{k-1}}} P(y_{i_1\, x_1}, ..., y_{i_{t_1-1}\, x_{t_1-1}}, \\
&y_{t_1\, x_{t_1}}, y_{i_{t_1+1}\, x_{t_1+1}}, ..., y_{i_k\, x_k}, x_{t_1}, y_{t_1} \mid z) \\
= &P(y_{t_0\, x_{t_0}} \mid z) + P(y_{t_1\, x_{t_1}} \mid z) - P(x_{t_0}, y_{t_0} \mid z) \\
&-P(x_{t_1}, y_{t_1} \mid z) \\
&+ \sum_{j=1}^{t_0-1} P(y_{t_0\, x_{t_0}}, x_j, y_{j+t_1-t_0\, x_{j+t_1-t_0}} \mid z) \\
&+P(y_{t_0\, x_{t_0}}, x_{t_0}, y_{t_1\, x_{t_1}} \mid z) \\
&+ \sum_{j=t_0+1}^{k-t_1+t_0} P(y_{t_0\, x_{t_0}}, x_j, y_{j+t_1-t_0\, x_{j+t_1-t_0}} \mid z) \\
&+ \sum_{j=1}^{t_1-t_0} P(y_{t_0\, x_{t_0}}, x_{k-t_1+t_0+j}, y_{j\, x_j} \mid z) \\
&+ \sum_{j=k+1}^{n} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j \mid z) \\
&- \sum_{\substack{\{i_1,...,i_{t_0-1}, i_{t_0+1},...,i_{k+2}\} \\ \in \{1,...,n\}^{k+1}}} P(y_{i_1\, x_1}, ..., y_{i_{t_0-1}\, x_{t_0-1}}, \\
&y_{t_0\, x_{t_0}}, y_{i_{t_0+1}\, x_{t_0+1}}, ..., y_{i_k\, x_k}, x_{i_{k+1}}, y_{i_{k+2}} \mid z) \\
&- \sum_{\substack{\{i_1,...,i_{t_1-1}, i_{t_1+1},...,i_{k+2}\} \\ \in \{1,...,n\}^{k+1}}} P(y_{i_1\, x_1}, ..., y_{i_{t_1-1}\, x_{t_1-1}}, \\
&y_{t_1\, x_{t_1}}, y_{i_{t_1+1}\, x_{t_1+1}}, ..., y_{i_k\, x_k}, x_{i_{k+1}}, y_{i_{k+2}} \mid z) \\
&+ \sum_{\substack{\{i_1,...,i_{t_0-1}, i_{t_0+1},...,i_k\} \\ \in \{1,...,n\}^{k-1}}} P(y_{i_1\, x_1}, ..., y_{i_{t_0-1}\, x_{t_0-1}}, \\
&y_{t_0\, x_{t_0}}, y_{i_{t_0+1}\, x_{t_0+1}}, ..., y_{i_k\, x_k}, x_{t_0}, y_{t_0} \mid z) \\
&+ \sum_{\substack{\{i_1,...,i_{t_1-1}, i_{t_1+1},...,i_k\} \\ \in \{1,...,n\}^{k-1}}} P(y_{i_1\, x_1}, ..., y_{i_{t_1-1}\, x_{t_1-1}}, \\
&y_{t_1\, x_{t_1}}, y_{i_{t_1+1}\, x_{t_1+1}}, ..., y_{i_k\, x_k}, x_{t_1}, y_{t_1} \mid z)
\end{aligned}$$

$$
\begin{aligned}
&= P(y_{t_0 x_{t_0}} \mid z) + P(y_{t_1 x_{t_1}} \mid z) - P(x_{t_0}, y_{t_0} \mid z) \\
&\quad -P(x_{t_1}, y_{t_1} \mid z) \\
&\quad - \sum_{\substack{\{i_1,\dots,i_{t_0-1},i_{t_0+1},\dots,i_{k+2}\} \\ \in\{1,\dots,n\}^{k+1}}} P(y_{i_1 x_1}, \dots, y_{i_{t_0-1} x_{t_0-1}}, \\
&\quad y_{t_0 x_{t_0}}, y_{i_{t_0+1} x_{t_0+1}}, \dots, y_{i_k x_k}, x_{i_{k+1}}, y_{i_{k+2}} \mid z) \\
&\quad + \Bigg[\sum_{j=1}^{t_0-1} P(y_{t_0 x_{t_0}}, x_j, y_{j+t_1-t_0 \, x_{j+t_1-t_0}} \mid z) \\
&\quad + \sum_{j=t_0+1}^{k-t_1+t_0} P(y_{t_0 x_{t_0}}, x_j, y_{j+t_1-t_0 \, x_{j+t_1-t_0}} \mid z) \\
&\quad + \sum_{j=1}^{t_1-t_0} P(y_{t_0 x_{t_0}}, x_{k-t_1+t_0+j}, y_{j x_j} \mid z) \\
&\quad + \sum_{j=k+1}^{n} P(y_{1 x_1}, \dots, y_{k x_k}, x_j \mid z) \\
&\quad + \sum_{\substack{\{i_1,\dots,i_{t_0-1},i_{t_0+1},\dots,i_k\} \\ \in\{1,\dots,n\}^{k-1}}} P(y_{i_1 x_1}, \dots, y_{i_{t_0-1} x_{t_0-1}}, \\
&\quad y_{t_0 x_{t_0}}, y_{i_{t_0+1} x_{t_0+1}}, \dots, y_{i_k x_k}, x_{t_0}, y_{t_0} \mid z) \Bigg] \\
&\quad - \sum_{\substack{\{i_1,\dots,i_{t_1-1},i_{t_1+1},\dots,i_{k+2}\} \\ \in\{1,\dots,n\}^{k+1}}} P(y_{i_1 x_1}, \dots, y_{i_{t_1-1} x_{t_1-1}}, \\
&\quad y_{t_1 x_{t_1}}, y_{i_{t_1+1} x_{t_1+1}}, \dots, y_{i_k x_k}, x_{i_{k+1}}, y_{i_{k+2}} \mid z) \\
&\quad + \Bigg[P(y_{t_0 x_{t_0}}, x_{t_0}, y_{t_1 x_{t_1}} \mid z) \\
&\quad + \sum_{\substack{\{i_1,\dots,i_{t_1-1},i_{t_1+1},\dots,i_k\} \\ \in\{1,\dots,n\}^{k-1}}} P(y_{i_1 x_1}, \dots, y_{i_{t_1-1} x_{t_1-1}}, \\
&\quad y_{t_1 x_{t_1}}, y_{i_{t_1+1} x_{t_1+1}}, \dots, y_{i_k x_k}, x_{t_1}, y_{t_1} \mid z) \Bigg] \qquad (3) \\
&\le P(y_{t_0 x_{t_0}} \mid z) + P(y_{t_1 x_{t_1}} \mid z) - P(x_{t_0}, y_{t_0} \mid z) \\
&\quad -P(x_{t_1}, y_{t_1} \mid z) \qquad (4)
\end{aligned}
$$

Here, the equal sign holds when $\exists 1 \le t_0 < t_1 \le k$, and $P(y_{t_0 x_{t_0}} \mid z) = 0$.
For $m = 2$, by applying equation (2), we can get:

$$
\begin{aligned}
& P(y_{1 x_1}, \dots, y_{k x_k} \mid z) \\
&= \frac{1}{2} \times \left[2 \sum_{j=1}^{n} P(y_{1 x_1}, \dots, y_{k x_k}, x_j \mid z) \right] \\
&= \frac{1}{2} \times \Big[\sum_{j=1}^{n} P(y_{1 x_1}, \dots, y_{k x_k}, x_j \mid z) \\
&\quad + \sum_{j=1}^{n} P(y_{1 x_1}, \dots, y_{k x_k}, x_j \mid z) \Big]
\end{aligned}
$$

Then W.L.O.G., let $1 \le t_0 < t_1 < t_2 \le k$. By applying equation (3), we have

$$
\begin{aligned}
& P(y_{1 x_1}, \dots, y_{k x_k}) \\
&\le \frac{1}{2} \times \Bigg\{ \Bigg[P(y_{t_0 x_{t_0}} \mid z) + P(y_{t_1 x_{t_1}} \mid z) \\
&\quad -P(x_{t_0}, y_{t_0} \mid z) - P(x_{t_1}, y_{t_1} \mid z) \\
&\quad - \sum_{\substack{\{i_1,\dots,i_{t_0-1},i_{t_0+1},\dots,i_{k+2}\} \\ \in\{1,\dots,n\}^{k+1}}} P(y_{i_1 x_1}, \dots, y_{i_{t_0-1} x_{t_0-1}}, \\
&\quad y_{t_0 x_{t_0}}, y_{i_{t_0+1} x_{t_0+1}}, \dots, y_{i_k x_k}, x_{i_{k+1}}, y_{i_{k+2}} \mid z) \\
&\quad + \Bigg[\sum_{j=1}^{t_0-1} P(y_{t_0 x_{t_0}}, x_j, y_{j+t_1-t_0 \, x_{j+t_1-t_0}} \mid z) \\
&\quad + \sum_{j=t_0+1}^{k-t_1+t_0} P(y_{t_0 x_{t_0}}, x_j, y_{j+t_1-t_0 \, x_{j+t_1-t_0}} \mid z) \\
&\quad + \sum_{j=1}^{t_1-t_0} P(y_{t_0 x_{t_0}}, x_{k-t_1+t_0+j}, y_{j x_j} \mid z) \\
&\quad + \sum_{j=k+1}^{n} P(y_{1 x_1}, \dots, y_{k x_k}, x_j \mid z) \\
&\quad + \sum_{\substack{\{i_1,\dots,i_{t_0-1},i_{t_0+1},\dots,i_k\} \\ \in\{1,\dots,n\}^{k-1}}} P(y_{i_1 x_1}, \dots, y_{i_{t_0-1} x_{t_0-1}}, \\
&\quad y_{t_0 x_{t_0}}, y_{i_{t_0+1} x_{t_0+1}}, \dots, y_{i_k x_k}, x_{t_0}, y_{t_0} \mid z) \Bigg] \\
&\quad - \sum_{\substack{\{i_1,\dots,i_{t_1-1},i_{t_1+1},\dots,i_{k+2}\} \\ \in\{1,\dots,n\}^{k+1}}} P(y_{i_1 x_1}, \dots, y_{i_{t_1-1} x_{t_1-1}}, \\
&\quad y_{t_1 x_{t_1}}, y_{i_{t_1+1} x_{t_1+1}}, \dots, y_{i_k x_k}, x_{i_{k+1}}, y_{i_{k+2}} \mid z) \\
&\quad + \Bigg[P(y_{t_0 x_{t_0}}, x_{t_0}, y_{t_1 x_{t_1}} \mid z) \\
&\quad + \sum_{\substack{\{i_1,\dots,i_{t_1-1},i_{t_1+1},\dots,i_k\} \\ \in\{1,\dots,n\}^{k-1}}} P(y_{i_1 x_1}, \dots, y_{i_{t_1-1} x_{t_1-1}}, \\
&\quad y_{t_1 x_{t_1}}, y_{i_{t_1+1} x_{t_1+1}}, \dots, y_{i_k x_k}, x_{t_1}, y_{t_1} \mid z) \Bigg] \Bigg] \\
&\quad + \Bigg[P(y_{t_2 x_{t_2}} \mid z) - P(x_{t_2}, y_{t_2} \mid z)
\end{aligned}
$$

$$
\begin{aligned}
& - \sum_{\substack{\{i_1,\ldots,i_{t_2-1},i_{t_2+1},\ldots,i_{k+2}\}\\ \in\{1,\ldots,n\}^{k+1}}} P(y_{i_1 x_1},...,y_{i_{t_2-1} x_{t_2-1}},\\
& y_{t_2 x_{t_2}}, y_{i_{t_2+1} x_{t_2+1}},...,y_{i_k x_k}, x_{i_{k+1}}, y_{i_{k+2}} \mid z)\\
& + \sum_{\substack{\{i_1,\ldots,i_{t_2-1},i_{t_2+1},\ldots,i_k\}\\ \in\{1,\ldots,n\}^{k-1}}} P(y_{i_1 x_1},...,y_{i_{t_2-1} x_{t_2-1}},\\
& y_{t_2 x_{t_2}}, y_{i_{t_2+1} x_{t_2+1}},...,y_{i_k x_k}, x_{t_2}, y_{t_2} \mid z)\\
& + \sum_{\substack{1\le j\le k\\ j\neq t_2}} P(y_{1_{x_1}},...,y_{k_{x_k}}, x_j \mid z)\\
& + P(y_{1_{x_1}},...,y_{t_2-1_{x_{t_2+1}}}, y_{t_2 x_{t_2}}, y_{t_2+1_{x+1}},...,y_{k_{x_k}},\\
& x_{t_2}, y_{t_2} \mid z)\\
& + \sum_{j=k+1}^{n} P(y_{1_{x_1}},...,y_{k_{x_k}}, x_j \mid z)\Bigg]\Bigg\}\\
\le\ & \frac{1}{2}\times\Bigg\{\Bigg[P(y_{t_0 x_{t_0}} \mid z) + P(y_{t_1 x_{t_1}} \mid z)\\
& - P(x_{t_0}, y_{t_0} \mid z) - P(x_{t_1}, y_{t_1} \mid z)\\
& - \sum_{\substack{\{i_1,\ldots,i_{t_0-1},i_{t_0+1},\ldots,i_{k+2}\}\\ \in\{1,\ldots,n\}^{k+1}}} P(y_{i_1 x_1},...,y_{i_{t_0-1} x_{t_0-1}},\\
& y_{t_0 x_{t_0}}, y_{i_{t_0+1} x_{t_0+1}},...,y_{i_k x_k}, x_{i_{k+1}}, y_{i_{k+2}} \mid z)\\
& + \Bigg[\sum_{j=1}^{t_0-1} P(y_{t_0 x_{t_0}}, x_j, y_{j+t_1-t_0\, x_{j+t_1-t_0}} \mid z)\\
& + \sum_{j=t_0+1}^{k-t_1+t_0} P(y_{t_0 x_{t_0}}, x_j, y_{j+t_1-t_0\, x_{j+t_1-t_0}} \mid z)\\
& + \sum_{j=1}^{t_1-t_0} P(y_{t_0 x_{t_0}}, x_{k-t_1+t_0+j}, y_{j_{x_j}} \mid z)\\
& + \sum_{j=k+1}^{n} P(y_{1_{x_1}},...,y_{k_{x_k}}, x_j \mid z)\\
& + \sum_{\substack{\{i_1,\ldots,i_{t_0-1},i_{t_0+1},\ldots,i_k\}\\ \in\{1,\ldots,n\}^{k-1}}} P(y_{i_1 x_1},...,y_{i_{t_0-1} x_{t_0-1}},\\
& y_{t_0 x_{t_0}}, y_{i_{t_0+1} x_{t_0+1}},...,y_{i_k x_k}, x_{t_0}, y_{t_0} \mid z)\Bigg]\\
& - \sum_{\substack{\{i_1,\ldots,i_{t_1-1},i_{t_1+1},\ldots,i_{k+2}\}\\ \in\{1,\ldots,n\}^{k+1}}} P(y_{i_1 x_1},...,y_{i_{t_1-1} x_{t_1-1}},\\
& y_{t_1 x_{t_1}}, y_{i_{t_1+1} x_{t_1+1}},...,y_{i_k x_k}, x_{i_{k+1}}, y_{i_{k+2}} \mid z)\\
& + \Bigg[P(y_{t_0 x_{t_0}}, x_{t_0}, y_{t_1 x_{t_1}} \mid z)\\
& + \sum_{\substack{\{i_1,\ldots,i_{t_1-1},i_{t_1+1},\ldots,i_k\}\\ \in\{1,\ldots,n\}^{k-1}}} P(y_{i_1 x_1},...,y_{i_{t_1-1} x_{t_1-1}},\\
& y_{t_1 x_{t_1}}, y_{i_{t_1+1} x_{t_1+1}},...,y_{i_k x_k}, x_{t_1}, y_{t_1} \mid z)\Bigg]\Bigg]\\
& + \Bigg[P(y_{t_2 x_{t_2}} \mid z) - P(x_{t_2}, y_{t_2} \mid z)\\
& - \sum_{\substack{\{i_1,\ldots,i_{t_2-1},i_{t_2+1},\ldots,i_{k+2}\}\\ \in\{1,\ldots,n\}^{k+1}}} P(y_{i_1 x_1},...,y_{i_{t_2-1} x_{t_2-1}},\\
& y_{t_2 x_{t_2}}, y_{i_{t_2+1} x_{t_2+1}},...,y_{i_k x_k}, x_{i_{k+1}}, y_{i_{k+2}} \mid z)\\
& + \sum_{\substack{\{i_1,\ldots,i_{t_2-1},i_{t_2+1},\ldots,i_k\}\\ \in\{1,\ldots,n\}^{k-1}}} P(y_{i_1 x_1},...,y_{i_{t_2-1} x_{t_2-1}},\\
& y_{t_2 x_{t_2}}, y_{i_{t_2+1} x_{t_2+1}},...,y_{i_k x_k}, x_{t_2}, y_{t_2} \mid z)\\
& + \sum_{\substack{1\le j\le k\\ j\neq t_2}} P(y_{1_{x_1}},...,y_{k_{x_k}}, x_j \mid z)\\
& + P(y_{t_1 x_{t_1}}, x_{t_2}, y_{t_2 x_{t_2}} \mid z)\\
& + \sum_{j=k+1}^{n} P(y_{1_{x_1}},...,y_{k_{x_k}}, x_j \mid z)\Bigg]\Bigg\}
\end{aligned}
$$

here, the equal sign holds when $\exists 1 \le t_1 < t_2 \le k$, $\forall P(y_{j_{x_j}} \mid z) = 0$ for $j \in [1,k], j \neq t_1$.

$$
\begin{aligned}
=\ & \frac{1}{2}\times\Bigg\{\Bigg[P(y_{t_0 x_{t_0}} \mid z) + P(y_{t_1 x_{t_1}} \mid z)\\
& + P(y_{t_2 x_{t_2}} \mid z) - P(x_{t_0}, y_{t_0} \mid z)\\
& - P(x_{t_1}, y_{t_1} \mid z) - P(x_{t_2}, y_{t_2} \mid z)\\
& - \sum_{\substack{\{i_1,\ldots,i_{t_0-1},i_{t_0+1},\ldots,i_{k+2}\}\\ \in\{1,\ldots,n\}^{k+1}}} P(y_{i_1 x_1},...,y_{i_{t_0-1} x_{t_0-1}},\\
& y_{t_0 x_{t_0}}, y_{i_{t_0+1} x_{t_0+1}},...,y_{i_k x_k}, x_{i_{k+1}}, y_{i_{k+2}} \mid z)\\
& + \Bigg[\sum_{j=1}^{t_0-1} P(y_{t_0 x_{t_0}}, x_j, y_{j+t_1-t_0\, x_{j+t_1-t_0}} \mid z)\\
& + \sum_{j=t_0+1}^{k-t_1+t_0} P(y_{t_0 x_{t_0}}, x_j, y_{j+t_1-t_0\, x_{j+t_1-t_0}} \mid z)\\
& + \sum_{j=1}^{t_1-t_0} P(y_{t_0 x_{t_0}}, x_{k-t_1+t_0+j}, y_{j_{x_j}} \mid z)\\
& + \sum_{j=k+1}^{n} P(y_{1_{x_1}},...,y_{k_{x_k}}, x_j \mid z)\\
& + \sum_{\substack{\{i_1,\ldots,i_{t_0-1},i_{t_0+1},\ldots,i_k\}\\ \in\{1,\ldots,n\}^{k-1}}} P(y_{i_1 x_1},...,y_{i_{t_0-1} x_{t_0-1}},\\
& y_{t_0 x_{t_0}}, y_{i_{t_0+1} x_{t_0+1}},...,y_{i_k x_k}, x_{t_0}, y_{t_0} \mid z)\Bigg]
\end{aligned}
$$

$$- \sum_{\substack{\{i_1,...,i_{t_1-1},i_{t_1+1},...,i_{k+2}\} \\ \in\{1,...,n\}^{k+1}}} P(y_{i_1 x_1}, ..., y_{i_{t_1-1} x_{t_1-1}},$$

$$y_{t_1 x_{t_1}}, y_{i_{t_1+1} x_{t_1+1}}, ..., y_{i_k x_k}, x_{i_{k+1}}, y_{i_{k+2}} \mid z)$$

$$+\Big[P(y_{t_0 x_{t_0}}, x_{t_0}, y_{t_1 x_{t_1}} \mid z)$$

$$+P(y_{t_1 x_{t_1}}, x_{t_2}, y_{t_2 x_{t_2}} \mid z)$$

$$+ \sum_{\substack{\{i_1,...,i_{t_1-1},i_{t_1+1},...,i_k\} \\ \in\{1,...,n\}^{k-1}}} P(y_{i_1 x_1}, ..., y_{i_{t_1-1} x_{t_1-1}},$$

$$y_{t_1 x_{t_1}}, y_{i_{t_1+1} x_{t_1+1}}, ..., y_{i_k x_k}, x_{t_1}, y_{t_1} \mid z)\Big]\Big]$$

$$- \sum_{\substack{\{i_1,...,i_{t_2-1},i_{t_2+1},...,i_{k+2}\} \\ \in\{1,...,n\}^{k+1}}} P(y_{i_1 x_1}, ..., y_{i_{t_2-1} x_{t_2-1}},$$

$$y_{t_2 x_{t_2}}, y_{i_{t_2+1} x_{t_2+1}}, ..., y_{i_k x_k}, x_{i_{k+1}}, y_{i_{k+2}} \mid z)$$

$$+\Big[\sum_{\substack{\{i_1,...,i_{t_2-1},i_{t_2+1},...,i_k\} \\ \in\{1,...,n\}^{k-1}}} P(y_{i_1 x_1}, ..., y_{i_{t_2-1} x_{t_2-1}},$$

$$y_{t_2 x_{t_2}}, y_{i_{t_2+1} x_{t_2+1}}, ..., y_{i_k x_k}, x_{t_2}, y_{t_2} \mid z)$$

$$+ \sum_{\substack{1\le j\le k \\ j\ne t_2}} P(y_{1 x_1}, ..., y_{k x_k}, x_j \mid z)$$

$$+ \sum_{j=k+1}^{n} P(y_{1 x_1}, ..., y_{k x_k}, x_j \mid z)\Big]\Big]\Big\}$$

$$\begin{aligned} \le\ & \frac{1}{2} \times \Big[P(y_{t_0 x_{t_0}} \mid z) + P(y_{t_1 x_{t_1}} \mid z) \\ & +P(y_{t_2 x_{t_2}} \mid z) - P(x_{t_0}, y_{t_0} \mid z) \\ & -P(x_{t_1}, y_{t_1} \mid z) - P(x_{t_2}, y_{t_2} \mid z)\Big] \end{aligned}$$

Here, the equal sign holds when $\exists 1 \le t_0 < t_1 \le k$, and $P(y_{t_0 x_{t_0}} \mid z) = P(y_{t_1 x_{t_1}} \mid z) = 0$. This is just a sufficient condition illustrating tightness, while the equality can also hold in other cases.

For $3 \le m \le k-1$, W.L.O.G., let $1 \le t_0 < ... < t_m \le k$. By applying equation (2), we can get

$$\begin{aligned} & P(y_{1 x_1}, ..., y_{k x_k} \mid z) \\ =\ & \frac{1}{m} \times \Big[\sum_{j=1}^{n} P(y_{1 x_1}, ..., y_{k x_k}, x_j \mid z) \\ & +(m-1)\sum_{j=1}^{n} P(y_{1 x_1}, ..., y_{k x_k}, x_j \mid z)\Big] \end{aligned}$$

By applying equation (4), we have

$$\begin{aligned} & P(y_{1 x_1}, ..., y_{k x_k} \mid z) \\ \le\ & \frac{1}{m} \times \Big[P(y_{t_0 x_{t_0}} \mid z) + P(y_{t_1 x_{t_1}} \mid z) \\ & -P(x_{t_0}, y_{t_0} \mid z) - P(x_{t_1}, y_{t_1} \mid z) \\ & +(m-1)\sum_{j=1}^{n} P(y_{1 x_1}, ..., y_{k x_k}, x_j \mid z)\Big] \end{aligned}$$

Similar to the proof when $m = 2$, we can derive results for $3 \le m \le k-1$:

$$\begin{aligned} & P(y_{1 x_1}, ..., y_{k x_k} \mid z) \\ \le\ & \frac{1}{m} \times \Big[P(y_{t_0 x_{t_0}} \mid z) + P(y_{t_1 x_{t_1}} \mid z) \\ & -P(x_{t_0}, y_{t_0} \mid z) - P(x_{t_1}, y_{t_1} \mid z) \\ & +\sum_{j=2}^{m}\Big[P(y_{t_j x_{t_j}} \mid z) - P(x_{t_j}, y_{t_j} \mid z)\Big]\Big] \\ =\ & \frac{1}{m} \times \sum_{j=0}^{m}\Big[P(y_{t_j x_{t_j}} \mid z) - P(x_{t_j}, y_{t_j} \mid z)\Big] \end{aligned}$$

Overall, we have proved the third bound for $m \in [1, k-1]$.

By substituting

$$\max\left\{\begin{array}{c} 0, \\ \sum_{j=1}^{k} P(y_{j_{x_j}} \mid z) - k + 1, \\ \text{For } i \in \{1, ..., k\}: \\ \sum_{\substack{1\le j\le k \\ j\ne i}} \Big[P(y_{j_{x_j}} \mid z) + P(x_j \mid z) - \\ -P(x_j, y_j \mid z)\Big] + P(x_i, y_i \mid z) - k + 1 \end{array}\right\}$$
$$\le P(y_{1 x_1}, ..., y_{k x_k} \mid z)$$

$$\min\left\{\begin{array}{c} \sum_{j=1}^{k} P(x_j, y_j \mid z) + \sum_{j=k+1}^{n} P(x_j \mid z), \\ \text{For } j \in \{1, ..., k\}: \\ P(y_{j_{x_j}} \mid z), \\ \text{For } m \in \{1, ..., k-1\}, \\ t_j \in \{1, ..., k\}: \\ \frac{1}{m}\Big[\sum_{j=0}^{m} P(y_{t_j x_{t_j}} \mid z) - P(x_{t_j}, y_{t_j} \mid z)\Big] \end{array}\right\}$$
$$\ge P(y_{1 x_1}, ..., y_{k x_k} \mid z)$$

into equation (1), and applying law of total probability, we have

$$\begin{aligned}
&\sum_z P(y_{1_{x_1}},...,y_{k_{x_k}} \mid z) \times P(z) \\
\geq\ & \sum_z 0 \times P(z) \\
=\ & 0
\end{aligned}$$

$$\begin{aligned}
&\sum_z P(y_{1_{x_1}},...,y_{k_{x_k}} \mid z) \times P(z) \\
\geq\ & \sum_z \left[\sum_{j=1}^{k} P(y_{j_{x_j}} \mid z) - k + 1\right] \times P(z) \\
=\ & \sum_{j=1}^{k} P(y_{j_{x_j}}) - k + 1
\end{aligned}$$

$$\begin{aligned}
&\sum_z P(y_{1_{x_1}},...,y_{k_{x_k}} \mid z) \times P(z) \\
\geq\ & \sum_z \Bigg\{ \sum_{\substack{1\leq j\leq k \\ j\neq i}} \Big[P(y_{j_{x_j}} \mid z) + P(x_j \mid z) \\
& -P(x_j, y_j \mid z)\Big] + P(x_i, y_i \mid z) - k + 1 \Bigg\} \times P(z) \\
=\ & \sum_{\substack{1\leq j\leq k \\ j\neq i}} \Big[P(y_{j_{x_j}}) + P(x_j) - P(x_j, y_j)\Big] \\
& + P(x_i, y_i) - k + 1
\end{aligned}$$

$$\begin{aligned}
&\sum_z P(y_{1_{x_1}},...,y_{k_{x_k}} \mid z) \times P(z) \\
\leq\ & \sum_z \left[\sum_{j=1}^{k} P(x_j, y_j \mid z) + \sum_{j=k+1}^{n} P(x_j \mid z)\right] \times P(z) \\
=\ & \sum_{j=1}^{k} P(x_j, y_j) + \sum_{j=k+1}^{n} P(x_j)
\end{aligned}$$

$$\begin{aligned}
&\sum_z P(y_{1_{x_1}},...,y_{k_{x_k}} \mid z) \times P(z) \\
\leq\ & \sum_z P(y_{j_{x_j}} \mid z) \times P(z) \\
=\ & P(y_{j_{x_j}})
\end{aligned}$$

$$\begin{aligned}
&\sum_z P(y_{1_{x_1}},...,y_{k_{x_k}} \mid z) \times P(z) \\
\leq\ & \sum_z \left\{ \frac{1}{m} \left[\sum_{j=0}^{m} P(y_{t_{j_{x_{t_j}}}} \mid z) - P(x_{t_j}, y_{t_j} \mid z)\right]\right\} \\
& \times P(z) \\
=\ & \frac{1}{m}\left[\sum_{j=0}^{m} P(y_{t_{j_{x_{t_j}}}}) - P(x_{t_j}, y_{t_j})\right]
\end{aligned}$$

Thus, we can guarantee that the proposed lower and upper bounds are no looser than the lower and upper bounds in Shu, Wang, and Li (2026). Following the notation in Mueller, Li, and Pearl (2021), $P(y_{j_{x_j}} \mid z)$ denotes experimental data within the subpopulation characterized by z. □

Proof of Theorem 3

Proof.

$$\begin{aligned}
PSub(k,p) &= P(y_{1_{x_1}},...,y_{k_{x_k}}, x_p) \\
&= \sum_z P(y_{1_{x_1}},...,y_{k_{x_k}}, x_p \mid z) \\
&\quad \times P(z)
\end{aligned} \tag{5}$$

First, we need to prove:

$$\max\left\{\begin{array}{c} 0, \\ \sum_{j=1}^{k}\Big[P(y_{j_{x_j}} \mid z) + P(x_j \mid z) - \\ -P(x_j, y_j \mid z)\Big] + P(x_p \mid z) - k \end{array}\right\} \leq P(y_{1_{x_1}},...,y_{k_{x_k}}, x_p \mid z)$$

$$\min\left\{\begin{array}{c} P(x_p \mid z), \\ \\ \text{For } j \in \{1,...,k\}: \\ P(y_{j_{x_j}} \mid z) - P(x_j, y_j \mid z) \end{array}\right\} \geq P(y_{1_{x_1}},...,y_{k_{x_k}}, x_p \mid z)$$

By the Fréchet Inequalities, for any z with $P(z) > 0$, we can obtain the first lower bound and the first upper bound,

$$\begin{aligned}
P(y_{1_{x_1}},...,y_{k_{x_k}}, x_p \mid z) &\geq 0 \\
P(y_{1_{x_1}},...,y_{k_{x_k}}, x_p \mid z) &\leq P(x_p \mid z).
\end{aligned}$$

The equality of the first lower bound holds when $\exists j \in [1,k]$, that $P(y_{j_{x_j}} \mid z) = 0$ or $P(x_p \mid z) = 0$, $p \neq j$.

The equality of the first upper bound holds when $P(y_{j_{x_j}} \mid z) = 1$ for $\forall j \in [1,k]$, $j \neq p$.

For the second lower bound

$$\begin{aligned}
& P(y_{1_{x_1}},...,y_{k_{x_k}}, x_p \mid z) \\
=\ & P(y_{1_{x_1}},...,y_{k_{x_k}}, x_p \mid z) \\
& + \sum_{j=1}^{n} P(y_{1_{x_1}},...,y_{k_{x_k}}, x_j \mid z) \\
& - \sum_{j=1}^{n} P(y_{1_{x_1}},...,y_{k_{x_k}}, x_j \mid z) \\
=\ & P(y_{1_{x_1}},...,y_{k_{x_k}} \mid z) + P(y_{1_{x_1}},...,y_{k_{x_k}}, x_p \mid z) \\
& - \sum_{j=1}^{n} P(y_{1_{x_1}},...,y_{k_{x_k}}, x_j \mid z)
\end{aligned}$$

$$
\begin{aligned}
&= P(y_{1_{x_1}},...,y_{k_{x_k}} \mid z) + P(y_{1_{x_1}},...,y_{k_{x_k}},x_p \mid z) \\
&\quad + \sum_{j=1}^{n} P(x_j \mid z) - 1 - \sum_{j=1}^{n} P(y_{1_{x_1}},...,y_{k_{x_k}},x_j \mid z) \\
&= P(y_{1_{x_1}},...,y_{k_{x_k}} \mid z) - 1 \\
&\quad + P(y_{1_{x_1}},...,y_{k_{x_k}},x_p \mid z) \\
&\quad + \sum_{j=1}^{k} P(x_j \mid z) - \sum_{j=1}^{k} P(y_{1_{x_1}},...,y_{k_{x_k}},x_j \mid z) \\
&\quad + \sum_{j=k+1}^{n} P(x_j \mid z) \\
&\quad - \sum_{j=k+1}^{n} P(y_{1_{x_1}},...,y_{k_{x_k}},x_j \mid z) \\
&= P(y_{1_{x_1}},...,y_{k_{x_k}} \mid z) - 1 \\
&\quad + \sum_{j=1}^{k} P(x_j \mid z) \\
&\quad - \sum_{j=1}^{k} P(y_{1_{x_1}},...,y_{j-1_{x_{j-1}}},y_{j+1_{x_{j+1}}},...,y_{k_{x_k}}, \\
&\quad x_j, y_j \mid z) \\
&\quad + \sum_{j=k+1}^{n} P(x_j \mid z) \\
&\quad - \sum_{j=k+1}^{n} P(y_{1_{x_1}},...,y_{k_{x_k}},x_j \mid z) \\
&\quad + P(y_{1_{x_1}},...,y_{k_{x_k}},x_p \mid z) \\
&= P(y_{1_{x_1}},...,y_{k_{x_k}} \mid z) - 1 \\
&\quad + \sum_{j=1}^{k} P(x_j \mid z) \\
&\quad - \sum_{j=1}^{k} P(y_{1_{x_1}},...,y_{j-1_{x_{j-1}}},y_{j+1_{x_{j+1}}},...,y_{k_{x_k}}, \\
&\quad x_j, y_j \mid z) \\
&\quad + \sum_{j=k+1}^{n} P(x_j \mid z) \\
&\quad - \sum_{\substack{k+1 \le j \le n, \\ j \neq p}} P(y_{1_{x_1}},...,y_{k_{x_k}},x_j \mid z) \\
&\geq \sum_{j=1}^{k} P(y_{j_{x_j}} \mid z) - (k-1) - 1 + \sum_{j=1}^{k} P(x_j \mid z) \\
&\quad - \sum_{j=1}^{k} P(x_j, y_j \mid z) + \sum_{j=k+1}^{n} P(x_j \mid z) \\
&\quad - \sum_{\substack{k+1 \le j \le n, \\ j \neq p}} P(x_j \mid z)
\end{aligned}
$$

here, the equal sign holds when $\exists j \in [1,n]$, and $P(y_{i_{x_i}} \mid z) = 1$ for $\forall i \in [1,k], i \neq j$.

$$
\begin{aligned}
&= \sum_{j=1}^{k} P(y_{j_{x_j}} \mid z) - k + \sum_{j=1}^{k} P(x_j \mid z) \\
&\quad - \sum_{j=1}^{k} P(x_j, y_j \mid z) + P(x_p \mid z) \\
&= \sum_{j=1}^{k} \Big[P(y_{j_{x_j}} \mid z) + P(x_j \mid z) - P(x_j, y_j \mid z) \Big] \\
&\quad + P(x_p \mid z) - k
\end{aligned}
$$

The equality of the second lower bound holds when $\exists j \in [1,n], P(y_{i_{x_i}} \mid z) = 1$ for $\forall i \in [1,k], i \neq j$.

For the remaining upper bounds, $\forall j \in [1,k]$:

$$
\begin{aligned}
&P(y_{1_{x_1}},...,y_{k_{x_k}},x_p \mid z) \\
&= P(y_{1_{x_1}},...,y_{k_{x_k}},x_p \mid z) + P(y_{j_{x_j}} \mid z) \\
&\quad - P(y_{j_{x_j}} \mid z) \\
&= P(y_{1_{x_1}},...,y_{k_{x_k}},x_p \mid z) + P(y_{j_{x_j}} \mid z) \\
&\quad - \sum_{\substack{\{i_1,...,i_{j-1},i_{j+1},...,i_{k+1}\} \\ \in \{1,...,n\}^k}} P(y_{i_1{}_{x_1}},...,y_{i_{j-1}{}_{x_{j-1}}}, \\
&\quad y_{j_{x_j}}, y_{i_{j+1}{}_{x_{j+1}}},...,y_{i_k{}_{x_k}}, x_{i_{k+1}} \mid z)
\end{aligned}
$$

Since $p \neq j$ for $1 \le j \le k$,

$$
\begin{aligned}
&P(y_{1_{x_1}},...,y_{k_{x_k}},x_p \mid z) \\
&\le P(y_{j_{x_j}} \mid z) \\
&\quad - \sum_{\substack{\{i_1,...,i_{j-1},i_{j+1},...,i_k\} \\ \in \{1,...,n\}^{k-1}}} P(y_{i_1{}_{x_1}},...,y_{i_{j-1}{}_{x_{j-1}}}, y_{j_{x_j}}, \\
&\quad y_{i_{j+1}{}_{x_{j+1}}},...,y_{i_k{}_{x_k}}, x_j \mid z)
\end{aligned}
$$

here, the equal sign holds when $P(x_j \mid z) = 0$ for $\forall j \in [k+1,n]$.

$$
\begin{aligned}
&= P(y_{j_{x_j}} \mid z) - P(y_{j_{x_j}}, x_j \mid z) \\
&= P(y_{j_{x_j}} \mid z) - P(x_j, y_j \mid z)
\end{aligned}
$$

The equality of the second upper bound holds when $P(x_j \mid z) = 0$ for $\forall j \in [k+1,n]$.

By substituting

$$
\max \left\{ \begin{array}{c} 0, \\ \sum_{j=1}^{k} \Big[P(y_{j_{x_j}} \mid z) + P(x_j \mid z) - \\ -P(x_j, y_j \mid z) \Big] + P(x_p \mid z) - k \end{array} \right\}
\le P(y_{1_{x_1}},...,y_{k_{x_k}},x_p \mid z)
$$

$$\min\left\{\begin{array}{c} P(x_p \mid z), \\ \\ \text{For } j \in \{1,...,k\}: \\ P(y_{j_{x_j}} \mid z) - P(x_j, y_j \mid z) \end{array}\right\} \geq P(y_{1_{x_1}},...,y_{k_{x_k}}, x_p \mid z)$$

into equation (5), and applying law of total probability, we have

$$\begin{aligned} & \sum_z P(y_{1_{x_1}},...,y_{k_{x_k}}, x_p \mid z) \times P(z) \\ \geq & \sum_z 0 \times P(z) \\ = & \ 0 \end{aligned}$$

$$\begin{aligned} & \sum_z P(y_{1_{x_1}},...,y_{k_{x_k}}, x_p \mid z) \times P(z) \\ \geq & \sum_z \left\{ \sum_{j=1}^{k} \Big[P(y_{j_{x_j}} \mid z) + P(x_j \mid z) \right. \\ & \left. -P(x_j, y_j \mid z) \Big] + P(x_p \mid z) - k \right\} \times P(z) \\ = & \sum_{j=1}^{k} \Big[P(y_{j_{x_j}}) + P(x_j) - P(x_j, y_j) \Big] \\ & +P(x_p) - k \end{aligned}$$

$$\begin{aligned} & \sum_z P(y_{1_{x_1}},...,y_{k_{x_k}}, x_p \mid z) \times P(z) \\ \leq & \ P(x_p \mid z) \times P(z) \\ = & \ P(x_p) \end{aligned}$$

$$\begin{aligned} & \sum_z P(y_{1_{x_1}},...,y_{k_{x_k}}, x_p \mid z) \times P(z) \\ \leq & \Big[P(y_{j_{x_j}} \mid z) - P(x_j, y_j \mid z) \Big] \times P(z) \\ = & \ P(y_{j_{x_j}}) - P(x_j, y_j) \end{aligned}$$

Thus, we can guarantee that the proposed lower and upper bounds are no looser than those of Shu, Wang, and Li (2026). Following the notation in Mueller, Li, and Pearl (2021), $P(y_{j_{x_j}} \mid z)$ denotes experimental data within the subpopulation characterized by z. ☐

Proof of Theorem 4

Proof.

$$\begin{aligned} PRep(k,q) &= P(y_{1_{x_1}},...,y_{k_{x_k}}, y_q) \\ &= \sum_z P(y_{1_{x_1}},...,y_{k_{x_k}}, y_q \mid z) \\ & \quad \times P(z) \end{aligned} \quad (6)$$

First, we need to prove:

$$\max\left\{\begin{array}{c} 0, \\ \\ \sum_{j=1}^{k} \Big[P(y_{j_{x_j}} \mid z) + P(x_j \mid z) - \\ -P(x_j, y_j \mid z) \Big] + \sum_{\substack{k+1 \leq j \leq n \\ j \neq q}} P(x_j, y_q \mid z) + \\ +P(x_q, y_q \mid z) - k, \\ \\ \text{If } q \in \{1,...,k\}: \\ \sum_{\substack{1 \leq j \leq k \\ j \neq q}} \Big[P(y_{j_{x_j}} \mid z) + P(x_j \mid z) - \\ -P(x_j, y_j \mid z) \Big] + P(x_q, y_q \mid z) - (k-1) \end{array}\right\} \leq P(y_{1_{x_1}},...,y_{k_{x_k}}, y_q \mid z)$$

$$\min\left\{\begin{array}{c} \text{If } q \in \{1,...,k\}: \\ P(y_{q_{x_q}} \mid z), \\ \\ P(x_q, y_q \mid z) + \sum_{\substack{k+1 \leq j \leq n \\ j \neq q}} P(x_j, y_q \mid z), \\ \\ \text{For } j \in \{1,...,k\}, \text{ and } j \neq q \\ P(y_{j_{x_j}} \mid z) - P(x_j, y_j \mid z), \end{array}\right\} \geq P(y_{1_{x_1}},...,y_{k_{x_k}}, y_q \mid z)$$

By the Fréchet Inequalities, for any z with $P(z) > 0$, we can obtain the first lower bound and the first upper bound,

$$\begin{aligned} P(y_{1_{x_1}},...,y_{k_{x_k}}, y_q \mid z) & \geq 0 \\ P(y_{1_{x_1}},...,y_{k_{x_k}}, y_q \mid z) & \leq P(y_{q_{x_q}} \mid z), \forall 1 \leq q \leq k. \end{aligned}$$

The equality of the first lower bound holds when $\exists j \in [1,k]$, that $P(y_{j_{x_j}} \mid z) = 0$ or $P(y_q \mid z) = 0$.

The equality of the first upper bound holds when $P(y_{j_{x_j}} \mid z) = 1, P(y_q \mid z) = 1$ for $\forall j \in [1,k], j \neq q$.

For the second lower bound

$$\begin{aligned} & P(y_{1_{x_1}},...,y_{k_{x_k}}, y_q \mid z) \\ = & \ P(y_{1_{x_1}},...,y_{k_{x_k}}, y_q \mid z) + P(y_{1_{x_1}},...,y_{k_{x_k}} \mid z) \\ & - \sum_{j=1}^{n} \sum_{l=1}^{n} P(y_{1_{x_1}},...,y_{k_{x_k}}, x_j, y_l \mid z) \\ = & \ P(y_{1_{x_1}},...,y_{k_{x_k}}, y_q \mid z) + P(y_{1_{x_1}},...,y_{k_{x_k}} \mid z) \\ & - \sum_{j=1}^{k} P(y_{1_{x_1}},...,y_{k_{x_k}}, x_j, y_j \mid z) \\ & - \sum_{j=k+1}^{n} \sum_{l=1}^{n} P(y_{1_{x_1}},...,y_{k_{x_k}}, x_j, y_l \mid z) \end{aligned}$$

$$
\begin{aligned}
&= P(y_{1_{x_1}},...,y_{k_{x_k}},y_q \mid z) + P(y_{1_{x_1}},...,y_{k_{x_k}} \mid z) \\
&\quad + \sum_{j=1}^{n} P(x_j \mid z) - 1 \\
&\quad - \sum_{j=1}^{k} P(y_{1_{x_1}},...,y_{k_{x_k}},x_j,y_j \mid z) \\
&\quad - \sum_{j=k+1}^{n} \sum_{l=1}^{n} P(y_{1_{x_1}},...,y_{k_{x_k}},x_j,y_l \mid z) \\
&= \sum_{j=1}^{n} P(y_{1_{x_1}},...,y_{k_{x_k}},x_j,y_q \mid z) \\
&\quad + P(y_{1_{x_1}},...,y_{k_{x_k}} \mid z) - 1 \\
&\quad + \sum_{j=1}^{k} P(x_j \mid z) - \sum_{j=1}^{k} P(y_{1_{x_1}},...,y_{k_{x_k}},x_j,y_j \mid z) \\
&\quad + \sum_{j=k+1}^{n} P(x_j \mid z) \\
&\quad - \sum_{j=k+1}^{n} \sum_{l=1}^{n} P(y_{1_{x_1}},...,y_{k_{x_k}},x_j,y_l \mid z)
\end{aligned}
$$

If $q \in [1,k]$,

$$
\begin{aligned}
&P(y_{1_{x_1}},...,y_{k_{x_k}},y_q \mid z) \\
&= P(y_{1_{x_1}},...,y_{k_{x_k}} \mid z) - 1 \\
&\quad + \sum_{j=1}^{k} P(x_j \mid z) - \sum_{j=1}^{k} P(y_{1_{x_1}},...,y_{k_{x_k}},x_j,y_j \mid z) \\
&\quad + P(y_{1_{x_1}},...,y_{k_{x_k}},x_q,y_q \mid z) + \sum_{j=k+1}^{n} P(x_j \mid z) \\
&\quad - \sum_{j=k+1}^{n} \sum_{l=1}^{n} P(y_{1_{x_1}},...,y_{k_{x_k}},x_j,y_l \mid z) \\
&\quad + \sum_{j=k+1}^{n} P(y_{1_{x_1}},...,y_{k_{x_k}},x_j,y_q \mid z) \\
&= P(y_{1_{x_1}},...,y_{k_{x_k}} \mid z) - 1 \\
&\quad + \sum_{j=1}^{k} P(x_j \mid z) \\
&\quad - \sum_{\substack{1\le j\le k,\\ j\neq q}} P(y_{1_{x_1}},...,y_{k_{x_k}},x_j,y_j \mid z) \\
&\quad + \sum_{j=k+1}^{n} P(x_j \mid z) \\
&\quad - \sum_{j=k+1}^{n} \sum_{\substack{1\le l\le n,\\ l\neq q}} P(y_{1_{x_1}},...,y_{k_{x_k}},x_j,y_l \mid z) \\
&\geq \sum_{j=1}^{k} P(y_{j_{x_j}} \mid z) - (k-1) - 1 \\
&\quad + \sum_{j=1}^{k} P(x_j \mid z) - \sum_{\substack{1\le j\le k,\\ j\neq q}} P(x_j,y_j \mid z) \\
&\quad + \sum_{j=k+1}^{n} P(x_j \mid z) - \sum_{j=k+1}^{n} \sum_{\substack{1\le l\le n,\\ l\neq q}} P(x_j,y_l \mid z)
\end{aligned}
$$

here, the equal sign holds when $\exists j \in [1,n]$, and $P(y_{i_{x_i}} \mid z) = 1$ for $\forall i \in [1,k], i \neq j$.

$$
\begin{aligned}
&= \sum_{j=1}^{k} P(y_{j_{x_j}} \mid z) - k + \sum_{j=1}^{k} P(x_j \mid z) \\
&\quad - \sum_{j=1}^{k} P(x_j,y_j \mid z) + P(x_q,y_q \mid z) \\
&\quad + \sum_{j=k+1}^{n} P(x_j,y_q \mid z) \\
&= \sum_{j=1}^{k} \Big[P(y_{j_{x_j}} \mid z) + P(x_j \mid z) - P(x_j,y_j \mid z) \Big] \\
&\quad + \sum_{\substack{k+1\le j\le n,\\ j\neq q}} P(x_j,y_q \mid z) + P(x_q,y_q \mid z) - k
\end{aligned}
$$

If $q \in [k+1,n]$,

$$
\begin{aligned}
&P(y_{1_{x_1}},...,y_{k_{x_k}},y_q \mid z) \\
&= P(y_{1_{x_1}},...,y_{k_{x_k}} \mid z) - 1 + \sum_{j=1}^{k} P(x_j \mid z) \\
&\quad - \sum_{j=1}^{k} P(y_{1_{x_1}},...,y_{k_{x_k}},x_j,y_j \mid z) \\
&\quad + \sum_{j=k+1}^{n} P(x_j \mid z) \\
&\quad - \sum_{j=k+1}^{n} \sum_{l=1}^{n} P(y_{1_{x_1}},...,y_{k_{x_k}},x_j,y_l \mid z) \\
&\quad + \sum_{j=k+1}^{n} P(y_{1_{x_1}},...,y_{k_{x_k}},x_j,y_q \mid z) \\
&= P(y_{1_{x_1}},...,y_{k_{x_k}} \mid z) - 1 + \sum_{j=1}^{k} P(x_j \mid z) \\
&\quad - \sum_{j=1}^{k} P(y_{1_{x_1}},...,y_{k_{x_k}},x_j,y_j \mid z) \\
&\quad + \sum_{j=k+1}^{n} P(x_j \mid z)
\end{aligned}
$$

$$
\begin{aligned}
& -\sum_{j=k+1}^{n} \sum_{\substack{1 \le l \le n, \\ l \ne q}} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j, y_l \mid z) \\
\geq \quad & \sum_{j=1}^{k} P(y_{j_{x_j}} \mid z) - (k-1) - 1 + \sum_{j=1}^{k} P(x_j \mid z) \\
& - \sum_{j=1}^{k} P(x_j, y_j \mid z) \\
& + \sum_{j=k+1}^{n} P(x_j \mid z) - \sum_{j=k+1}^{n} \sum_{\substack{1 \le l \le n, \\ l \ne q}} P(x_j, y_l \mid z) \\
& \text{here, the equal sign holds when } \exists j \in [1,n], \\
& \text{ and } P(y_{i_{x_i}} \mid z) = 1 \text{ for } \forall i \in [1,k], i \ne j. \\
= \quad & \sum_{j=1}^{k} P(y_{j_{x_j}} \mid z) - k + \sum_{j=1}^{k} P(x_j \mid z) \\
& - \sum_{j=1}^{k} P(x_j, y_j \mid z) + \sum_{j=k+1}^{n} P(x_j, y_q \mid z) \\
= \quad & \sum_{j=1}^{k} \Big[P(y_{j_{x_j}} \mid z) + P(x_j \mid z) - P(x_j, y_j \mid z) \Big] \\
& + \sum_{\substack{k+1 \le j \le n, \\ j \ne q}} P(x_j, y_q \mid z) + P(x_q, y_q \mid z) - k
\end{aligned}
$$

To summarize

$$
\begin{aligned}
& P(y_{1_{x_1}}, ..., y_{k_{x_k}}, y_q \mid z) \\
\geq \quad & \sum_{j=1}^{k} \Big[P(y_{j_{x_j}} \mid z) + P(x_j \mid z) - P(x_j, y_j \mid z) \Big] \\
& + \sum_{\substack{k+1 \le j \le n \\ j \ne q}} P(x_j, y_q \mid z) + P(x_q, y_q \mid z) - k
\end{aligned}
$$

and the equality of the second lower bound holds when $\exists j \in [1,n]$, and $P(y_{i_{x_i}} \mid z) = 1$ for $\forall i \in [1,k], i \ne j$.

For the third lower bound, if $1 \le q \le k$

$$
\begin{aligned}
& P(y_{1_{x_1}}, ..., y_{k_{x_k}}, y_q \mid z) \\
= \quad & \sum_{j=1}^{n} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j, y_q \mid z) \\
= \quad & P(y_{1_{x_1}}, ..., y_{q-1_{x_{q-1}}}, y_{q+1_{x_{q+1}}}, ..., y_{k_{x_k}}, x_q, y_q \mid z) \\
& + \sum_{j=k+1}^{n} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j, y_q \mid z) \\
= \quad & P(y_{1_{x_1}}, ..., y_{q-1_{x_{q-1}}}, y_{q+1_{x_{q+1}}}, ..., y_{k_{x_k}}, x_q, y_q \mid z) \\
& + \sum_{j=k+1}^{n} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j, y_q \mid z) \\
& + P(y_{1_{x_1}}, ..., y_{q-1_{x_{q-1}}}, y_{q+1_{x_{q+1}}}, ..., y_{k_{x_k}} \mid z) \\
& - \sum_{j=1}^{n} \sum_{l=1}^{n} P(y_{1_{x_1}}, ..., y_{q-1_{x_{q-1}}}, y_{q+1_{x_{q+1}}}, ..., y_{k_{x_k}}, \\
& x_j, y_l \mid z) \\
& + \sum_{j=1}^{n} P(x_j \mid z) - 1 \\
= \quad & P(y_{1_{x_1}}, ..., y_{q-1_{x_{q-1}}}, y_{q+1_{x_{q+1}}}, ..., y_{k_{x_k}} \mid z) - 1 \\
& + \sum_{j=1}^{k} P(x_j \mid z) \\
& - \sum_{\substack{1 \le j \le k, \\ j \ne q}} P(y_{1_{x_1}}, ..., y_{q-1_{x_{q-1}}}, y_{q+1_{x_{q+1}}}, ..., y_{k_{x_k}}, \\
& x_j, y_j \mid z) \\
& - \sum_{l=1}^{n} P(y_{1_{x_1}}, ..., y_{q-1_{x_{q-1}}}, y_{q+1_{x_{q+1}}}, ..., y_{k_{x_k}}, \\
& x_q, y_l \mid z) \\
& + P(y_{1_{x_1}}, ..., y_{q-1_{x_{q-1}}}, y_{q+1_{x_{q+1}}}, ..., y_{k_{x_k}}, x_q, \\
& y_q \mid z) \\
& + \sum_{j=k+1}^{n} P(x_j \mid z) \\
& - \sum_{j=k+1}^{n} \sum_{l=1}^{n} P(y_{1_{x_1}}, ..., y_{q-1_{x_{q-1}}}, y_{q+1_{x_{q+1}}}, ..., \\
& y_{k_{x_k}}, x_j, y_l \mid z) \\
& + \sum_{j=k+1}^{n} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j, y_q \mid z) \\
= \quad & P(y_{1_{x_1}}, ..., y_{q-1_{x_{q-1}}}, y_{q+1_{x_{q+1}}}, ..., y_{k_{x_k}} \mid z) - 1 \\
& + \sum_{j=1}^{k} P(x_j \mid z) \\
& - \sum_{\substack{1 \le j \le k, \\ j \ne q}} P(y_{1_{x_1}}, ..., y_{q-1_{x_{q-1}}}, y_{q+1_{x_{q+1}}}, ..., y_{k_{x_k}}, \\
& x_j, y_j \mid z) \\
& - \sum_{\substack{1 \le l \le n, \\ l \ne q}} P(y_{1_{x_1}}, ..., y_{q-1_{x_{q-1}}}, y_{q+1_{x_{q+1}}}, ..., y_{k_{x_k}}, \\
& x_q, y_l \mid z) \\
& + \sum_{j=k+1}^{n} P(x_j \mid z) \\
& - \sum_{j=k+1}^{n} \sum_{\substack{1 \le l \le n, \\ l \ne q}} P(y_{1_{x_1}}, ..., y_{q-1_{x_{q-1}}}, y_{q+1_{x_{q+1}}}, ..., \\
& y_{k_{x_k}}, x_j, y_l \mid z)
\end{aligned}
$$

$$
\begin{aligned}
\geq\ & \sum_{\substack{1\leq j\leq k,\\ j\neq q}} P(y_{j_{x_j}} \mid z) - (k-2) - 1 \\
& + \sum_{j=1}^{k} P(x_j \mid z) - \sum_{\substack{1\leq j\leq k,\\ j\neq q}} P(x_j, y_j \mid z) \\
& - \sum_{\substack{1\leq l\leq n,\\ l\neq q}} P(x_q, y_l \mid z) + \sum_{j=k+1}^{n} P(x_j \mid z) \\
& - \sum_{j=k+1}^{n} \sum_{\substack{1\leq l\leq n,\\ l\neq q}} P(x_j, y_l \mid z) \\
& \text{here, the equal sign holds when } \exists q \in [1,k], \\
& \text{ and } P(y_{i_{x_i}} \mid z) = 1 \text{ for } \forall i \in [1,k], i \neq q. \\
=\ & \sum_{\substack{1\leq j\leq k,\\ j\neq q}} P(y_{j_{x_j}} \mid z) - (k-1) \\
& + \sum_{\substack{1\leq j\leq k,\\ j\neq q}} P(x_j \mid z) + P(x_q \mid z) \\
& - \sum_{\substack{1\leq j\leq k,\\ j\neq q}} P(x_j, y_j \mid z) - \sum_{\substack{1\leq l\leq n,\\ l\neq q}} P(x_q, y_l \mid z) \\
& + \sum_{j=k+1}^{n} P(x_j, y_q \mid z) \\
=\ & \sum_{\substack{1\leq j\leq k,\\ j\neq q}} \Big[P(y_{j_{x_j}} \mid z) + P(x_j \mid z) - P(x_j, y_j \mid z) \Big] \\
& -(k-1) + P(x_q \mid z) - \sum_{\substack{1\leq l\leq n,\\ l\neq q}} P(x_q, y_l \mid z) \\
& + \sum_{j=k+1}^{n} P(x_j, y_q \mid z) \\
=\ & \sum_{\substack{1\leq j\leq k,\\ j\neq q}} \Big[P(y_{j_{x_j}} \mid z) + P(x_j \mid z) - P(x_j, y_j \mid z) \Big] \\
& -(k-1) + P(x_q, y_q \mid z) + \sum_{j=k+1}^{n} P(x_j, y_q \mid z) \\
\geq\ & \sum_{\substack{1\leq j\leq k,\\ j\neq q}} \Big[P(y_{j_{x_j}} \mid z) + P(x_j \mid z) - P(x_j, y_j \mid z) \Big] \\
& + P(x_q, y_q \mid z) - (k-1) \\
& \text{here, the equal sign holds when } P(x_j \mid z) = 0 \\
& \text{ for } \forall j \in [k+1, n].
\end{aligned}
$$

The equality of the third upper bound holds when $\exists q \in [1,k]$, and $P(y_{i_{x_i}} \mid z) = 1, P(x_j \mid z) = 0$ for $\forall i \in [1,k], j \in [k+1,n], i \neq q$.

For the second upper bound

$$
\begin{aligned}
& P(y_{1_{x_1}}, ..., y_{k_{x_k}}, y_q \mid z) \\
=\ & \sum_{j=1}^{n} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j, y_q \mid z) \\
=\ & \sum_{j=1}^{k} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j, y_q \mid z) \\
& + \sum_{j=k+1}^{n} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j, y_q \mid z)
\end{aligned}
$$

If $q \in [1,k]$,

$$
\begin{aligned}
& P(y_{1_{x_1}}, ..., y_{k_{x_k}}, y_q \mid z) \\
=\ & P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_q, y_q \mid z) \\
& + \sum_{j=k+1}^{n} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j, y_q \mid z) \\
\leq\ & P(x_q, y_q \mid z) + \sum_{j=k+1}^{n} P(x_j, y_q \mid z) \\
& \text{here, the equal sign holds when } P(y_{i_{x_i}} \mid z) = 1 \\
& \text{ for } \forall i \in [1,k]. \\
=\ & P(x_q, y_q \mid z) + \sum_{\substack{k+1\leq j\leq n,\\ j\neq q}} P(x_j, y_q \mid z)
\end{aligned}
$$

If $q \in [k+1,n]$,

$$
\begin{aligned}
& P(y_{1_{x_1}}, ..., y_{k_{x_k}}, y_q \mid z) \\
=\ & \sum_{j=k+1}^{n} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j, y_q \mid z) \\
\leq\ & \sum_{j=k+1}^{n} P(x_j, y_q \mid z) \\
& \text{here, the equal sign holds when } P(y_{i_{x_i}} \mid z) = 1 \\
& \text{ for } \forall i \in [1,k]. \\
=\ & P(x_q, y_q \mid z) + \sum_{\substack{k+1\leq j\leq n,\\ j\neq q}} P(x_j, y_q \mid z)
\end{aligned}
$$

To summarize

$$
\begin{aligned}
& P(y_{1_{x_1}}, ..., y_{k_{x_k}}, y_q \mid z) \\
\leq\ & P(x_q, y_q \mid z) + \sum_{\substack{k+1\leq j\leq n\\ j\neq q}} P(x_j, y_q \mid z)
\end{aligned}
$$

and the equality of the second upper bound holds when $P(y_{i_{x_i}} \mid z) = 1$ for $\forall i \in [1,k]$.

For the remaining upper bounds, $\forall j \in [1, k]$:

$$\begin{aligned} & P(y_{1_{x_1}}, ..., y_{k_{x_k}}, y_q \mid z) \\ = & \sum_{i=1}^{n} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_i, y_q \mid z) + P(y_{j_{x_j}} \mid z) \\ & -P(y_{j_{x_j}} \mid z) \\ = & \sum_{i=1}^{n} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_i, y_q \mid z) + P(y_{j_{x_j}} \mid z) \\ & - \sum_{\substack{\{i_1,...,i_{j-1},i_{j+1},...,i_{k+2}\} \\ \in \{1,...,n\}^{k+1}}} P(y_{i_1 x_1}, ..., y_{i_{j-1} x_{j-1}}, \\ & y_{j_{x_j}}, y_{i_{j+1} x_{j+1}}, ..., y_{i_k x_k}, x_{i_{k+1}}, y_{i_{k+2}} \mid z) \end{aligned}$$

Since $q \neq j$ for $1 \leq j \leq k$,

$$\begin{aligned} & P(y_{1_{x_1}}, ..., y_{k_{x_k}}, y_q \mid z) \\ \leq & P(y_{j_{x_j}} \mid z) \\ & - \sum_{\substack{\{i_1,...,i_{j-1},i_{j+1},...,i_k\} \\ \in \{1,...,n\}^{k-1}}} P(y_{i_1 x_1}, ..., y_{i_{j-1} x_{j-1}}, y_{j_{x_j}}, \\ & y_{i_{j+1} x_{j+1}}, ..., y_{i_k x_k}, x_j, y_j \mid z) \\ & \text{here, the equal sign holds when } P(x_j \mid z) = 0, \\ & P(y_j \mid z) = 0 \text{ and } P(x_{t_1}, y_{t_2} \mid z) = 0 \\ & \text{ for } \forall j \in [k+1, n], \forall t_1, t_2 \in [1, k] \text{ and } t_1 \neq t_2. \\ = & P(y_{j_{x_j}} \mid z) - P(y_{j_{x_j}}, x_j, y_j \mid z) \\ = & P(y_{j_{x_j}} \mid z) - P(x_j, y_j \mid z) \end{aligned}$$

The equality of the third upper bound holds when $P(x_j \mid z) = 0, P(y_j \mid z) = 0$ and $P(x_{t_1}, y_{t_2} \mid z) = 0$ for $\forall j \in [k+1, n], t_1, t_2 \in [1, k]$ and $t_1 \neq t_2$.

By substituting

$$\max \left\{ \begin{array}{c} 0, \\ \\ \sum_{j=1}^{k} \Big[P(y_{j_{x_j}} \mid z) + P(x_j \mid z) - \\ -P(x_j, y_j \mid z) \Big] + \sum_{\substack{k+1 \leq j \leq n \\ j \neq q}} P(x_j, y_q \mid z) + \\ +P(x_q, y_q \mid z) - k, \\ \\ \text{If } q \in \{1, ..., k\} : \\ \sum_{\substack{1 \leq j \leq k \\ j \neq q}} \Big[P(y_{j_{x_j}} \mid z) + P(x_j \mid z) - \\ -P(x_j, y_j \mid z) \Big] + P(x_q, y_q \mid z) - (k-1) \end{array} \right\}$$
$$\leq P(y_{1_{x_1}}, ..., y_{k_{x_k}}, y_q \mid z)$$

$$\min \left\{ \begin{array}{c} \text{If } q \in \{1, ..., k\} : \\ P(y_{q_{x_q}} \mid z), \\ \\ P(x_q, y_q \mid z) + \sum_{\substack{k+1 \leq j \leq n \\ j \neq q}} P(x_j, y_q \mid z), \\ \\ \text{For } j \in \{1, ..., k\}, \text{ and } j \neq q \\ P(y_{j_{x_j}} \mid z) - P(x_j, y_j \mid z), \end{array} \right\}$$
$$\geq P(y_{1_{x_1}}, ..., y_{k_{x_k}}, y_q \mid z)$$

into equation (6), and applying law of total probability, we have

$$\begin{aligned} & \sum_z P(y_{1_{x_1}}, ..., y_{k_{x_k}}, y_q \mid z) \times P(z) \\ \geq & \sum_z 0 \times P(z) \\ = & 0 \end{aligned}$$

$$\begin{aligned} & \sum_z P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_p \mid z) \times P(z) \\ \geq & \sum_z \Bigg\{ \sum_{j=1}^{k} \Big[P(y_{j_{x_j}} \mid z) + P(x_j \mid z) \\ & -P(x_j, y_j \mid z) \Big] + \sum_{\substack{k+1 \leq j \leq n \\ j \neq q}} P(x_j, y_q \mid z) \\ & +P(x_q, y_q \mid z) - k \Bigg\} \times P(z) \\ = & \sum_{j=1}^{k} \Big[P(y_{j_{x_j}}) + P(x_j) - P(x_j, y_j) \Big] \\ & + \sum_{\substack{k+1 \leq j \leq n \\ j \neq q}} P(x_j, y_q) + P(x_q, y_q) - k \end{aligned}$$

$$\begin{aligned} & \sum_z P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_p \mid z) \times P(z) \\ \geq & \sum_z \Bigg\{ \sum_{\substack{1 \leq j \leq k \\ j \neq q}} \Big[P(y_{j_{x_j}} \mid z) + P(x_j \mid z) \\ & -P(x_j, y_j \mid z) \Big] + P(x_q, y_q \mid z) - (k-1) \Bigg\} \\ & \times P(z) \\ = & \sum_{\substack{1 \leq j \leq k \\ j \neq q}} \Big[P(y_{j_{x_j}}) + P(x_j) - P(x_j, y_j) \Big] \\ & +P(x_q, y_q) - (k-1) \end{aligned}$$

$$
\begin{aligned}
& \sum_z P(y_{1_{x_1}}, ..., y_{k_{x_k}}, y_q \mid z) \times P(z) \\
\leq \;& \sum_z P(y_{q_{x_q}} \mid z) \times P(z) \\
= \;& P(y_{q_{x_q}})
\end{aligned}
$$

$$
\begin{aligned}
& \sum_z P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_p \mid z) \times P(z) \\
\leq \;& \sum_z \left[P(x_q, y_q \mid z) + \sum_{\substack{k+1 \leq j \leq n \\ j \neq q}} P(x_j, y_q \mid z) \right] \\
& \times P(z) \\
= \;& P(x_q, y_q) + \sum_{\substack{k+1 \leq j \leq n \\ j \neq q}} P(x_j, y_q)
\end{aligned}
$$

$$
\begin{aligned}
& \sum_z P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_p \mid z) \times P(z) \\
\leq \;& \sum_z \Big[P(y_{j_{x_j}} \mid z) - P(x_j, y_j \mid z) \Big] \times P(z) \\
= \;& P(y_{j_{x_j}}) - P(x_j, y_j)
\end{aligned}
$$

Thus, we can guarantee that the proposed lower and upper bounds are no looser than those of Shu, Wang, and Li (2026). Following the notation in Mueller, Li, and Pearl (2021), $P(y_{j_{x_j}} \mid z)$ denotes experimental data within the subpopulation characterized by z. □

Proof of Theorem 5

Proof.

$$
\begin{aligned}
PN(k,p,q) \;&=\; P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_p, y_q) \\
&=\; \sum_z P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_p, y_q \mid z) \\
&\quad\; \times P(z) \qquad (7)
\end{aligned}
$$

First, we need to prove:

$$
\max \left\{ \begin{array}{c} 0, \\ \sum_{j=1}^{k} \Big[P(y_{j_{x_j}} \mid z) + P(x_j \mid z) - \\ -P(x_j, y_j \mid z) \Big] + P(x_p, y_q \mid z) - k \end{array} \right\} \leq P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_p, y_q \mid z)
$$

$$
\min \left\{ \begin{array}{c} P(x_p, y_q \mid z), \\ \\ \text{For } j \in \{1, ..., k\}: \\ P(y_{j_{x_j}} \mid z) - P(x_j, y_j \mid z) \end{array} \right\} \geq P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_p, y_q \mid z)
$$

By the Fréchet Inequalities, for any z with $P(z) > 0$, we can obtain the first lower bound and the first upper bound,

$$
\begin{aligned}
P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_p, y_q \mid z) \;&\geq\; 0 \\
P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_p, y_q \mid z) \;&\leq\; P(x_p, y_q \mid z).
\end{aligned}
$$

The equality of the first lower bound holds when $\exists j \in [1, k]$, that $P(y_{j_{x_j}} \mid z) = 0$ or $P(x_p \mid z) = 0$ or $P(y_q \mid z) = 0, p \neq j$.

The equality of the first upper bound holds when $P(y_{j_{x_j}} \mid z) = 1$ for $\forall j \in [1, k]$.

For the second lower bound

$$
\begin{aligned}
& P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_p, y_q \mid z) \\
= \;& P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_p, y_q \mid z) + P(y_{1_{x_1}}, ..., y_{k_{x_k}} \mid z) \\
& -P(y_{1_{x_1}}, ..., y_{k_{x_k}} \mid z) \\
= \;& P(y_{1_{x_1}}, ..., y_{k_{x_k}} \mid z) + P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_p, y_q \mid z) \\
& -\sum_{j=1}^{n} \sum_{l=1}^{n} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j, y_l \mid z) \\
= \;& P(y_{1_{x_1}}, ..., y_{k_{x_k}} \mid z) + P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_p, y_q \mid z) \\
& +\sum_{j=1}^{n} P(x_j \mid z) - 1 \\
& -\sum_{j=1}^{k} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j, y_j \mid z) \\
& -\sum_{j=k+1}^{n} \sum_{l=1}^{n} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j, y_l \mid z) \\
= \;& P(y_{1_{x_1}}, ..., y_{k_{x_k}} \mid z) - 1 \\
& +\sum_{j=1}^{k} P(x_j \mid z) - \sum_{j=1}^{k} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j, y_j \mid z) \\
& +\sum_{j=k+1}^{n} P(x_j \mid z) \\
& -\sum_{j=k+1}^{n} \sum_{l=1}^{n} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j, y_l \mid z) \\
& +P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_p, y_q \mid z) \\
= \;& P(y_{1_{x_1}}, ..., y_{k_{x_k}} \mid z) - 1 \\
& +\sum_{j=1}^{k} P(x_j \mid z) - \sum_{j=1}^{k} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j, y_j \mid z) \\
& +\sum_{j=k+1}^{n} P(x_j \mid z) \\
& -\sum_{\substack{k+1 \leq j \leq n, \\ j \neq p}} \sum_{l=1}^{n} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j, y_l \mid z) \\
& -\sum_{\substack{1 \leq l \leq n, \\ l \neq p}} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_p, y_l \mid z)
\end{aligned}
$$

$$
\begin{aligned}
\geq\ & \sum_{j=1}^{k} P(y_{j_{x_j}} \mid z) - (k-1) - 1 + \sum_{j=1}^{k} P(x_j \mid z) \\
& - \sum_{j=1}^{k} P(x_j, y_j \mid z) + \sum_{j=k+1}^{n} P(x_j \mid z) \\
& - \sum_{\substack{k+1 \leq j \leq n, \\ j \neq p}} P(x_j \mid z) - \sum_{\substack{1 \leq l \leq n, \\ l \neq p}} P(x_p, y_l \mid z) \\
& \text{here, the equal sign holds when } \exists j \in [1, n], \\
& \text{ and } P(y_{i_{x_i}} \mid z) = 1 \text{ for } \forall i \in [1, k], i \neq j. \\
=\ & \sum_{j=1}^{k} P(y_{j_{x_j}} \mid z) - k + \sum_{j=1}^{k} P(x_j \mid z) \\
& - \sum_{j=1}^{k} P(x_j, y_j \mid z) + P(x_p \mid z) \\
& - \sum_{\substack{1 \leq l \leq n, \\ l \neq p}} P(x_p, y_l \mid z) \\
=\ & \sum_{j=1}^{k} \Big[P(y_{j_{x_j}} \mid z) + P(x_j \mid z) - P(x_j, y_j \mid z) \Big] \\
& + P(x_p, y_q \mid z) - k
\end{aligned}
$$

The equality of the second lower bound holds when $\exists j \in [1, n], P(y_{i_{x_i}} \mid z) = 1$ for $\forall i \in [1, k], i \neq j$.

For the remaining upper bounds, $\forall j \in [1, k]$:

$$
\begin{aligned}
& P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_p, y_q \mid z) \\
=\ & P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_p, y_q \mid z) + P(y_{j_{x_j}} \mid z) \\
& - P(y_{j_{x_j}} \mid z) \\
=\ & P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_p, y_q \mid z) + P(y_{j_{x_j}} \mid z) \\
& - \sum_{\substack{\{i_1, ..., i_{j-1}, i_{j+1}, ..., i_{k+2}\} \\ \in \{1, ..., n\}^{k+1}}} P(y_{{i_1}_{x_1}}, ..., y_{{i_{j-1}}_{x_{j-1}}}, \\
& y_{j_{x_j}}, y_{{i_{j+1}}_{x_{j+1}}}, ..., y_{{i_k}_{x_k}}, x_{i_{k+1}}, y_{i_{k+2}} \mid z)
\end{aligned}
$$

Since $p \neq j$ for $1 \leq j \leq k$,

$$
\begin{aligned}
& P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_p, y_q \mid z) \\
\leq\ & P(y_{j_{x_j}} \mid z) - \sum_{\substack{\{i_1, ..., i_{j-1}, i_{j+1}, ..., i_k\} \\ \in \{1, ..., n\}^{k-1}}} P(y_{{i_1}_{x_1}}, ..., \\
& y_{{i_{j-1}}_{x_{j-1}}}, y_{j_{x_j}}, y_{{i_{j+1}}_{x_{j+1}}}, ..., y_{{i_k}_{x_k}}, x_j, y_j \mid z) \\
& \text{here, the equal sign holds when } P(x_j \mid z) = 0, \\
& P(y_j \mid z) = 0 \text{ and } P(x_{t_1}, y_{t_2} \mid z) = 0 \\
& \text{ for } \forall j \in [k+1, n], \forall t_1, t_2 \in [1, k] \text{ and } t_1 \neq t_2. \\
=\ & P(y_{j_{x_j}} \mid z) - P(y_{j_{x_j}}, x_j, y_j \mid z) \\
=\ & P(y_{j_{x_j}} \mid z) - P(x_j, y_j \mid z)
\end{aligned}
$$

The equality of the second upper bound holds when $P(x_j \mid z) = 0, P(y_j \mid z) = 0$ and $P(x_{t_1}, y_{t_2} \mid z) = 0$ for $\forall j \in [k+1, n], t_1, t_2 \in [1, k]$ and $t_1 \neq t_2$.

By substituting

$$
\max \left\{ \begin{array}{c} 0, \\ \sum_{j=1}^{k} \Big[P(y_{j_{x_j}} \mid z) + P(x_j \mid z) - \\ - P(x_j, y_j \mid z) \Big] + P(x_p, y_q \mid z) - k \end{array} \right\}
$$
$$
\leq P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_p, y_q \mid z)
$$

$$
\min \left\{ \begin{array}{c} P(x_p, y_q \mid z), \\ \\ \text{For } j \in \{1, ..., k\}: \\ P(y_{j_{x_j}} \mid z) - P(x_j, y_j \mid z) \end{array} \right\}
$$
$$
\geq P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_p, y_q \mid z)
$$

into equation (7), and applying law of total probability, we have

$$
\begin{aligned}
& \sum_z P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_p, y_q \mid z) \times P(z) \\
\geq\ & \sum_z 0 \times P(z) \\
=\ & 0 \\
& \sum_z P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_p, y_q \mid z)) \times P(z) \\
\geq\ & \sum_z \left\{ \sum_{j=1}^{k} \Big[P(y_{j_{x_j}} \mid z) + P(x_j \mid z) \right. \\
& \left. - P(x_j, y_j \mid z) \Big] + P(x_p, y_q \mid z) - k \right\} \times P(z) \\
=\ & \sum_{j=1}^{k} \Big[P(y_{j_{x_j}}) + P(x_j) - P(x_j, y_j) \Big] \\
& + P(x_p, y_q) - k
\end{aligned}
$$

$$
\begin{aligned}
& \sum_z P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_p, y_q \mid z) \times P(z) \\
\leq\ & P(x_p, y_q \mid z) \times P(z) \\
=\ & P(x_p, y_q) \\
& \sum_z P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_p, y_q \mid z) \times P(z) \\
\leq\ & \Big[P(y_{j_{x_j}} \mid z) - P(x_j, y_j \mid z) \Big] \times P(z) \\
=\ & P(y_{j_{x_j}}) - P(x_j, y_j))
\end{aligned}
$$

Thus, we can guarantee that the proposed lower and upper bounds are no looser than those of Shu, Wang, and Li (2026). Following the notation in Mueller, Li, and Pearl (2021), $P(y_{j_{x_j}} \mid z)$ denotes experimental data within the subpopulation characterized by z. □

Proof of Theorem 6

Proof.

$$
\begin{aligned}
& PNS(k) \\
= \; & P(y_{1_{x_1}}, ..., y_{k_{x_k}}) \\
= \; & \sum_{\substack{z_1,...,z_k \\ \in\{1,...,n\}^k}} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, z_{1_{x_1}}, ..., z_{k_{x_k}}) \\
= \; & \sum_{\substack{z_1,...,z_k \\ \in\{1,...,n\}^k}} P(y_{1_{x_1}}, ..., y_{k_{x_k}} \mid z_{1_{x_1}}, ..., z_{k_{x_k}}) \\
& \times P(z_{1_{x_1}}, ..., z_{k_{x_k}}) \\
\leq \; & \sum_{\substack{z_1,...,z_k \\ \in\{1,...,n\}^k}} \min\Big\{P(y_{1_{x_1}} \mid z_{1_{x_1}}, ..., z_{k_{x_k}}), ..., \\
& P(y_{k_{x_k}} \mid z_{1_{x_1}}, ..., z_{k_{x_k}})\Big\} \\
& \times \min\Big\{P(z_{1_{x_1}}), ..., P(z_{k_{x_k}})\Big\} \\
& \text{the equality sign holds when for } \forall j \in [1,k], \\
& P(y_{j_{x_j}} \mid z_{1_{x_1}}, \ldots, z_{k_{x_k}}) = 0 \text{ or } P(z_{j_{x_j}}) = 0 \\
= \; & \sum_{\substack{z_1,...,z_k \\ \in\{1,...,n\}^k}} \min\Big\{P(y_{1_{x_1}} \mid z_{1_{x_1}}), ..., \\
& P(y_{k_{x_k}} \mid z_{k_{x_k}})\Big\} \times \min\Big\{P(z_{1_{x_1}}), ..., P(z_{k_{x_k}})\Big\} \\
& \text{it follows from the cross-world conditional} \\
& \text{independences that derive from graph:} \\
& Y_{x_j} \perp\!\!\!\perp \{Z_{x_i} : i \neq j\} \mid Z_{x_j}, \qquad j = 1, \ldots, k. \\
= \; & \sum_{\substack{z_1,...,z_k \\ \in\{1,...,n\}^k}} \min\Big\{P(y_1 \mid z_{1_{x_1}}, x_1), ..., \\
& P(y_k \mid z_{k_{x_k}}, x_k)\Big\} \times \min\Big\{P(z_{1_{x_1}}), ..., P(z_{k_{x_k}})\Big\} \\
& \text{since for } \forall x_j,\ Y_{x_j} \perp\!\!\!\perp X \mid Z_{x_j}. \\
= \; & \sum_{\substack{z_1,...,z_k \\ \in\{1,...,n\}^k}} \min\Big\{P(y_1 \mid z_1, x_1), ..., \\
& P(y_k \mid z_k, x_k)\Big\} \times \min\Big\{P(z_{1_{x_1}}), ..., P(z_{k_{x_k}})\Big\}
\end{aligned}
$$

Hence, we can say for $j \in \{1, ..., k\}$,

$$
\begin{aligned}
& PNS(k) \\
\leq & \sum_{\substack{z_1,...,z_k \\ \in\{1,...,n\}^k}} \min_j\{P(y_j \mid x_j, z_j)\} \\
& \times \min_j\{P(z_{j_{x_j}})\}
\end{aligned}
$$

□

Proof of Theorem 7

Proof.

$$
\begin{aligned}
& PSub(k,p) \\
= \; & P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_p) \\
= \; & \sum_{\substack{z_1,...,z_k \\ \in\{1,...,n\}^k}} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_p, z_{1_{x_1}}, ..., z_{k_{x_k}}) \\
= \; & \sum_{\substack{z_1,...,z_k \\ \in\{1,...,n\}^k}} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_p \mid z_{1_{x_1}}, ..., z_{k_{x_k}}) \\
& \times P(z_{1_{x_1}}, ..., z_{k_{x_k}}) \\
= \; & \sum_{\substack{z_1,...,z_k \\ \in\{1,...,n\}^k}} P(y_{1_{x_1}}, ..., y_{k_{x_k}} \mid z_{1_{x_1}}, ..., z_{k_{x_k}}) \\
& \times P(x_p \mid z_{1_{x_1}}, ..., z_{k_{x_k}}) \times P(z_{1_{x_1}}, ..., z_{k_{x_k}}) \\
& \text{since } (Y_{x_1}, \ldots, Y_{x_k}) \perp\!\!\!\perp X \mid (Z_{x_1}, \ldots, Z_{x_k}) \\
= \; & \sum_{\substack{z_1,...,z_k \\ \in\{1,...,n\}^k}} P(y_{1_{x_1}}, ..., y_{k_{x_k}} \mid z_{1_{x_1}}, ..., z_{k_{x_k}}) \\
& \times P(z_{1_{x_1}}, ..., z_{k_{x_k}}, x_p) \\
\leq \; & \sum_{\substack{z_1,...,z_k \\ \in\{1,...,n\}^k}} \min\Big\{P(y_{1_{x_1}} \mid z_{1_{x_1}}, ..., z_{k_{x_k}}), ..., \\
& P(y_{k_{x_k}} \mid z_{1_{x_1}}, ..., z_{k_{x_k}})\Big\} \\
& \times \min\Big\{P(z_{1_{x_1}}), ..., P(z_{k_{x_k}}), P(x_p)\Big\} \\
& \text{the equality sign holds when for } \forall j \in [1,k], \\
& P(y_{j_{x_j}} \mid z_{1_{x_1}}, \ldots, z_{k_{x_k}}) = 0 \\
& \text{ or } P(z_{j_{x_j}}) = 0 \text{ or } P(x_p) = 0 \\
= \; & \sum_{\substack{z_1,...,z_k \\ \in\{1,...,n\}^k}} \min\Big\{P(y_{1_{x_1}} \mid z_{1_{x_1}}), ..., \\
& P(y_{k_{x_k}} \mid z_{k_{x_k}})\Big\} \\
& \times \min\Big\{P(z_{1_{x_1}}), ..., P(z_{k_{x_k}}), P(x_p)\Big\} \\
& \text{as for } j \in [1,k]\text{: } Y_{x_j} \perp\!\!\!\perp \{Z_{x_i} : i \neq j\} \mid Z_{x_j} \\
= \; & \sum_{\substack{z_1,...,z_k \\ \in\{1,...,n\}^k}} \min\Big\{P(y_1 \mid z_{1_{x_1}}, x_1), ..., \\
& P(y_k \mid z_{k_{x_k}}, x_k)\Big\} \\
& \times \min\Big\{P(z_{1_{x_1}}), ..., P(z_{k_{x_k}}), P(x_p)\Big\} \\
& \text{since for } \forall x_j,\ Y_{x_j} \perp\!\!\!\perp X \mid Z_{x_j}. \\
= \; & \sum_{\substack{z_1,...,z_k \\ \in\{1,...,n\}^k}} \min\Big\{P(y_1 \mid z_1, x_1), ..., \\
& P(y_k \mid z_k, x_k)\Big\} \\
& \times \min\Big\{P(z_{1_{x_1}}), ..., P(z_{k_{x_k}}), P(x_p)\Big\}
\end{aligned}
$$

Hence, we can say for $j \in \{1, ..., k\}$,

$$
\begin{aligned}
& PSub(k,p) \\
\leq & \sum_{\substack{z_1,\ldots,z_k \\ \in\{1,\ldots,n\}^k}} \min_j\{P(y_j \mid x_j, z_j)\} \\
& \times \min_j\{P(z_{j_{x_j}}), P(x_p)\}
\end{aligned}
$$

□

Proof of Theorem 8

Proof.

$$
\begin{aligned}
& PRep(k,q) \\
= \ & P(y_{1_{x_1}}, ..., y_{k_{x_k}}, y_q) \\
\leq \ & P(y_{1_{x_1}}, ..., y_{k_{x_k}}) \\
& \text{the equality sign holds when } P(y_q)=0 \\
\leq \ & \sum_{\substack{z_1,\ldots,z_k \\ \in\{1,\ldots,n\}^k}} \min_j\{P(y_j \mid x_j, z_j)\} \times \min_j\{P(z_{j_{x_j}})\}
\end{aligned}
$$

Hence, we can say for $j \in \{1, ..., k\}$,

$$
\begin{aligned}
& PRep(k,q) \\
\leq & \sum_{\substack{z_1,\ldots,z_k \\ \in\{1,\ldots,n\}^k}} \min_j\{P(y_j \mid x_j, z_j)\} \times \min_j\{P(z_{j_{x_j}})\}
\end{aligned}
$$

□

Proof of Theorem 9

Proof.

$$
\begin{aligned}
& PN(k,p,q) \\
= \ & P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_p, y_q) \\
= \ & P(y_{1_{x_1}}, ..., y_{k_{x_k}}, y_{q_{x_p}}, x_p) \\
= \ & \sum_{\substack{z_1,\ldots,z_k,z_p \\ \in\{1,\ldots,n\}^{k+1}}} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, y_{q_{x_p}}, x_p, z_{1_{x_1}}, ..., \\
& z_{k_{x_k}}, z_{p_{x_p}}) \\
= \ & \sum_{\substack{z_1,\ldots,z_k,z_p \\ \in\{1,\ldots,n\}^{k+1}}} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, y_{q_{x_p}}, x_p \mid z_{1_{x_1}}, ..., \\
& z_{k_{x_k}}, z_{p_{x_p}}) \\
& \times P(z_{1_{x_1}}, ..., z_{k_{x_k}}, z_{p_{x_p}}) \\
= \ & \sum_{\substack{z_1,\ldots,z_k,z_p \\ \in\{1,\ldots,n\}^{k+1}}} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, y_{q_{x_p}} \mid z_{1_{x_1}}, ..., z_{k_{x_k}}, \\
& z_{p_{x_p}}) \\
& \times P(x_p \mid z_{1_{x_1}}, ..., z_{k_{x_k}}, z_{p_{x_p}}) \\
& \times P(z_{1_{x_1}}, ..., z_{k_{x_k}}, z_{p_{x_p}}) \\
& \text{since } \left(Y_{x_1}, \ldots, Y_{x_k}, Y_{x_p}\right) \perp\!\!\!\perp X \mid (Z_{x_1}, \ldots, Z_{x_k}, \\
& Z_{x_p}) \\
= \ & \sum_{\substack{z_1,\ldots,z_k,z_p \\ \in\{1,\ldots,n\}^{k+1}}} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, y_{q_{x_p}} \mid z_{1_{x_1}}, ..., z_{k_{x_k}}, \\
& z_{p_{x_p}}) \\
& \times P(z_{1_{x_1}}, ..., z_{k_{x_k}}, z_{p_{x_p}}, x_p) \\
\leq \ & \sum_{\substack{z_1,\ldots,z_k,z_p \\ \in\{1,\ldots,n\}^{k+1}}} \min\Big\{P(y_{1_{x_1}} \mid z_{1_{x_1}}, ..., z_{k_{x_k}}, z_{p_{x_p}}), \\
& ..., P(y_{k_{x_k}} \mid z_{1_{x_1}}, ..., z_{k_{x_k}}, z_{p_{x_p}}), \\
& P(y_{q_{x_p}} \mid z_{1_{x_1}}, ..., z_{k_{x_k}}, z_{p_{x_p}})\Big\} \\
& \times \min\Big\{P(z_{1_{x_1}}), ..., P(z_{k_{x_k}}), P(z_{p_{x_p}}), P(x_p)\Big\} \\
& \text{the equality sign holds when for } \forall j \in [1,k], \\
& P(y_{j_{x_j}} \mid z_{1_{x_1}}, \ldots, z_{k_{x_k}}, z_{p_{x_p}}) = 0 \\
& \text{ or } P(y_{q_{x_p}} \mid z_{1_{x_1}}, \ldots, z_{k_{x_k}}, z_{p_{x_p}}) = 0 \\
& \text{ or } P(z_{j_{x_j}}) = 0 \text{ or } P(z_{p_{x_p}}) = 0 \text{ or } P(x_p) = 0 \\
= \ & \sum_{\substack{z_1,\ldots,z_k,z_p \\ \in\{1,\ldots,n\}^{k+1}}} \min\Big\{P(y_{1_{x_1}} \mid z_{1_{x_1}}), ..., \\
& P(y_{k_{x_k}} \mid z_{k_{x_k}}), P(y_{q_{x_p}} \mid z_{p_{x_p}})\Big\} \\
& \times \min\Big\{P(z_{1_{x_1}}), ..., P(z_{k_{x_k}}), P(z_{p_{x_p}}), P(x_p)\Big\} \\
& \text{as for } j \in \{1, \ldots, k, p\}\text{: } Y_{x_j} \perp\!\!\!\perp \{Z_{x_i} : i \neq j\} \mid Z_{x_j} \\
= \ & \sum_{\substack{z_1,\ldots,z_k,z_p \\ \in\{1,\ldots,n\}^{k+1}}} \min\Big\{P(y_1 \mid z_{1_{x_1}}, x_1), ..., \\
& P(y_k \mid z_{k_{x_k}}, x_k), P(y_q \mid z_{p_{x_p}}, x_p)\Big\} \\
& \times \min\Big\{P(z_{1_{x_1}}), ..., P(z_{k_{x_k}}), P(z_{p_{x_p}}), P(x_p)\Big\} \\
& \text{since for } \forall x_j,\ Y_{x_j} \perp\!\!\!\perp X \mid Z_{x_j}. \\
= \ & \sum_{\substack{z_1,\ldots,z_k,z_p \\ \in\{1,\ldots,n\}^{k+1}}} \min\Big\{P(y_1 \mid z_1, x_1), ..., \\
& P(y_k \mid z_k, x_k), P(y_q \mid z_p, x_p)\Big\} \\
& \times \min\Big\{P(z_{1_{x_1}}), ..., P(z_{k_{x_k}}), P(z_{p_{x_p}}), P(x_p)\Big\}
\end{aligned}
$$

Hence, we can say for $j \in \{1, ..., k\}$,

$$
\begin{aligned}
& PN(k,p,q) \\
\leq & \sum_{\substack{z_1,\ldots,z_k,z_p \\ \in\{1,\ldots,n\}^{k+1}}} \min_j\{P(y_j \mid x_j, z_j), P(y_q \mid x_p, z_p)\} \\
& \times \min_j\{P(z_{j_{x_j}}), P(z_{p_{x_p}}), P(x_p)\}
\end{aligned}
$$

□

Proof of Theorem 10

Proof.

$$
\begin{aligned}
& PNS(k) \\
= \; & P(y_{1_{x_1}}, ..., y_{k_{x_k}}) \\
= \; & \sum_{\substack{z_1,...,z_k \\ \in \{1,...,n\}^k}} P(y_{1_{z_1}}, ..., y_{k_{z_k}}, z_{1_{x_1}}, ..., z_{k_{x_k}}) \\
= \; & \sum_{z_1 \neq ... \neq z_k} P(y_{1_{z_1}}, ..., y_{k_{z_k}}) \times P(z_{1_{x_1}}, ..., z_{k_{x_k}}) \\
\leq \; & \sum_{z_1 \neq ... \neq z_k} \min\{P(y_{1_{z_1}}), ..., P(y_{k_{z_k}})\} \\
& \times \min\{P(z_{1_{x_1}}), ..., P(z_{k_{x_k}})\} \\
& \text{the equality sign holds when for } \forall j \in [1,k], \\
& P(y_{j_{z_j}}) = 0 \text{ or } P(z_{j_{x_j}}) = 0 \\
= \; & \sum_{z_1 \neq ... \neq z_k} \min\{P(y_1 \mid z_1), ..., P(y_k \mid z_k)\} \\
& \times \min\{P(z_1 \mid x_1), ..., P(z_k \mid x_k)\}
\end{aligned}
$$

Hence, we can say for $j \in \{1, ..., k\}$,

$$
\begin{aligned}
& PNS(k) \\
\leq \; & \sum_{\substack{z_1 \neq ... \neq z_k \\ \in \{1,...,n\}^k}} \min_j\{P(y_j \mid z_j)\} \times \min_j\{P(z_j \mid x_j)\}
\end{aligned}
$$

□

Proof of Theorem 11

Proof.

$$
\begin{aligned}
& PSub(k,p) \\
= \; & P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_p) \\
= \; & \sum_{\substack{z_1,...,z_k \\ \in \{1,...,n\}^k}} P(y_{1_{z_1}}, ..., y_{k_{z_k}}, x_p, z_{1_{x_1}}, ..., z_{k_{x_k}}) \\
= \; & \sum_{z_1 \neq ... \neq z_k} P(y_{1_{z_1}}, ..., y_{k_{z_k}}) \times P(z_{1_{x_1}}, ..., z_{k_{x_k}}) \\
& \times P(x_p) \\
& \text{as } X \perp\!\!\!\perp \{Y_{z_j}, Z_{x_j}\} \\
\leq \; & \sum_{z_1 \neq ... \neq z_k} \min\{P(y_{1_{z_1}}), ..., P(y_{k_{z_k}})\} \\
& \times \min\{P(z_{1_{x_1}}), ..., P(z_{k_{x_k}})\} \times P(x_p) \\
& \text{the equality sign holds when for } \forall j \in [1,k], \\
& P(y_{j_{z_j}}) = 0 \text{ or } P(z_{j_{x_j}}) = 0 \\
= \; & \sum_{z_1 \neq ... \neq z_k} \min\{P(y_1 \mid z_1), ..., P(y_k \mid z_k)\} \\
& \times \min\{P(z_1 \mid x_1), ..., P(z_k \mid x_k)\} \times P(x_p)
\end{aligned}
$$

Hence, we can say for $j \in \{1, ..., k\}$,

$$
\begin{aligned}
& PSub(k,p) \\
\leq \; & \sum_{\substack{z_1 \neq ... \neq z_k \\ \in \{1,...,n\}^k}} \min_j\{P(y_j \mid z_j)\} \\
& \times \min_j\{P(z_j \mid x_j)\} \times P(x_p)
\end{aligned}
$$

□

Proof of Theorem 12

Proof.

$$
\begin{aligned}
& PRep(k,q) \\
= \; & P(y_{1_{x_1}}, ..., y_{k_{x_k}}, y_q) \\
\leq \; & P(y_{1_{x_1}}, ..., y_{k_{x_k}}) \\
& \text{the equality sign holds when } P(y_q) = 0 \\
\leq \; & \sum_{\substack{z_1 \neq ... \neq z_k \\ \in \{1,...,n\}^k}} \min_j\{P(y_j \mid z_j)\} \times \min_j\{P(z_j \mid x_j)\}
\end{aligned}
$$

Hence, we can say for $j \in \{1, ..., k\}$,

$$
\begin{aligned}
& PRep(k,q) \\
\leq \; & \sum_{\substack{z_1 \neq ... \neq z_k \\ \in \{1,...,n\}^k}} \min_j\{P(y_j \mid z_j)\} \times \min_j\{P(z_j \mid x_j)\}
\end{aligned}
$$

□

Proof of Theorem 13

Proof.

$$
\begin{aligned}
& PN(k,p,q) \\
= \; & P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_p, y_q) \\
= \; & P(y_{1_{x_1}}, ..., y_{k_{x_k}}, y_{q_{x_p}}, x_p) \\
= \; & \sum_{\substack{z_1,...,z_k,z_p \\ \in \{1,...,n\}^{k+1}}} P(y_{1_{z_1}}, ..., y_{k_{z_k}}, y_{q_{z_p}}, z_{1_{x_1}}, ..., z_{k_{x_k}}, \\
& z_{p_{x_p}}, x_p) \\
= \; & \sum_{z_1 \neq ... \neq z_k \neq z_p} P(y_{1_{z_1}}, ..., y_{k_{z_k}}, y_{q_{z_p}}) \\
& \times P(z_{1_{x_1}}, ..., z_{k_{x_k}}, z_{p_{x_p}}) \times P(x_p) \\
& \text{as } X \perp\!\!\!\perp \{Y_{z_j}, Z_{x_j}\} \\
\leq \; & \sum_{z_1 \neq ... \neq z_k \neq z_p} \min\{P(y_{1_{z_1}}), ..., P(y_{k_{z_k}}), P(y_{q_{z_p}})\} \\
& \times \min\{P(z_{1_{x_1}}), ..., P(z_{k_{x_k}}), P(z_{p_{x_p}})\} \times P(x_p) \\
& \text{the equality sign holds when for } \forall j \in [1,k], \\
& P(y_{j_{z_j}}) = 0 \text{ or } P(y_{q_{z_p}}) = 0 \\
& \text{or } P(z_{j_{x_j}}) = 0 \text{ or } P(z_{p_{x_p}}) = 0
\end{aligned}
$$

$$= \sum_{z_1 \neq \ldots \neq z_k \neq z_p} \min\{P(y_1 \mid z_1), ..., P(y_k \mid z_k), P(y_q \mid z_p)\} \times \min\{P(z_1 \mid x_1), ..., P(z_k \mid x_k), P(z_p \mid x_p)\} \times P(x_p)$$

Hence, we can say for $j \in \{1, ..., k\}$,

$$PN(k, p, q) \leq \sum_{\substack{z_1 \neq \ldots \neq z_k \neq z_p \\ \in \{1,\ldots,n\}^{k+1}}} \min_j \{P(y_j \mid z_j), P(y_q \mid z_p)\} \times \min_j \{P(z_j \mid x_j), P(z_p \mid x_p)\} \times P(x_p)$$

□

Examples

Example 1: From Table 1, we can collect all data we want.

Since each entry in the table represents the count $n(x, y, z)$, for each fixed value $Z = z$, we have

$$P(x \mid z) = \frac{\sum_y n(x, y, z)}{\sum_{x,y} n(x, y, z)},$$

$$P(y \mid x, z) = \frac{n(x, y, z)}{\sum_y n(x, y, z)},$$

and

$$P(y, x \mid z) = \frac{n(x, y, z)}{\sum_{x,y} n(x, y, z)}.$$

These quantities satisfy

$$P(y, x \mid z) = P(y \mid x, z)P(x \mid z).$$

For z_1, we have

$$P(z_1) = \frac{2}{5},$$
$$P(x_1 \mid z_1) = \frac{1}{6}, \quad P(x_2 \mid z_1) = \frac{1}{3}, \quad P(x_3 \mid z_1) = \frac{1}{2}.$$

$$P(y_1 \mid x_1, z_1) = \frac{23}{30}, \qquad P(y_1 \mid x_2, z_1) = \frac{1}{30},$$
$$P(y_1 \mid x_3, z_1) = \frac{9}{30}, \qquad P(y_2 \mid x_1, z_1) = \frac{6}{30},$$
$$P(y_2 \mid x_2, z_1) = \frac{28}{30}, \qquad P(y_2 \mid x_3, z_1) = \frac{20}{30},$$
$$P(y_3 \mid x_1, z_1) = \frac{1}{30}, \qquad P(y_3 \mid x_2, z_1) = \frac{1}{30},$$
$$P(y_3 \mid x_3, z_1) = \frac{1}{30}.$$

$$P(x_1, y_1 \mid z_1) = \frac{23}{180}, \qquad P(x_2, y_1 \mid z_1) = \frac{2}{180},$$
$$P(x_3, y_1 \mid z_1) = \frac{27}{180}, \qquad P(x_1, y_2 \mid z_1) = \frac{6}{180},$$
$$P(x_2, y_2 \mid z_1) = \frac{56}{180}, \qquad P(x_3, y_2 \mid z_1) = \frac{60}{180},$$
$$P(x_1, y_3 \mid z_1) = \frac{1}{180}, \qquad P(x_2, y_3 \mid z_1) = \frac{2}{180},$$
$$P(x_3, y_3 \mid z_1) = \frac{3}{180}.$$

For z_2, we have

$$P(z_2) = \frac{1}{5},$$
$$P(x_1 \mid z_2) = \frac{1}{2}, \quad P(x_2 \mid z_2) = \frac{1}{6}, \quad P(x_3 \mid z_2) = \frac{1}{3}.$$

$$P(y_1 \mid x_1, z_2) = \frac{1}{30}, \qquad P(y_1 \mid x_2, z_2) = \frac{3}{30},$$
$$P(y_1 \mid x_3, z_2) = \frac{1}{30}, \qquad P(y_2 \mid x_1, z_2) = \frac{25}{30},$$
$$P(y_2 \mid x_2, z_2) = \frac{25}{30}, \qquad P(y_2 \mid x_3, z_2) = \frac{1}{30},$$
$$P(y_3 \mid x_1, z_2) = \frac{4}{30}, \qquad P(y_3 \mid x_2, z_2) = \frac{2}{30},$$
$$P(y_3 \mid x_3, z_2) = \frac{28}{30}.$$

$$P(x_1, y_1 \mid z_2) = \frac{3}{180}, \qquad P(x_2, y_1 \mid z_2) = \frac{3}{180},$$
$$P(x_3, y_1 \mid z_2) = \frac{2}{180}, \qquad P(x_1, y_2 \mid z_2) = \frac{75}{180},$$
$$P(x_2, y_2 \mid z_2) = \frac{25}{180}, \qquad P(x_3, y_2 \mid z_2) = \frac{2}{180},$$
$$P(x_1, y_3 \mid z_2) = \frac{12}{180}, \qquad P(x_2, y_3 \mid z_2) = \frac{2}{180},$$
$$P(x_3, y_3 \mid z_2) = \frac{56}{180}.$$

For z_3, we have

$$P(z_3) = \frac{2}{5},$$
$$P(x_1 \mid z_3) = \frac{2}{3}, \quad P(x_2 \mid z_3) = \frac{1}{6}, \quad P(x_3 \mid z_3) = \frac{1}{6}.$$

$$P(y_1 \mid x_1, z_3) = \frac{24}{30}, \qquad P(y_1 \mid x_2, z_3) = \frac{22}{30},$$
$$P(y_1 \mid x_3, z_3) = \frac{2}{30}, \qquad P(y_2 \mid x_1, z_3) = \frac{3}{30},$$
$$P(y_2 \mid x_2, z_3) = \frac{1}{30}, \qquad P(y_2 \mid x_3, z_3) = \frac{1}{30},$$
$$P(y_3 \mid x_1, z_3) = \frac{3}{30}, \qquad P(y_3 \mid x_2, z_3) = \frac{7}{30},$$
$$P(y_3 \mid x_3, z_3) = \frac{27}{30}.$$

$$P(x_1,y_1 \mid z_3) = \frac{96}{180}, \qquad P(x_2,y_1 \mid z_3) = \frac{22}{180},$$
$$P(x_3,y_1 \mid z_3) = \frac{2}{180}, \qquad P(x_1,y_2 \mid z_3) = \frac{12}{180},$$
$$P(x_2,y_2 \mid z_3) = \frac{1}{180}, \qquad P(x_3,y_2 \mid z_3) = \frac{1}{180},$$
$$P(x_1,y_3 \mid z_3) = \frac{12}{180}, \qquad P(x_2,y_3 \mid z_3) = \frac{7}{180},$$
$$P(x_3,y_3 \mid z_3) = \frac{27}{180}.$$

After applying the back-door adjustment formula, which gives

$$P(y_{j_{x_j}} \mid z) = P(y_j \mid x_j, z).$$

Substituting this equality into Theorems 2 yields a new theorem that requires only observational data, without the need for experimental data. The new equation is listed below:

$$\sum_z \max \left\{ \begin{array}{c} 0, \\ \\ \sum_{j=1}^{k} P(y_j \mid x_j, z) - k + 1, \\ \\ \text{For } i \in \{1,...,k\}: \\ \sum_{\substack{1 \le j \le k \\ j \ne i}} \Big[P(y_j \mid x_j, z) + \\ + P(x_j \mid z) - P(x_j, y_j \mid z) \Big] + \\ + P(x_i, y_i \mid z) - k + 1 \end{array} \right\} \times P(z) \le PNS(k)$$

$$\sum_z \min \left\{ \begin{array}{c} \sum_{j=1}^{k} P(x_j, y_j \mid z) + \\ + \sum_{j=k+1}^{n} P(x_j \mid z), \\ \\ \text{For } j \in \{1,...,k\}: \\ P(y_j \mid x_j, z), \\ \\ \text{For } m \in \{1,...,k-1\}, \\ t_j \in \{1,...,k\}: \\ \frac{1}{m} \Big[\sum_{j=0}^{m} P(y_{t_j} \mid x_{t_j}, z) - \\ - P(x_{t_j}, y_{t_j} \mid z) \Big] \end{array} \right\} \times P(z) \ge PNS(k)$$

By applying the new bounds, we can derive

$$\sum_z \max \left\{ \begin{array}{c} 0, \\ P(y_1 \mid x_1, z) + P(y_2 \mid x_2, z) \\ + P(y_3 \mid x_3, z) - 2, \\ \Big[P(y_2 \mid x_2, z) + P(x_2 \mid z) \\ - P(x_2, y_2 \mid z) \Big] + \Big[P(y_3 \mid x_3, z) \\ + P(x_3 \mid z) - P(x_3, y_3 \mid z) \Big] \\ + P(x_1, y_1 \mid z) - 2, \\ \Big[P(y_1 \mid x_1, z) + P(x_1 \mid z) \\ - P(x_1, y_1 \mid z) \Big] + \Big[P(y_3 \mid x_3, z) \\ + P(x_3 \mid z) - P(x_3, y_3 \mid z) \Big] \\ + P(x_2, y_2 \mid z) - 2, \\ \Big[P(y_1 \mid x_1, z) + P(x_1 \mid z) \\ - P(x_1, y_1 \mid z) \Big] + \Big[P(y_2 \mid x_2, z) \\ + P(x_2 \mid z) - P(x_2, y_2 \mid z) \Big] \\ + P(x_3, y_3 \mid z) - 2 \end{array} \right\} \times P(z) \le PNS(k)$$

$$\sum_z \min \left\{ \begin{array}{c} P(x_1, y_1 \mid z) + P(x_2, y_2 \mid z) \\ + P(x_3, y_3 \mid z), \\ P(y_1 \mid x_1, z), \\ P(y_2 \mid x_2, z), \\ P(y_3 \mid x_3, z), \\ \Big[P(y_1 \mid x_1, z) - P(x_1, y_1 \mid z) \\ + P(y_2 \mid x_2, z) - P(x_2, y_2 \mid z) \Big], \\ \Big[P(y_1 \mid x_1, z) - P(x_1, y_1 \mid z) \\ + P(y_3 \mid x_3, z) - P(x_3, y_3 \mid z) \Big], \\ \Big[P(y_2 \mid x_2, z) - P(x_2, y_2 \mid z) \\ + P(y_3 \mid x_3, z) - P(x_3, y_3 \mid z) \Big], \\ \frac{1}{2} \Big[P(y_1 \mid x_1, z) - P(x_1, y_1 \mid z) \\ + P(y_2 \mid x_2, z) - P(x_2, y_2 \mid z) \\ + P(y_3 \mid x_3, z) - P(x_3, y_3 \mid z) \Big] \end{array} \right\} \times P(z) \ge PNS(k)$$

After applying all the required data we obtained before, we can derive

$$0 \le PNS(3) \le 0.033.$$

Example 2: From Table 2, we can collect all data we want.

Since each cell in the table represents the joint count $n(x,y,z)$, we obtain

$$P(z \mid x) = \frac{\sum_y n(x,y,z)}{\sum_{z,y} n(x,y,z)}.$$

That is, for a fixed $X = x$, we first sum over Y within each level $Z = z$ and then divide by the total number of individuals with $X = x$.

Similarly,

$$P(y \mid z) = \frac{\sum_x n(x,y,z)}{\sum_{x,y} n(x,y,z)}.$$

That is, for a fixed $Z = z$, we sum over X for each outcome $Y = y$ and then divide by the total number of individuals in the stratum $Z = z$.

$$\begin{aligned}
P(z_1 \mid x_1) &= \frac{28}{30}, & P(z_2 \mid x_1) &= \frac{1}{30},\\
P(z_3 \mid x_1) &= \frac{1}{30}, & P(z_1 \mid x_2) &= \frac{19}{30},\\
P(z_2 \mid x_2) &= \frac{8}{30}, & P(z_3 \mid x_2) &= \frac{3}{30},\\
P(z_1 \mid x_3) &= \frac{1}{30}, & P(z_2 \mid x_3) &= \frac{7}{30},\\
P(z_3 \mid x_3) &= \frac{22}{30}.
\end{aligned}$$

$$\begin{aligned}
P(y_1 \mid z_1) &= \frac{16}{30}, & P(y_2 \mid z_1) &= \frac{13}{30},\\
P(y_3 \mid z_1) &= \frac{1}{30}, & P(y_1 \mid z_2) &= \frac{2}{30},\\
P(y_2 \mid z_2) &= \frac{27}{30}, & P(y_3 \mid z_2) &= \frac{1}{30},\\
P(y_1 \mid z_3) &= \frac{6}{30}, & P(y_2 \mid z_3) &= \frac{3}{30},\\
P(y_3 \mid z_3) &= \frac{21}{30}.
\end{aligned}$$

Following the example, we can apply Thm. 10:

$$\min\left\{\begin{array}{c}
PNS_{UB},\\[2ex]
\min\{P(y_1 \mid z_1), P(y_2 \mid z_2), P(y_3 \mid z_3)\}\times\\
\min\{P(z_1 \mid x_1), P(z_2 \mid x_2), P(z_3 \mid x_3)\}\\
+\\
+\min\{P(y_1 \mid z_1), P(y_2 \mid z_3), P(y_3 \mid z_2)\}\times\\
\min\{P(z_1 \mid x_1), P(z_3 \mid x_2), P(z_2 \mid x_3)\}\\
+\\
+\min\{P(y_1 \mid z_2), P(y_2 \mid z_1), P(y_3 \mid z_3)\}\times\\
\min\{P(z_2 \mid x_1), P(z_1 \mid x_2), P(z_3 \mid x_3)\}\\
+\\
+\min\{P(y_1 \mid z_2), P(y_2 \mid z_3), P(y_3 \mid z_1)\}\times\\
\min\{P(z_2 \mid x_1), P(z_3 \mid x_2), P(z_1 \mid x_3)\}\\
+\\
+\min\{P(y_1 \mid z_3), P(y_2 \mid z_1), P(y_3 \mid z_2)\}\times\\
\min\{P(z_3 \mid x_1), P(z_1 \mid x_2), P(z_2 \mid x_3)\}\\
+\\
+\min\{P(y_1 \mid z_3), P(y_2 \mid z_2), P(y_3 \mid z_1)\}\times\\
\min\{P(z_3 \mid x_1), P(z_2 \mid x_2), P(z_1 \mid x_3)\}
\end{array}\right\} \geq PNS(3)$$

By applying the data, we have:

$$\begin{aligned}
&\min\left\{\begin{array}{c}
0.507,\\
\min\left\{\frac{16}{30},\frac{27}{30},\frac{21}{30}\right\}\times\min\left\{\frac{28}{30},\frac{8}{30},\frac{22}{30}\right\}\\
+\min\left\{\frac{16}{30},\frac{3}{30},\frac{1}{30}\right\}\times\min\left\{\frac{28}{30},\frac{3}{30},\frac{7}{30}\right\}\\
+\min\left\{\frac{2}{30},\frac{13}{30},\frac{21}{30}\right\}\times\min\left\{\frac{1}{30},\frac{19}{30},\frac{22}{30}\right\}\\
+\min\left\{\frac{2}{30},\frac{3}{30},\frac{1}{30}\right\}\times\min\left\{\frac{1}{30},\frac{3}{30},\frac{1}{30}\right\}\\
+\min\left\{\frac{6}{30},\frac{13}{30},\frac{1}{30}\right\}\times\min\left\{\frac{1}{30},\frac{19}{30},\frac{7}{30}\right\}\\
+\min\left\{\frac{6}{30},\frac{27}{30},\frac{1}{30}\right\}\times\min\left\{\frac{1}{30},\frac{8}{30},\frac{1}{30}\right\}
\end{array}\right\}\\
&=\min\left\{\begin{array}{c}
0.507,\\[1ex]
\frac{16}{30}\frac{8}{30}+\frac{1}{30}\frac{3}{30}+\frac{2}{30}\frac{1}{30}+\frac{1}{30}\frac{1}{30}+\frac{1}{30}\frac{1}{30}\\[1ex]
+\frac{1}{30}\frac{1}{30}
\end{array}\right\}\\
&=0.151.
\end{aligned}$$

Hence, we can conclude:

$$0 \leq \mathrm{PNS}(3) \ \leq 0.151.$$

Simulation Algorithm

We used the following algorithm to generate samples and conduct the simulations. Q selects the causal quantity; G and Z select the structure. Every theorem in the paper is one choice of (Q, G, Z). Following Mueller, Li, and Pearl (2021), we use the same procedure to generate the conditional probability tables.

Algorithm 1: Generate simulation data for Q under G

Input: Number of output samples n
Causal diagram G
Variable to condition on Z
Quantity Q, where
$Q \in \{\mathrm{PNS}(k), \mathrm{PSub}(k,p), \mathrm{PRep}(k,q), \mathrm{PN}(k,p,q)\}$

Output: List of 4-tuples containing the general lower bound, graph-based lower bound, graph-based upper bound, and general upper bound

for $i \leftarrow 1$ to n **do**
  $\mathrm{cpt} \leftarrow$ GENERATE-CPT$(G, \mathrm{Exp}(1))$
  // General (Shu et al.) lower and upper bounds
  $(\mathrm{lb}, \mathrm{ub}) \leftarrow$ Q-BOUNDS(Q, cpt)
  // Graph-based lower and upper bounds
  $(\mathrm{lb}_G, \mathrm{ub}_G) \leftarrow$ Q-GRAPH(Q, cpt, G, Z)
  APPEND-RESULT$(\mathrm{lb}, \mathrm{lb}_G, \mathrm{ub}_G, \mathrm{ub})$
end for
return output list