Identification of Probabilities of Causation: A Complete Characterization

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Abstract

Probabilities of causation are fundamental to modern decision-making. Pearl first introduced three binary probabilities of causation, and Tian and Pearl later derived tight bounds for them using Balke's linear programming. The theoretical characterization of probabilities of causation with multi-valued treatments and outcomes has remained unresolved for decades, limiting the scope of causality-based decision-making. In this paper, we resolve this foundational gap by proposing a complete set of representative probabilities of causation and proving that they are sufficient to characterize all possible probabilities of causation within the framework of Structural Causal Models (SCMs). We then formally derive tight bounds for these representative quantities using formal mathematical proofs. Finally, we demonstrate the practical relevance of our results through illustrative toy examples.

1 Introduction

In fields such as healthcare, finance, and energy, probabilities of causation can enable effective, accurate, and explainable decision-making in complex scenarios. This causality-based approach addresses key challenges, including selection bias, counterfactual reasoning, individualized decision-making, and proper credit assignment—ensuring that outcomes are attributed to the treatments or factors that actually caused them. For example, Li and Pearl [2019] proposed a unit selection framework that uses a linear combination of probabilities of causation to identify individuals who are most likely to respond as desired, while also evaluating the associated rewards and costs. Similarly, Mueller and Pearl [2022] demonstrated how probabilities of causation can guide personalized medical decisions in alignment with the ethical principle of "do no harm."

The development of probabilities of causation began in the early 2000s, when Pearl [1999] first introduced three key binary measures: the probability of necessity (PN), the probability of sufficiency (PS), and the probability of necessity and sufficiency (PNS) in the Structural Causal Models (SCMs) [Galles and Pearl, 1998, Halpern, 2000]. Tian and Pearl [2000] then derived tight bounds for these quantities using Balke's linear programming method [Balke, 1995]. Decades later, Li and Pearl [2019, 2022b] formally proved the validity of these bounds. Building on this foundation, Mueller et al. [2021], along with Dawid et al. [2017], further narrowed the bounds by incorporating covariate information and leveraging underlying causal structures.

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The aforementioned studies are all restricted to binary treatments and outcomes, which poses significant limitations for real-world applications. In contrast, extending probabilities of causation to the non-binary case enables a more detailed and informative assessment. For example, in a binary setting, physicians can only determine whether a medication is effective or not, leading to a simple yes-or-no prescription decision. However, with multi-valued treatments x_i (e.g., different dosage levels, where $1 \leq i \leq n$ and $n \in \mathbb{N}$), doctors can evaluate which dosage level yields the optimal therapeutic effect for a particular patient. This finer-grained understanding supports more personalized and effective treatment decisions.

Efforts to address non-binary cases have continued in recent work. Zhang et al. [2022], as well as Li and Pearl [2022a], proposed numerical methods for computing non-binary probabilities of causation using nonlinear programming techniques. More recently, Li and Pearl [2024] introduced the recursive-form and un-tight theoretical bounds for these probabilities. However, numerical methods are constrained by computational complexity, and recursive forms often lack sharpness—particularly in high-dimensional settings—indicating that this line of research still requires substantial advancement.

In this paper, we present tight, non-recursive, closed-form theoretical bounds for arbitrary non-binary probabilities of causation without imposing any structural restrictions. We further verified these bounds using Balke's linear programming framework [Balke, 1995] in low-dimensional settings (specifically, when the number of values for the treatment and outcome are three or four). Our approach first identifies a small set of powerful non-binary probabilities of causation that are sufficient to represent any others, and then derives tight bounds for this representative set.

1.1 Key Contributions

The contributions of our paper are summarized as follows:

- We provide a complete characterization of all nonbinary probabilities of causation in Structural Causal Models (SCMs) through a small set of representative probabilities.
- We first derive tight, closed-form bounds for these representative probabilities of causation using formal mathematical reasoning.
- We offer the first theoretical insight into the equivalence classes of probabilities of causation.
- We establish the complete theoretical foundation for discrete probabilities of causation, laying the groundwork for causality-based decision making.

2 Preliminaries

We begin by reviewing the basic definitions of probabilities of causation and the associated notation in Structural Causal Models (SCMs) [Galles and Pearl, 1998, Halpern, 2000]. Readers already familiar with SCMs may choose to skip this section.

Counterfactuals are well defined within the SCM framework. A counterfactual statement such as "Variable Y would have the value y had X been x" is denoted as $Y_x = y$. Here, the subscript x refers to a hypothetical event, which is well-defined in SCMs. For brevity, we will use y_x, $y_{x'}$, y'_x, and $y'_{x'}$ throughout the paper to represent the events $Y_x = y$, $Y_{x'} = y$, $Y_x = y'$, and $Y_{x'} = y'$, respectively. Unless otherwise specified, we assume that experimental data are available in the form of causal effects (e.g., $P(y_x)$), while observational data are provided as joint probabilities (e.g., $P(x, y)$). In our notation, X denotes the treatment variable and Y denotes the outcome or effect.

Let X and Y be two binary variables in a causal model M, where x denotes the proposition $X =$ true, x' denotes $X =$ false, y denotes $Y =$ true, and y' denotes $Y =$ false. The three basic binary probabilities of causation—PN, PS, and PNS—are defined as follows [Pearl, 1999]:

Definition 1 (Probabilities of Causation)**.** *[Pearl, 1999]*

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

PNS stands for the probability that y would respond to x both ways, and therefore measures both the sufficiency and necessity of x to produce y.

Tian and Pearl [2000] then derived tight bounds for the PN, PS, and PNS using Balke's linear programming approach [Balke, 1995]. These bounds were later given a formal theoretical proof by Li and Pearl [2019, 2022b].

The tight bounds for binary PNS,PN, and PS, are given as follows:

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

$$\max\left\{\begin{array}{c} 0, \\ \frac{P(y)-P(y_{x'})}{P(x,y)} \end{array}\right\} \leq \text{PN} \leq \min\left\{\begin{array}{c} 1, \\ \frac{P(y'_{x'})-P(x',y')}{P(x,y)} \end{array}\right\}$$

$$\max\left\{\begin{array}{c} 0, \\ \frac{P(y')-P(y'_{x})}{P(x',y')} \end{array}\right\} \leq \text{PS} \leq \min\left\{\begin{array}{c} 1, \\ \frac{P(y_x)-P(x,y)}{P(x',y')} \end{array}\right\}$$

Regarding non-binary probabilities of causation, Li and Pearl [2024] recently provided eight theorems establishing theoretical (though not tight) recursive-form bounds for cases where both the treatment and the effect are non-binary. Specifically, when the treatment variable X takes m values and the outcome variable Y takes n values, the following set of non-binary probabilities of causation are defined and bounded. (We omit the detailed bounds here; interested readers may refer to [Li and Pearl, 2024] for full derivations.)

Probability of preservation(i, j): $P(y_{i_{x_j}}, y_i)$, $s.t., 1 \leq i \leq n, 1 \leq j \leq m$

Probability of replacement(i, j, k): $P(y_{i_{x_j}}, y_k)$, $s.t., 1 \leq i, k \leq n, 1 \leq j \leq m, i \neq k$

Probability of substitute(i, j, k): $P(y_{i_{x_j}}, x_k)$, $s.t., 1 \leq i \leq n, 1 \leq j, k \leq m, j \neq k$

Probability of necessity(i, j, k, p): $P(y_{i_{x_j}}, y_k, x_p)$, $s.t., 1 \leq i, k \leq n, 1 \leq j, p \leq m, j \neq p$

Probability of necessity and sufficiency(k): $P(y_{i_1 x_{j_1}}, ..., y_{i_k x_{j_k}})$, $s.t., 1 \leq i_1, ..., i_k \leq n,$ $1 \leq j_1, ..., j_k \leq m, j_1 \neq ... \neq j_k$

Probability of substitute(k,p): $P(y_{i_1 x_{j_1}}, ..., y_{i_k x_{j_k}}, x_p)$, $s.t., 1 \leq i_1, ..., i_k \leq n,$ $1 \leq j_1, ..., j_k, p \leq m, j_1 \neq ... \neq j_k \neq p$

Probability of replacement(k,q): $P(y_{i_1 x_{j_1}}, ..., y_{i_k x_{j_k}}, y_q)$, $s.t., 1 \leq i_1, ..., i_k, q \leq n,$ $1 \leq j_1, ..., j_k \leq m, j_1 \neq ... \neq j_k$

Probability of necessity(k, p, q): $P(y_{i_1 x_{j_1}}, ..., y_{i_k x_{j_k}}, x_p, y_q)$, $s.t., 1 \leq i_1, ..., i_k, q \leq n, 1 \leq j_1, ..., j_k,$ $p \leq m, j_1 \neq ... \neq j_k \neq p.$

In this paper, we will provide closed-form tight bounds for a subset of the modified probabilities defined above and demonstrate that these selected probabilities are sufficient to represent all discrete probabilities of causation within SCMs.

3 Main Results

In this section, we first simplify the definitions of the Probability of Necessity and Sufficiency(k), Probability of Substitute(k,p), Probability of Replacement(k,q), and Probability of Necessity(k,p,q) defined by Li and Pearl [2024] into their most concise forms, while retaining their ability to represent all discrete probabilities of causation in Structural Causal Models (SCMs).

3.1 Probability of necessity and sufficiency(k)

The Probability of Necessity and Sufficiency(k) is simplified to the form $P(y_{1_{x_1}}, \ldots, y_{k_{x_k}})$, where $|X| = |Y| = n$, and the values of X and Y are arranged in increasing order within the probability expression. This simplification yields the most straightforward closed-form representation. We will later demonstrate that this simplification preserves generality. The tight bounds for the modified Probability of Necessity and Sufficiency(k) are presented in the following theorem, where "tight" indicates that for every value within the bounds, there exists at least one SCM compatible with the data that realizes it. This interpretation of tightness will apply throughout the remainder of the paper. All theorem proofs are provided in the appendix.

Theorem 2 (Probability of necessity and sufficiency(k) (PNS(k))). *Suppose variable X has n values $x_1, ..., x_n$ and Y has n values $y_1, ..., y_n$, $k \leq n$, then the probability of necessity and sufficiency(k) $P(y_{1_{x_1}}, ..., y_{k_{x_k}})$ is bounded as following:*

$$\max \left\{ \begin{array}{cc} 0, & \\ \sum_{j=1}^{k} P(y_{j_{x_j}}) - k + 1, & \\ \sum_{\substack{1 \leq j \leq k \\ j \neq i}} \left[P(y_{j_{x_j}}) + P(x_j) - P(x_j, y_j) \right] + & \\ +P(x_i, y_i) - k + 1, & i \in \{1, ..., k\} \end{array} \right\} \leq P(y_{1_{x_1}}, ..., y_{k_{x_k}})$$

$$\min \left\{ \begin{array}{cc} \sum_{j=1}^{k} P(x_j, y_j) + \sum_{j=k+1}^{n} P(x_j), & \\ P(y_{j_{x_j}}), & j \in \{1, ..., k\}, \\ \frac{1}{m} \left[\sum_{j=0}^{m} P(y_{t_j \, x_{t_j}}) - P(x_{t_j}, y_{t_j}) \right], & m \in \{1, ..., k-1\}, \\ & t_j \in \{1, ..., k\} \end{array} \right\} \geq P(y_{1_{x_1}}, ..., y_{k_{x_k}})$$

Note that PNS(k) is a nonbinary, higher-order generalization of the original PNS. For example, PNS(2)—which reduces to the binary PNS—represents the probability that y_1 would respond to x_1 and y_2 would respond to x_2, formally written as $P(y_{1_{x_1}}, y_{2_{x_2}})$. Bounds for similar probabilities, such as $P(y_{2_{x_1}}, y_{1_{x_2}})$, can also be derived by leveraging the replaceability property of the probabilities of causation, as described in Theorem 7.

The proof of tightness—that is, the conditions under which the bounds are achieved with equality—is provided in the appendix. We will also present toy examples to illustrate how tightness enhances decision-making capabilities. While some may argue that the previous definition of PNS(k) is more general, we will later demonstrate their equivalence in expressive power in Theorem 6.

3.2 Probability of substitute(k, p)

Similar to the Probability of Necessity and Sufficiency(k), the Probability of Substitute(k, p) is simplified as stated in the following theorem:

Theorem 3 (Probability of substitute(k, p) (PSub(k, p))). *Suppose variable X has n values $x_1, ..., x_n$ and Y has n values $y_1, ..., y_n$, $k \leq n$, then the probability $P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_p)$, s.t., $p \neq j$ for $1 \leq j \leq k$ is bounded as following:*

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

$$\min \left\{ \begin{array}{cc} P(x_p), & \\ P(y_{j_{x_j}}) - P(x_j, y_j), & j \in \{1, ..., k\} \end{array} \right\} \geq P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_p)$$

3.3 Probability of replacement(k, q)

Then, the Probability of replacement(k, q) is simplified as stated in the following theorem:

Theorem 4 (Probability of replacement(k, q) (PRep(k, q)))**.** *Suppose variable X has n values $x_1, ..., x_n$ and Y has n values $y_1, ..., y_n$, $k \leq n$, then the probability $P(y_{1_{x_1}}, ..., y_{k_{x_k}}, y_q)$ is bounded as following:*

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

$$\min\left\{\begin{array}{cc} P(y_{q_{x_q}}), & q \in \{1, ..., k\}, \\ \displaystyle P(x_q, y_q) + \sum_{\substack{k+1 \leq j \leq n \\ j \neq q}} P(x_j, y_q), & \\ P(y_{j_{x_j}}) - P(x_j, y_j), & j \in \{1, ..., k\}, j \neq q \end{array}\right\} \geq P(y_{1_{x_1}}, ..., y_{k_{x_k}}, y_q)$$

3.4 Probability of necessity(k, p, q)

Finally, the Probability of necessity(k, p, q) is simplified as stated in the following theorem:

Theorem 5 (Probability of necessity(k, p, q) (PN(k, p, q)))**.** *Suppose variable X has n values $x_1, ..., x_n$ and Y has n values $y_1, ..., y_n$, $k \leq n$, then the probability $P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_p, y_q)$, s.t., $p \neq j$ for $1 \leq j \leq k$ is bounded as following:*

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

$$\min\left\{\begin{array}{cc} P(x_p, y_q), & \\ P(y_{j_{x_j}}) - P(x_j, y_j), & j \in \{1, ..., k\} \end{array}\right\} \geq P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_p, y_q)$$

3.5 Equivalence Class in Probability of Causation

We now proceed to demonstrate the generality of the above modified probabilities of causation through the next two theorems.

Theorem 6 (Equivalence classes in probabilities of causation)**.** *Suppose variable X has n values $x_1, ..., x_n$, Y has m values $y_1, ..., y_m$:*

- ***Case 1:*** *Let Y' have n values $y'_1, ..., y'_n$. W.L.O.G., let $k \leq m < n$.*
  Then the bounds of the probability, $P(y_{1_{x_1}}, ..., y_{k_{x_k}})$, is exactly the same as the bounds of the probability, $P(y'_{1_{x_1}}, ..., y'_{k_{x_k}})$, where
  $$P(y'_{l_{x_j}}) = 0, P(y'_l) = 0, \text{ for } m+1 \leq l \leq n, 1 \leq j \leq n,$$
  $$\text{and, } P(y'_{l_{x_j}}) = P(y_{l_{x_j}}), P(x_j, y'_l) = P(x_j, y_l), \text{ for } 1 \leq l \leq m, 1 \leq j \leq n.$$

- ***Case 2:*** *Let X' have m values $x'_1, ..., x'_m$. W.L.O.G., let $k \leq m < n$.*
  Then the bounds of the probability, $P(y_{1_{x_1}}, ..., y_{k_{x_k}})$, is exactly the same as the bounds of the probability, $P(y'_{1_{x_1}}, ..., y'_{k_{x_k}})$, where
  $$P(y_{j_{x_l}}) = 0, P(y_{m_{x_l}}) = 1, P(x_l) = 0, \text{ for } m+1 \leq l \leq n, 1 \leq j \leq m-1,$$
  $$\text{and, } P(y_{j_{x_l}}) = P(y_{j_{x'_l}}), P(x_l, y_j) = P(x'_l, y_j) \text{ for } 1 \leq l \leq m, 1 \leq j \leq m.$$

3.6 Replaceability in Probability of Causation

Theorem 7 (Replaceability in probabilities of causation)**.** *Suppose variable X has n values $x_1, ..., x_n$ and Y has n values $y_1, ..., y_n$, then the bounds of the probability, $P(y_{1_{x_1}}, ..., y_{i-1_{x_{i-1}}}, y_{\hat{i}_{x_i}}, y_{i+1_{x_{i+1}}}, ..., y_{k_{x_k}})$, can be obtained by replacing $y_{i_{x_i}}$ with $y_{\hat{i}_{x_i}}$ for any i, such that $1 \leq i \leq n$, in the bounds of the probability, $P(y_{1_{x_1}}, ..., y_{k_{x_k}})$.*

Note that both theorems apply to the cases of PNS(k), Psub(k, p), PRep(k, q), and PN(k, p, q). For instance, to derive the bounds for $P(y_x, y_{x'}, y''_{x''} \mid x, y)$, we can first apply PN$(3, 1, 1)$ to obtain $P(y_x, y'_{x'}, y''_{x''}, x, y)$. If $|X| \neq |Y|$, we should first apply Theorem 6. Then, using the replaceability property of probabilities of causation (Theorem 7), we can convert $P(y_x, y'_{x'}, y''_{x''}, x, y)$ into $P(y_x, y_{x'}, y''_{x''}, x, y)$. Finally, dividing by $P(x, y)$ yields the desired conditional probability: $P(y_x, y_{x'}, y''_{x''} \mid x, y)$.

4 Examples

In this section, we will discuss several examples to demonstrate the effectiveness and usefulness of our results.

4.1 Bundled Marketing Strategy

A beverage company is preparing to launch their new summer drinks, which are peachy-peachy, melonnon and durianna. Due to budget constraints, they will choose one of the drinks as the main product to promote this summer and determine an appropriate promotional strategy. Hence, the company implemented a soft launch of these new refreshments to evaluate user responses. A group of users was targeted with in-app advertisements, enabling the company to collect both experimental and observational data before the official release. Customers can choose to exit the app without taking further action, add the selected drink to their shopping cart and stop there, or proceed directly to purchase. One industry research expert suggests that peachy-peachy may be the most popular drink. So the company wants to know the probability that customers will pay directly if they choose peachy-peachy, that they will do nothing if they choose melonnon, and that they will just add drink into their cart if they choose durianna.

Let X denote the options of new summer drinks, where x_1 indicates peachy-peachy, x_2 indicate melonnon, and x_3 indicates durianna. Let Y denote the outcome of customers' reaction, where y_1 indicates no further reaction, y_2 indicates adding the selected drink into cart, and y_3 indicates do the payment directly. The probability that the company desires is $P(y_{3_{x_1}}, y_{1_{x_2}}, y_{2_{x_3}})$.

The marketing researchers provided an experimental study of 900 people in which each participants was exposed to only one of the three new beverages during the soft launch. The results are shown in Table 1.

	Peachy-peachy	Melonnon	Durianna
Inactive	46	270	40
Add to cart	23	8	223
Make a payment	231	22	37
Overall	300	300	300

Table 1: Experimental data collected by the marketing department. Here, 300 people were forced to choose Peachy-peachy, 300 people were forced to choose Melonnon, and 300 people were forced to choose Durianna.

The experimental data provide the following estimates:

$$P(y_{1_{x_1}}) = 46/300, P(y_{2_{x_1}}) = 23/300, P(y_{3_{x_1}}) = 231/300,$$
$$P(y_{1_{x_2}}) = 270/300, P(y_{2_{x_2}}) = 8/300, P(y_{3_{x_2}}) = 22/300,$$
$$P(y_{1_{x_3}}) = 40/300, P(y_{2_{x_3}}) = 223/300, P(y_{3_{x_3}}) = 37/300.$$

Here, all three experimental estimates, $P(y_{3_{x_1}})$, $P(y_{1_{x_2}})$, and $P(y_{2_{x_3}})$, in the target probability of causation are higher than 0.5, which may give us the sense that the target probability of causation, $P(y_{3_{x_1}}, y_{1_{x_2}}, y_{2_{x_3}})$, would be high.

The marketing researchers also conducted an observational study of 900 people in which all participants were exposed to all new beverages during the soft launch. They were willing to make selections and chose the flavor among three options themselves. The results are shown in Table 2.

	Peachy-peachy	Melonnon	Durianna
Inactive	131	45	38
Add to cart	68	22	483
Make a payment	1	51	61
Overall	200	118	582

Table 2: Observational data collected by the hospital. Here, 900 patients were free to choose one of the three treatments by themselves; 259 patients chose surgery, 142 patients chose chemotherapy, and 598 patients chose radiation.

The observational data provide the following estimates:

$$P(x_1, y_1) = 131/900, P(x_1, y_2) = 68/900, P(x_1, y_3) = 1/900,$$
$$P(x_2, y_1) = 45/900, P(x_2, y_2) = 22/900, P(x_2, y_3) = 51/900,$$
$$P(x_3, y_1) = 38/900, P(x_3, y_2) = 483/900, P(x_3, y_3) = 61/900.$$

We then plug the estimates into Theorem 2 and Theorem 7 (see appendix for detailed calculations). We obtain the bounds of the target probability of causation as follows:

$$0.509 \leq P(y_{3_{x_1}}, y_{1_{x_2}}, y_{2_{x_3}}) \leq 0.588$$

In Li and Pearl's paper[Li and Pearl, 2024], the probability lies in the range

$$0.428 \leq P(y_{3_{x_1}}, y_{1_{x_2}}, y_{2_{x_3}}) \leq 0.588,$$

we narrower the bounds and diminish the ambiguity about whether the probability will fall in the range above or below 0.5.

In conclusion, the probability that customers would pay if they chose peachy-peachy, that they would act inactive if they chose melonnon, and that they will add the drink to the cart if they chose durianna is above 0.509 and below 0.588, implying that the company should promote peachy-peachy, and consider offering coupons for durianna to incentive purchasing power (for example, offering half off peachy-peachy if the customer has purchased durianna). For personalized promotions, once considering the groups that share the same characteristics and conducting studies on the selected subgroups, we can tailor promotional strategy base on customers' preferences.

4.2 Personal Decision-Making on Supplement Use

Molly had just celebrated her 50th birthday, and she heard from a friend about a trending wellness product that claims to help people stay youthful. Intrigued but cautious, she made an appointment with her personal physician to ask for professional advice. Her doctor was trying to provide an honest and informed answer, thus he did some research online and found the company announced that this health supplement causes zero harm to the human body and people can safely double the dose of pill if they want to be more energetic. Based on his past clinical experience and some online reviews about the product, the doctor began to wonder if the health supplement will have some negative impacts on people.

Let X represent the daily intake, where x_1 indicates the person takes four pills a day, x_2 indicates two pills per day, x_3 indicates one pill per day, and x_4 indicates the person does not take the pill (people like Molly who have not tried it yet). Let Y represent the physical condition of the individual, where y_1 indicates poor health, y_2 indicates fair or stable condition, and y_3 indicates excellent health. Now, the doctor's question becomes the following probability of causation, $P(y_{1_{x_1}}, y_{2_{x_2}}, y_{2_{x_3}}|x_4, y_2)$. In words, among individuals like Molly who have not tried the wellness product and is under fair health condition, what is the probability that they would stay fair if they tried one or two pills daily, but would have experienced negative effects if taking four pills daily.

The physician obtained data from the company, which recorded changes in health conditions among elderly individuals over a six-month period during which they took different doses of the supplement while with a similar diet and routine. The physician subsequently summarized the results of experimental and observational studies into Table 3 and Table 4.

	Four pills	Two pills	One pill	None
Poor	195	11	80	100
Fair	51	266	198	147
Excellent	54	23	22	53
Overall	300	300	300	300

Table 3: Experimental data summarized by Molly's physician. Here, 300 older people were forced to take four pills per day, 300 older people were forced to take two pills per day, 300 older people were forced to take one pill per day, and 300 older people were forced to not take the pill.

	Four pills	Two pills	One pill	None
Poor	67	11	53	46
Fair	129	17	53	436
Excellent	193	87	70	38
Overall	389	115	176	520

Table 4: Observational data summarized by Molly's physician. Here, 1200 older people were open to all choices, 389 people chose to take four pills per day, 115 people chose to take two pills per day, 176 people chose to take one pill per day, and 520 people chose to not take the pill.

The experimental data provide the estimates:

$$P(y_{1_{x_1}}) = 195/300, P(y_{2_{x_1}}) = 51/300, P(y_{3_{x_1}}) = 54/300,$$
$$P(y_{1_{x_2}}) = 11/300, P(y_{2_{x_2}}) = 266/300, P(y_{3_{x_2}}) = 23/300,$$
$$P(y_{1_{x_3}}) = 80/300, P(y_{2_{x_3}}) = 198/300, P(y_{3_{x_3}}) = 22/300,$$
$$P(y_{1_{x_4}}) = 100/300, P(y_{2_{x_4}}) = 147/300, P(y_{3_{x_4}}) = 53/300$$

The observational data provide the estimates:

$$P(x_1, y_1) = 67/1200, P(x_1, y_2) = 129/1200, P(x_1, y_3) = 193/1200,$$
$$P(x_2, y_1) = 11/1200, P(x_2, y_2) = 17/1200, P(x_2, y_3) = 87/1200,$$
$$P(x_3, y_1) = 53/1200, P(x_3, y_2) = 53/1200, P(x_3, y_3) = 70/1200,$$
$$P(x_4, y_1) = 46/1200, P(x_4, y_2) = 436/1200, P(x_4, y_3) = 38/1200$$

Based on the observational study, the company reported that among elderly individuals taking four, two, or one pill per day, improvements in wellness were observed with estimated increases of 16%, 7.3%, and 5.8%, respectively. These findings suggest that the health supplement may have a beneficial effect.

Now, consider the following probability of causation:

$$P(y_{1_{x_1}}, y_{2_{x_2}}, y_{2_{x_3}} \mid x_4, y_2) = \frac{P(y_{1_{x_1}}, y_{2_{x_2}}, y_{2_{x_3}}, x_4, y_2)}{P(x_4, y_2)}$$

What is the probability that taking more health supplement would negatively affect people?

By applying the experimental and observational estimates to Theorem 5 and Theorem 7 (see the appendix), we derive the following bounds:

$$0.0125 \leq P(y_{1_{x_1}}, y_{2_{x_2}}, y_{2_{x_3}}, x_4, y_2) \leq 0.363$$

This range is tighter than the prior bounds reported in Li and Pearl [2024]:

$$0 \leq P(y_{1_{x_1}}, y_{2_{x_2}}, y_{2_{x_3}}, x_4, y_2) \leq 0.363$$

Given that $P(x_4, y_2) = \frac{436}{1200}$, we can further compute:

$$34.4\% \leq P(y_{1_{x_1}}, y_{2_{x_2}}, y_{2_{x_3}} \mid x_4, y_2) \leq 100\%$$

which provides more informative bounds compared to:

$$0\% \leq P(y_{1_{x_1}}, y_{2_{x_2}}, y_{2_{x_3}} \mid x_4, y_2) \leq 100\%$$

as shown in Li and Pearl [2024].

As a result, the physician can now confidently inform Molly that there is a significant risk associated with taking the supplement at higher doses.

5 Conclusion

This paper presents a complete representation of probabilities of causation using experimental and observational data, without imposing assumptions on the underlying data-generating process. We introduced the concept of equivalence classes among probabilities of causation, which not only simplifies their representation but also leads to more intuitive and compact formulations of their bounds. These bounds were proven to be tight and represent the fundamental limits of what can be inferred statistically. We verified our results using Balke's linear programming in low-dimensional settings (specifically for $n = 3$ and $n = 4$), where our derived values matched exactly. However, Balke's method becomes computationally infeasible for higher dimensions due to exponential growth in the number of variables.

Our examples demonstrate the practical value of multi-valued probabilities of causation in real-world scenarios, such as bundled marketing strategies and personalized decision-making. Unlike binary settings, multi-valued treatments allow for richer and more nuanced policies—such as targeting combinations of products or uncovering hidden user preferences. This helps reduce unnecessary marketing expenditures and supports more informed decisions. While the numerical improvements in our examples over existing bounds (e.g., [Li and Pearl, 2024]) may appear modest due to the ternary structure used, the advantages become more pronounced as the dimensionality of the treatment and outcome spaces increases. Moreover, such nonbinary frameworks can empower individuals to better interpret promotional claims and make decisions aligned with their interests.

Beyond marketing, real-world applications of probabilities of causation span complex domains such as policymaking, finance, energy, and education—where binary treatments are often insufficient. In these cases, cross-world counterfactual conjunctions and multi-level treatments offer a more realistic modeling tool. Incorporating covariates and explicit causal graphs may further refine these probabilities, leading to tighter bounds and more individualized inference. This direction—especially analyzing how bounds shift under covariate adjustment—remains an important avenue for future research.

Finally, although monotonicity assumptions have enabled identifiability in the binary case, extending such assumptions to nonbinary settings reveals that point identification is generally not achievable. One promising future direction is to apply the Monotonic Incremental Treatment Effect (MITE) framework to simplify and tighten the bounds in nonbinary settings. Altogether, this work lays a theoretical foundation for tight, closed-form, and interpretable bounds of probabilities of causation in multi-valued domains, enabling more effective, efficient, and explainable decision-making across a variety of real-world applications.

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A Appendix / supplemental material

A.1 Proof of Theorems

A.1.1 Probability of necessity and sufficiency(k)

Theorem 2 (Probability of necessity and sufficiency(k) (PNS(k))). *Suppose variable X has n values $x_1, ..., x_n$ and Y has n values $y_1, ..., y_n$, $k \leq n$, then the probability of necessity and sufficiency(k) $P(y_{1_{x_1}}, ..., y_{k_{x_k}})$ is bounded as following:*

$$\max \left\{ \begin{array}{ll} 0, & \\ \sum_{j=1}^{k} P(y_{j_{x_j}}) - k + 1, & \\ \sum_{\substack{1 \leq j \leq k \\ j \neq i}} \Big[P(y_{j_{x_j}}) + P(x_j) - P(x_j, y_j) \Big] + & \\ +P(x_i, y_i) - k + 1, & i \in \{1, ..., k\} \end{array} \right\} \leq P(y_{1_{x_1}}, ..., y_{k_{x_k}})$$

$$\min \left\{ \begin{array}{ll} \sum_{j=1}^{k} P(x_j, y_j) + \sum_{j=k+1}^{n} P(x_j), & \\ P(y_{j_{x_j}}), & j \in \{1, ..., k\}, \\ \frac{1}{m} \left[\sum_{j=0}^{m} P(y_{t_{j_{x_{t_j}}}}) - P(x_{t_j}, y_{t_j}) \right], & m \in \{1, ..., k-1\}, \\ & t_j \in \{1, ..., k\} \end{array} \right\} \geq P(y_{1_{x_1}}, ..., y_{k_{x_k}})$$

Proof. By Fréchet Inequalities, we have,

$$\begin{array}{rcl} P(A_1, ..., A_n) & \geq & \max \{0, P(A_1) + ... + P(A_n) - n + 1\}, \\ P(A_1, ..., A_n) & \leq & \min \{P(A_1), ..., P(A_n)\}. \end{array}$$

Thus, we can easily derive the first two lower bounds and the second upper bound,

$$\begin{array}{rcl} P(y_{1_{x_1}}, ..., y_{k_{x_k}}) & \geq & \max \left\{ 0, \sum_{j=1}^{k} P(y_{j_{x_j}}) - k + 1 \right\} \\ P(y_{1_{x_1}}, ..., y_{k_{x_k}}) & \leq & \min_{1 \leq j \leq k} \left\{ P(y_{j_{x_j}}) \right\}. \end{array}$$

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

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

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

To proof the remaining lower bound $\sum_{\substack{1 \leq j \leq k \\ i \neq j}} \Big[P(y_{j_{x_j}}) + P(x_j) - P(x_j, y_j) \Big] + P(x_i, y_i) - k + 1$, we start from

$$\begin{array}{rcl} P(y_{1_{x_1}}, ..., y_{k_{x_k}}) & = & \sum_{j=1}^{n} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j) \\ & = & \sum_{j=1}^{k} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j) + \sum_{j=k+1}^{n} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j) \\ & \geq & \sum_{j=1}^{k} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j) \end{array}$$

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

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

$$\begin{aligned}
\sum_{j=1}^{k} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j) &= P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_i) + \sum_{\substack{1\le j\le k\\ i\neq j}} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j) \\
&\geq P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_i)
\end{aligned}$$

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

thus, we have

$$\begin{aligned}
& P(y_{1_{x_1}}, ..., y_{k_{x_k}}) \\
\geq\ & P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_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_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_i) + \sum_{j=1}^{n} P(x_j) - 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) \\
& - \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) \\
=\ & 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) \\
& + \sum_{\substack{1\le j\le k\\ j\neq i}} P(x_j) + P(x_i) + \sum_{j=k+1}^{n} P(x_j) - 1 \\
& + P(y_{1_{x_1}}, ..., y_{i-1_{x_{i-1}}}, y_{i+1_{x_{i+1}}}, ..., y_{k_{x_k}}) \\
& - \sum_{\substack{1\le j\le 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) \\
& - \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) \\
& - \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) \\
=\ & P(y_{1_{x_1}}, ..., y_{i-1_{x_{i-1}}}, y_{i+1_{x_{i+1}}}, ..., y_{k_{x_k}}) - 1 \\
& + \sum_{\substack{1\le j\le k\\ j\neq i}} P(x_j) - \sum_{\substack{1\le j\le 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) \\
& + P(x_i) - \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) \\
& + 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) \\
& + \sum_{j=k+1}^{n} P(x_j) - \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) \\
=\ & P(y_{1_{x_1}}, ..., y_{i-1_{x_{i-1}}}, y_{i+1_{x_{i+1}}}, ..., y_{k_{x_k}}) - 1 \\
& + \sum_{\substack{1\le j\le k\\ j\neq i}} P(x_j) - \sum_{\substack{1\le j\le 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) \\
& + P(x_i) - \sum_{\substack{1\le q\le 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)
\end{aligned}$$

$$
\begin{aligned}
&+\sum_{j=k+1}^{n} P(x_j) - \sum_{j=k+1}^{n} P(y_{1_{x_1}}, ..., y_{i-1_{x_{i-1}}}, y_{i+1_{x_{i+1}}}, ..., y_{k_{x_k}}, x_j) \\
\geq\ & \sum_{\substack{1\leq j\leq k \\ i\neq j}} P(y_{j_{x_j}}) - (k-2) - 1 + \sum_{\substack{1\leq j\leq k \\ j\neq i}} P(x_j) - \sum_{\substack{1\leq j\leq k \\ j\neq i}} P(x_j, y_j) \\
&+P(x_i) - \sum_{\substack{1\leq q\leq n \\ q\neq i}} P(x_i, y_q) + \sum_{j=k+1}^{n} P(x_j) - \sum_{j=k+1}^{n} P(x_j) \\
&\text{here, the equal sign holds when } \exists i \in [1,k], \text{ and } P(y_{j_{x_j}}) = 1 \text{ for } \forall j \in [1,k], j \neq i. \\
=\ & \sum_{\substack{1\leq j\leq k \\ i\neq j}} \Big[P(y_{j_{x_j}}) + P(x_j) - P(x_j, y_j)\Big] + P(x_i, y_i) - k + 1
\end{aligned}
$$

The equality of the third lower bound holds when

- $\forall x_j = 0$ for $j \in [1, n]$ and $j \neq i$
- and $\exists i \in [1,k],$ and $P(y_{j_{x_j}}) = 1$ for $\forall j \in [1,k], j \neq i.$

To proof the first upper bound,

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

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

To proof the remaining upper bound $\frac{1}{m}\Big[\sum_{j=0}^{m} P(y_{t_j}{}_{x_{t_j}}) - P(x_{t_j}, y_{t_j})\Big]$, for $m \in \{1, ..., k-1\}$, $t_j \in \{1, ..., k\}$, we can first write PNS(k) into

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

For $m = 1$,

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

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

$$
\begin{aligned}
& P(y_{1_{x_1}}, ..., y_{k_{x_k}}) \\
= & \sum_{j=1}^{n} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j) \\
= & \sum_{j=1}^{k} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j) + \sum_{j=k+1}^{n} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j) \\
\leq & \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}}) + \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}}) \\
& + \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}}) + \sum_{j=k+1}^{n} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j) \\
& \text{here, the equal sign holds when } \exists 1 \leq t_0 < t_1 \leq k, \\
& \text{ and } P(y_{i_{x_i}}) = 1 \text{ for } \forall i \in [1,k], i \neq t_0, i \neq j+t_1-t_0 \text{ for } j \in [1, k-t_1+t_0]. \\
= & \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}}) + \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}}) \\
& + \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}}) + \sum_{j=k+1}^{n} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j) \\
& + P(y_{t_0 x_{t_0}}) + P(y_{t_1 x_{t_1}}) - P(x_{t_0}, y_{t_0}) - P(x_{t_1}, y_{t_1}) \\
& - \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}}) \\
& - \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}}) \\
& + \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}) \\
& + \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}) \\
= & P(y_{t_0 x_{t_0}}) + P(y_{t_1 x_{t_1}}) - P(x_{t_0}, y_{t_0}) - P(x_{t_1}, y_{t_1}) \\
& + \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}}) + P(y_{t_0 x_{t_0}}, x_{t_0}, y_{t_1 x_{t_1}}) \\
& + \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}}) + \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}}) \\
& + \sum_{j=k+1}^{n} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j) \\
& - \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}}) \\
& - \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}})
\end{aligned}
$$

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

here, the equal sign holds when $\exists 1 \leq t_0 < t_1 \leq k,$ and $P(y_{t_0 x_{t_0}}) = 0$.

(this is just a sufficient condition illustrating tightness, while the equality can also hold in other cases)

For $m = 2$, by applying equation (1), we can get:

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

Then W.L.O.G., let $1 \leq t_0 < t_1 < t_2 \leq k$. By applying equation (2), we have

$$
\begin{aligned}
& P(y_{1 x_1},\ldots,y_{k x_k}) \\
\leq \; & \frac{1}{2} \times \Bigg\{ \Bigg[P(y_{t_0 x_{t_0}}) + P(y_{t_1 x_{t_1}}) - P(x_{t_0},y_{t_0}) - P(x_{t_1},y_{t_1}) \\
& - \sum_{\substack{\{i_1,\ldots,i_{t_0-1},i_{t_0+1},\ldots,i_{k+2}\}\\ \in\{1,\ldots,n\}^{k+1}}} P(y_{i_1 x_1},\ldots,y_{i_{t_0-1} x_{t_0-1}},y_{t_0 x_{t_0}},y_{i_{t_0+1} x_{t_0+1}},\ldots,y_{i_k x_k},x_{i_{k+1}},y_{i_{k+2}})
\end{aligned}
$$

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

$$+\Bigg[P(y_{t_0 x_{t_0}}, x_{t_0}, y_{t_1 x_{t_1}})$$

$$+\sum_{\substack{\{i_1,\dots,i_{t_1-1},i_{t_1+1},\dots,i_k\}\\ \in\{1,\dots,n\}^{k-1}}} P(y_{i_1 x_1},\dots,y_{i_{t_1-1} x_{t_1-1}}, y_{t_1 x_{t_1}}, y_{i_{t_1+1} x_{t_1+1}},\dots,y_{i_k x_k}, x_{t_1}, y_{t_1})\Bigg]\Bigg]$$

$$+\Bigg[P(y_{t_2 x_{t_2}}) - P(x_{t_2}, y_{t_2})$$

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

$$+\sum_{\substack{\{i_1,\dots,i_{t_2-1},i_{t_2+1},\dots,i_k\}\\ \in\{1,\dots,n\}^{k-1}}} P(y_{i_1 x_1},\dots,y_{i_{t_2-1} x_{t_2-1}}, y_{t_2 x_{t_2}}, y_{i_{t_2+1} x_{t_2+1}},\dots,y_{i_k x_k}, x_{t_2}, y_{t_2})$$

$$+\sum_{\substack{1\le j\le k\\ j\ne t_2}} P(y_{1 x_1},\dots,y_{k x_k}, x_j) + P(y_{t_1 x_{t_1}}, x_{t_2}, y_{t_2 x_{t_2}}) + \sum_{j=k+1}^{n} P(y_{1 x_1},\dots,y_{k x_k}, x_j)\Bigg]\Bigg\}$$

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

$$= \frac{1}{2}\times\Bigg\{\Bigg[\Bigg[P(y_{t_0 x_{t_0}}) + P(y_{t_1 x_{t_1}}) + P(y_{t_2 x_{t_2}}) - P(x_{t_0}, y_{t_0}) - P(x_{t_1}, y_{t_1}) - P(x_{t_2}, y_{t_2})$$

$$-\sum_{\substack{\{i_1,\dots,i_{t_0-1},i_{t_0+1},\dots,i_{k+2}\}\\ \in\{1,\dots,n\}^{k+1}}} P(y_{i_1 x_1},\dots,y_{i_{t_0-1} x_{t_0-1}}, y_{t_0 x_{t_0}}, y_{i_{t_0+1} x_{t_0+1}},\dots,y_{i_k x_k}, x_{i_{k+1}}, y_{i_{k+2}})$$

$$+\Bigg[\sum_{j=1}^{t_0-1} P(y_{t_0 x_{t_0}}, x_j, y_{j+t_1-t_0\, x_{j+t_1-t_0}}) + \sum_{j=t_0+1}^{k-t_1+t_0} P(y_{t_0 x_{t_0}}, x_j, y_{j+t_1-t_0\, x_{j+t_1-t_0}})$$

$$+\sum_{j=1}^{t_1-t_0} P(y_{t_0 x_{t_0}}, x_{k-t_1+t_0+j}, y_{j x_j}) + \sum_{j=k+1}^{n} P(y_{1 x_1},\dots,y_{k x_k}, x_j)$$

$$+\sum_{\substack{\{i_1,\dots,i_{t_0-1},i_{t_0+1},\dots,i_k\}\\ \in\{1,\dots,n\}^{k-1}}} P(y_{i_1 x_1},\dots,y_{i_{t_0-1} x_{t_0-1}}, y_{t_0 x_{t_0}}, y_{i_{t_0+1} x_{t_0+1}},\dots,y_{i_k x_k}, x_{t_0}, y_{t_0})\Bigg]$$

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

$$+\Bigg[P(y_{t_0 x_{t_0}}, x_{t_0}, y_{t_1 x_{t_1}}) + P(y_{t_1 x_{t_1}}, x_{t_2}, y_{t_2 x_{t_2}})$$

$$+\sum_{\substack{\{i_1,\dots,i_{t_1-1},i_{t_1+1},\dots,i_k\}\\ \in\{1,\dots,n\}^{k-1}}} P(y_{i_1 x_1},\dots,y_{i_{t_1-1} x_{t_1-1}}, y_{t_1 x_{t_1}}, y_{i_{t_1+1} x_{t_1+1}},\dots,y_{i_k x_k}, x_{t_1}, y_{t_1})\Bigg]\Bigg]$$

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

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

$$+\sum_{\substack{1\le j\le k\\ j\ne t_2}} P(y_{1_{x_1}},...,y_{k_{x_k}},x_j)+\sum_{j=k+1}^{n} P(y_{1_{x_1}},...,y_{k_{x_k}},x_j)\Big]\Big\}$$

$$\le \frac{1}{2}\times\Big[P(y_{t_0 x_{t_0}})+P(y_{t_1 x_{t_1}})+P(y_{t_2 x_{t_2}})-P(x_{t_0},y_{t_0})-P(x_{t_1},y_{t_1})-P(x_{t_2},y_{t_2})\Big]$$

here, the equal sign holds when $\exists 1\le t_0 < t_1 \le k,$ and $P(y_{t_0 x_{t_0}}) = P(y_{t_1 x_{t_1}}) = 0$.

(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 (1), we can get

$$P(y_{1_{x_1}},...,y_{k_{x_k}}) = \frac{1}{m}\times\left[\sum_{j=1}^{n} P(y_{1_{x_1}},...,y_{k_{x_k}},x_j)+(m-1)\sum_{j=1}^{n} P(y_{1_{x_1}},...,y_{k_{x_k}},x_j)\right]$$

By applying equation (3), we have

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

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

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

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

A.1.2 Probability of substitute(k,p)

Theorem 3 (Probability of substitute(k,p) (PSub(k,p))). *Suppose variable X has n values $x_1,...,x_n$ and Y has n values $y_1,...,y_n$, $k\le n$, then the probability $P(y_{1_{x_1}},...,y_{k_{x_k}},x_p)$, s.t., $p\ne j$ for $1\le j\le k$ is bounded as following:*

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

$$\min\left\{\begin{array}{c}P(x_p),\\ P(y_{j_{x_j}})-P(x_j,y_j),\quad j\in\{1,...,k\}\end{array}\right\}\ge P(y_{1_{x_1}},...,y_{k_{x_k}},x_p)$$

Proof. By Fréchet Inequalities, we have,

$$\begin{aligned}P(A_1,...,A_n) &\ge 0,\\ P(A_1,...,A_n) &\le P(A_j),\ \text{for } \forall 1\le j\le n.\end{aligned}$$

Thus, we can obtain the first lower bound and the first upper bound,

$$\begin{aligned}P(y_{1_{x_1}},...,y_{k_{x_k}},x_p) &\ge 0\\ P(y_{1_{x_1}},...,y_{k_{x_k}},x_p) &\le P(x_p).\end{aligned}$$

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

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

For the second lower bound

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

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

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

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

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

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

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

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

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

A.1.3 Probability of replacement(k, q)

Theorem 4 (Probability of replacement(k, q) (PRep(k, q)))**.** *Suppose variable X has n values $x_1, ..., x_n$ and Y has n values $y_1, ..., y_n$, $k \leq n$, then the probability $P(y_{1_{x_1}}, ..., y_{k_{x_k}}, y_q)$ is bounded as following:*

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

$$\min \left\{ \begin{array}{ll} P(y_{q_{x_q}}), & q \in \{1, ..., k\}, \\ P(x_q, y_q) + \sum_{\substack{k+1 \leq j \leq n \\ j \neq q}} P(x_j, y_q), & \\ P(y_{j_{x_j}}) - P(x_j, y_j), & j \in \{1, ..., k\}, j \neq q \end{array} \right\} \geq P(y_{1_{x_1}}, ..., y_{k_{x_k}}, y_q)$$

Proof. By Fréchet Inequalities, we have,

$$\begin{aligned}
P(A_1, ..., A_n) &\geq 0, \\
P(A_1, ..., A_n) &\leq P(A_j), \text{ for } \forall 1 \leq j \leq n.
\end{aligned}$$

Thus, we can obtain the first lower bound and the first upper bound,

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

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

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

For the second lower bound

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

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

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

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

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

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

To summarize

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

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

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

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

$$
\begin{aligned}
& +P(y_{1_{x_1}}, ..., y_{q-1_{x_{q-1}}}, y_{q+1_{x_{q+1}}}, ..., y_{k_{x_k}}) \\
& -\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) \\
& +\sum_{j=1}^{n} P(x_j) - 1 \\
= \; & P(y_{1_{x_1}}, ..., y_{q-1_{x_{q-1}}}, y_{q+1_{x_{q+1}}}, ..., y_{k_{x_k}}) - 1 \\
& +\sum_{j=1}^{k} P(x_j) - \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) \\
& -\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) \\
& +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) \\
& +\sum_{j=k+1}^{n} P(x_j) - \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) \\
& +\sum_{j=k+1}^{n} P(y_{1_{x_1}}, ..., y_{k_{x_k}}, x_j, y_q) \\
= \; & P(y_{1_{x_1}}, ..., y_{q-1_{x_{q-1}}}, y_{q+1_{x_{q+1}}}, ..., y_{k_{x_k}}) - 1 \\
& +\sum_{j=1}^{k} P(x_j) - \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) \\
& -\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) \\
& +\sum_{j=k+1}^{n} P(x_j) - \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) \\
\ge \; & \sum_{\substack{1\le j\le k,\\ j\ne q}} P(y_{j_{x_j}}) - (k-2) - 1 \\
& +\sum_{j=1}^{k} P(x_j) - \sum_{\substack{1\le j\le k,\\ j\ne q}} P(x_j, y_j) - \sum_{\substack{1\le l\le n,\\ l\ne q}} P(x_q, y_l) + \sum_{j=k+1}^{n} P(x_j) - \sum_{j=k+1}^{n}\sum_{\substack{1\le l\le n,\\ l\ne q}} P(x_j, y_l) \\
& \text{here, the equal sign holds when } \exists q \in [1,k], \text{ and } P(y_{i_{x_i}}) = 1 \text{ for } \forall i \in [1,k], i \ne q. \\
= \; & \sum_{\substack{1\le j\le k,\\ j\ne q}} P(y_{j_{x_j}}) - (k-1) \\
& +\sum_{\substack{1\le j\le k,\\ j\ne q}} P(x_j) + P(x_q) - \sum_{\substack{1\le j\le k,\\ j\ne q}} P(x_j, y_j) - \sum_{\substack{1\le l\le n,\\ l\ne q}} P(x_q, y_l) + \sum_{j=k+1}^{n} P(x_j, y_q) \\
= \; & \sum_{\substack{1\le j\le k,\\ j\ne q}} \Big[P(y_{j_{x_j}}) + P(x_j) - P(x_j, y_j)\Big] - (k-1)
\end{aligned}
$$

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

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

For the second upper bound

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

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

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

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

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

To summarize

$$
P(y_{1_{x_1}}, ..., y_{k_{x_k}}, y_q) \leq P(x_q, y_q) + \sum_{\substack{k+1\le j\le n\\ j\neq q}} P(x_j, y_q)
$$

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

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

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

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

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

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

A.1.4 Probability of necessity(k,p,q)

Theorem 5 (Probability of necessity(k,p,q) (PN(k,p,q)))**.** *Suppose variable X has n values $x_1,...,x_n$ and Y has n values $y_1,...,y_n$, $k \leq n$, then the probability $P(y_{1_{x_1}},...,y_{k_{x_k}},x_p,y_q)$, s.t., $p \neq j$ for $1 \leq j \leq k$ is bounded as following:*

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

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

Proof. By Fréchet Inequalities, we have,

$$\begin{aligned}
P(A_1,...,A_n) &\geq 0, \\
P(A_1,...,A_n) &\leq P(A_j), \text{ for } \forall 1 \leq j \leq n.
\end{aligned}$$

Thus, we can obtain the first lower bound and the first upper bound,

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

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

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

For the second lower bound

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

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

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

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

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

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

A.1.5 Equivalence Class in Probability of Causation

Theorem 6 (Equivalence classes in probabilities of causation)**.** *Suppose variable X has n values $x_1, ..., x_n$, Y has m values $y_1, ..., y_m$:*

- ***Case 1:*** *Let Y' have n values $y'_1, ..., y'_n$. W.L.O.G., let $k \leq m < n$.*
  Then the bounds of the probability, $P(y_{1_{x_1}}, ..., y_{k_{x_k}})$, is exactly the same as the bounds of the probability, $P(y'_{1_{x_1}}, ..., y'_{k_{x_k}})$, where

  $$P(y'_{l_{x_j}}) = 0, P(y'_l) = 0, \textit{ for } m+1 \leq l \leq n, 1 \leq j \leq n,$$

  $$\textit{and, } P(y'_{l_{x_j}}) = P(y_{l_{x_j}}), P(x_j, y'_l) = P(x_j, y_l), \textit{ for } 1 \leq l \leq m, 1 \leq j \leq n.$$

- ***Case 2:*** *Let X' have m values $x'_1, ..., x'_m$. W.L.O.G., let $k \leq m < n$.*
  Then the bounds of the probability, $P(y_{1_{x_1}}, ..., y_{k_{x_k}})$, is exactly the same as the bounds of the probability, $P(y'_{1_{x_1}}, ..., y'_{k_{x_k}})$, where

  $$P(y_{j_{x_l}}) = 0, P(y_{m_{x_l}}) = 1, P(x_l) = 0, \textit{ for } m+1 \leq l \leq n, 1 \leq j \leq m-1,$$

  $$\textit{and, } P(y_{j_{x_l}}) = P(y_{j_{x'_l}}), P(x_l, y_j) = P(x'_l, y_j) \textit{ for } 1 \leq l \leq m, 1 \leq j \leq m.$$

Proof.

Case 1:

Following Tian and Pearl [2000], the bounds of PNS are determined by a corresponding linear programming formulation. Therefore, to prove this theorem, we will show that the two probabilities share exactly the same linear programming formulation.

First, the bounds of PNS of treatment X with outcome Y' are determined by the following Linear programming formulation:

$$\pm min \sum_{\substack{\{j_{k+1},...,j_n,j_{n+1}\} \\ \in\{1,...,n\}^{n-k+1}}} P_{12...kj_{k+1}...j_nj_{n+1}}$$

and along with linear constraints:

$$
\begin{aligned}
\sum_{\substack{\{j_1,...,j_n,j_{n+1}\} \\ \in\{1,...,n\}^{n+1}}} P_{j_1j_2...j_nj_{n+1}} &= 1 \\
P_{j_1j_2...j_nj_{n+1}} &\geq 0
\end{aligned}
$$

$$
\begin{aligned}
\sum_{\substack{\{j_2,\dots j_n,j_{n+1}\}\\ \in\{1,\dots,n\}^n}} P_{1j_2\dots j_n j_{n+1}} &= P(y'_{1_{x_1}})\\
\sum_{\substack{\{j_2,\dots,j_n,j_{n+1}\}\\ \in\{1,\dots,n\}^n}} P_{2j_2\dots j_n j_{n+1}} &= P(y'_{2_{x_1}})\\
&\vdots\\
\sum_{\substack{\{j_2,\dots,j_n,j_{n+1}\}\\ \in\{1,\dots,n\}^n}} P_{n-1j_2\dots j_n j_{n+1}} &= P(y'_{n-1_{x_1}})\\
\sum_{\substack{\{j_1,j_3,\dots,j_n,j_{n+1}\}\\ \in\{1,\dots,n\}^n}} P_{j_1 1 j_3\dots j_n j_{n+1}} &= P(y'_{1_{x_2}})\\
&\vdots\\
\sum_{\substack{\{j_1,j_3,\dots,j_n,j_{n+1}\}\\ \in\{1,\dots,n\}^n}} P_{j_1 n-1 j_3\dots j_n j_{n+1}} &= P(y'_{n-1_{x_2}})\\
&\vdots\\
&\vdots\\
\sum_{\substack{\{j_1,\dots,j_{n-1},j_{n+1}\}\\ \in\{1,\dots,n\}^n}} P_{j_1 j_2\dots j_{n-1} 1 j_{n+1}} &= P(y'_{1_{x_n}})\\
&\vdots\\
\sum_{\substack{\{j_1,\dots,j_{n-1},j_{n+1}\}\\ \in\{1,\dots,n\}^n}} P_{j_1 j_2\dots j_{n-1} n-1 j_{n+1}} &= P(y'_{n-1_{x_n}})
\end{aligned}
$$

$$
\begin{aligned}
\sum_{\substack{\{j_2,\dots j_n\}\\ \in\{1,\dots,n\}^{n-1}}} P_{1j_2\dots j_n 1} &= P(x_1,y'_1)\\
\sum_{\substack{\{j_2,\dots,j_n\}\\ \in\{1,\dots,n\}^{n-1}}} P_{2j_2\dots j_n 1} &= P(x_1,y'_2)\\
&\vdots\\
\sum_{\substack{\{j_2,\dots,j_n\}\\ \in\{1,\dots,n\}^{n-1}}} P_{nj_2\dots j_n 1} &= P(x_1,y'_n)\\
\sum_{\substack{\{j_1,j_3,\dots,j_n\}\\ \in\{1,\dots,n\}^{n-1}}} P_{j_1 1 j_3\dots j_n 2} &= P(x_2,y'_1)\\
&\vdots
\end{aligned}
$$

$$\vdots$$

$$\sum_{\substack{\{j_1,j_3,\ldots,j_n\}\\ \in\{1,\ldots,n\}^{n-1}}} P_{j_1nj_3\ldots j_n2} = P(x_2, y'_n)$$

$$\vdots$$

$$\sum_{\substack{\{j_1,\ldots,j_{n-1}\}\\ \in\{1,\ldots,n\}^{n-1}}} P_{j_1j_2\ldots j_{n-1}1n} = P(x_n, y'_1)$$

$$\vdots$$

$$\sum_{\substack{\{j_1,\ldots,j_{n-1}\}\\ \in\{1,\ldots,n\}^{n-1}}} P_{j_1j_2\ldots j_{n-1}n-1n} = P(x_n, y'_{n-1})$$

Second, the bounds of PNS of treatment X with outcome Y are determined by the following Linear programming formulation:

$$\pm min \sum_{\substack{\{j_{k+1},\ldots,j_n\}\\ \in\{1,\ldots,m\}^{n-k}}} \sum_{j_{n+1}=1}^{n} P_{12\ldots kj_{k+1}\ldots j_nj_{n+1}}$$

and along with linear constraints:

$$\sum_{\substack{\{j_1,\ldots,j_n\}\\ \in\{1,\ldots,m\}^{n}}} \sum_{j_{n+1}=1}^{n} P_{j_1j_2\ldots j_nj_{n+1}} = 1$$

$$P_{j_1j_2\ldots j_nj_{n+1}} \geq 0$$

$$\sum_{\substack{\{j_2,\ldots j_n\}\\ \in\{1,\ldots,m\}^{n-1}}} \sum_{j_{n+1}=1}^{n} P_{1j_2\ldots j_nj_{n+1}} = P(y_{1_{x_1}})$$

$$\sum_{\substack{\{j_2,\ldots,j_n\}\\ \in\{1,\ldots,m\}^{n-1}}} \sum_{j_{n+1}=1}^{n} P_{2j_2\ldots j_nj_{n+1}} = P(y_{2_{x_1}})$$

$$\vdots$$

$$\sum_{\substack{\{j_2,\ldots,j_n\}\\ \in\{1,\ldots,m\}^{n-1}}} \sum_{j_{n+1}=1}^{n} P_{mj_2\ldots j_nj_{n+1}} = P(y_{m_{x_1}})$$

$$\sum_{\substack{\{j_1,j_3,\ldots,j_n\}\\ \in\{1,\ldots,m\}^{n-1}}} \sum_{j_{n+1}=1}^{n} P_{j_11j_3\ldots j_nj_{n+1}} = P(y_{1_{x_2}})$$

$$\vdots$$

$$\begin{aligned}
\sum_{\substack{\{j_1,j_3,\ldots,j_n\}\\ \in\{1,\ldots,m\}^{n-1}}} \sum_{j_{n+1}=1}^{n} P_{j_1 m j_3 \ldots j_n j_{n+1}} &= P(y_{m_{x_2}}) \\
&\vdots \\
\sum_{\substack{\{j_1,\ldots,j_{n-1}\}\\ \in\{1,\ldots,m\}^{n-1}}} \sum_{j_{n+1}=1}^{n} P_{j_1 j_2 \ldots j_{n-1} 1 j_{n+1}} &= P(y_{1_{x_n}}) \\
&\vdots \\
\sum_{\substack{\{j_1,\ldots,j_{n-1}\}\\ \in\{1,\ldots,m\}^{n-1}}} \sum_{j_{n+1}=1}^{n} P_{j_1 j_2 \ldots j_{n-1} m j_{n+1}} &= P(y_{m_{x_n}}) \\
\sum_{\substack{\{j_2,\ldots j_n\}\\ \in\{1,\ldots,m\}^{n-1}}} P_{1 j_2 \ldots j_n 1} &= P(x_1, y_1) \\
\sum_{\substack{\{j_2,\ldots,j_n\}\\ \in\{1,\ldots,m\}^{n-1}}} P_{2 j_2 \ldots j_n 1} &= P(x_1, y_2) \\
&\vdots \\
\sum_{\substack{\{j_2,\ldots,j_n\}\\ \in\{1,\ldots,m\}^{n-1}}} P_{m j_2 \ldots j_n 1} &= P(x_1, y_m) \\
\sum_{\substack{\{j_1,j_3,\ldots,j_n\}\\ \in\{1,\ldots,m\}^{n-1}}} P_{j_1 1 j_3 \ldots j_n 2} &= P(x_2, y_1) \\
&\vdots \\
\sum_{\substack{\{j_1,j_3,\ldots,j_n\}\\ \in\{1,\ldots,m\}^{n-1}}} P_{j_1 m j_3 \ldots j_n 2} &= P(x_2, y_m) \\
&\vdots \\
\sum_{\substack{\{j_1,\ldots,j_{n-1}\}\\ \in\{1,\ldots,m\}^{n-1}}} P_{j_1 j_2 \ldots j_{n-1} 1 n} &= P(x_n, y_1) \\
&\vdots
\end{aligned}$$

$$\sum_{\substack{\{j_1,\ldots,j_{n-1}\}\\ \in\{1,\ldots,m\}^{n-1}}} P_{j_1 j_2 \ldots j_{n-1} m-1 n} = P(x_n, y_{m-1})$$

$$\sum_{\substack{\{j_1,\ldots,j_{n-1}\}\\ \in\{1,\ldots,m\}^{n-1}}} P_{j_1 j_2 \ldots j_{n-1} m n} = P(x_n, y_m)$$

By setting

$$P(y'_{l_{x_j}}) = 0, P(y'_l) = 0$$

for $m+1 \leq l \leq n$ and $1 \leq j \leq n$, and keeping

$$P(y'_{l_{x_j}}) = P(y_{l_{x_j}}), P(x_j, y'_l) = P(x_j, y_l)$$

for $1 \leq l \leq m$ and $1 \leq j \leq n$, the two formulations are identical.

Case 2:

Again the bounds of PNS of treatment X' with outcome Y are determined by the following Linear programming formulation,

$$\pm min \sum_{\substack{\{j_{k+1},\ldots,j_m\}\\ \in\{1,\ldots,m\}^{m-k}}} \sum_{j_{n+1}=1}^{m} P_{12\ldots k j_{k+1}\ldots j_m n \ldots n j_{n+1}}$$

and along with linear constraints:

$$\sum_{\substack{\{j_1,\ldots,j_m\}\\ \in\{1,\ldots,m\}^{m}}} \sum_{j_{n+1}=1}^{m} P_{j_1 j_2 \ldots j_m n \ldots n j_{n+1}} = 1$$

$$P_{j_1 j_2 \ldots j_m n \ldots n j_{n+1}} \geq 0$$

$$\sum_{\substack{\{j_2,\ldots j_m\}\\ \in\{1,\ldots,m\}^{m-1}}} \sum_{j_{n+1}=1}^{m} P_{1 j_2 \ldots j_m n \ldots n j_{n+1}} = P(y_{1_{x'_1}})$$

$$\sum_{\substack{\{j_2,\ldots,j_m\}\\ \in\{1,\ldots,m\}^{m-1}}} \sum_{j_{n+1}=1}^{m} P_{2 j_2 \ldots j_m n \ldots n j_{n+1}} = P(y_{2_{x'_1}})$$

$$\vdots$$

$$\sum_{\substack{\{j_2,\ldots,j_m\}\\ \in\{1,\ldots,m\}^{m-1}}} \sum_{j_{n+1}=1}^{m} P_{m-1 j_2 \ldots j_m n \ldots n j_{n+1}} = P(y_{m-1_{x'_1}})$$

$$\sum_{\substack{\{j_1,j_3,\ldots,j_m\}\\ \in\{1,\ldots,m\}^{m-1}}} \sum_{j_{n+1}=1}^{m} P_{j_1 1 j_3 \ldots j_m n \ldots n j_{n+1}} = P(y_{1_{x'_2}})$$

$$\vdots$$

$$\sum_{\substack{\{j_1,j_3,\ldots,j_m\}\\ \in\{1,\ldots,m\}^{m-1}}} \sum_{j_{n+1}=1}^{m} P_{j_1 m-1 j_3 \ldots j_m n \ldots n j_{n+1}} = P(y_{m-1_{x'_2}})$$

$$\vdots$$

$$\sum_{\substack{\{j_1,\dots,j_{m-1}\}\\ \in\{1,\dots,m\}^{m-1}}} \sum_{j_{n+1}=1}^{m} P_{j_1 j_2 \dots j_{m-1} 1 n \dots n j_{n+1}} = P(y_{1_{x'_m}})$$

$$\vdots$$

$$\sum_{\substack{\{j_1,\dots,j_{m-1}\}\\ \in\{1,\dots,m\}^{m-1}}} \sum_{j_{n+1}=1}^{m} P_{j_1 j_2 \dots j_{m-1} m-1 n \dots n j_{n+1}} = P(y_{m-1_{x'_m}})$$

$$\sum_{\substack{\{j_2,\dots j_m\}\\ \in\{1,\dots,m\}^{m-1}}} P_{1 j_2 \dots j_m n \dots n 1} = P(x_1, y_1)$$

$$\sum_{\substack{\{j_2,\dots,j_m\}\\ \in\{1,\dots,m\}^{m-1}}} P_{2 j_2 \dots j_m n \dots n 1} = P(x'_1, y_2)$$

$$\vdots$$

$$\sum_{\substack{\{j_2,\dots,j_m\}\\ \in\{1,\dots,m\}^{m-1}}} P_{m j_2 \dots j_m n \dots n 1} = P(x'_1, y_m)$$

$$\sum_{\substack{\{j_1,j_3,\dots,j_m\}\\ \in\{1,\dots,m\}^{m-1}}} P_{j_1 1 j_3 \dots j_m n \dots n 2} = P(x'_2, y_1)$$

$$\vdots$$

$$\sum_{\substack{\{j_1,j_3,\dots,j_m\}\\ \in\{1,\dots,m\}^{m-1}}} P_{j_1 m j_3 \dots j_m n \dots n 2} = P(x'_2, y_m)$$

$$\vdots$$

$$\sum_{\substack{\{j_1,\dots,j_{m-1}\}\\ \in\{1,\dots,m\}^{m-1}}} P_{j_1 j_2 \dots j_{m-1} 1 n \dots n m} = P(x'_m, y_1)$$

$$\vdots$$

$$\sum_{\substack{\{j_1,\dots,j_{m-1}\}\\ \in\{1,\dots,m\}^{m-1}}} P_{j_1 j_2 \dots j_{m-1} m-1 n \dots n m} = P(x'_m, y_{m-1})$$

$$\sum_{\substack{\{j_1,\ldots,j_{m-1}\}\\ \in\{1,\ldots,m\}^{m-1}}} P_{j_1 j_2 \ldots j_{m-1} mn \ldots nm} = P(x'_m, y_m)$$

And the bounds of PNS of treatment X and outcome Y are determined by the following Linear programming formulation:

$$\pm min \sum_{\substack{\{j_{k+1},\ldots,j_n\}\\ \in\{1,\ldots,m\}^{n-k}}} \sum_{j_{n+1}=1}^{n} P_{12\ldots k j_{k+1}\ldots j_n j_{n+1}}$$

and along with linear constraints:

$$\begin{aligned}
\sum_{\substack{\{j_1,\ldots,j_n\}\\ \in\{1,\ldots,m\}^{n}}} \sum_{j_{n+1}=1}^{n} P_{j_1 j_2 \ldots j_n j_{n+1}} &= 1\\
P_{j_1 j_2 \ldots j_n j_{n+1}} &\geq 0\\
\sum_{\substack{\{j_2,\ldots j_n\}\\ \in\{1,\ldots,m\}^{n-1}}} \sum_{j_{n+1}=1}^{n} P_{1 j_2 \ldots j_n j_{n+1}} &= P(y_{1_{x_1}})\\
\sum_{\substack{\{j_2,\ldots,j_n\}\\ \in\{1,\ldots,m\}^{n-1}}} \sum_{j_{n+1}=1}^{n} P_{2 j_2 \ldots j_n j_{n+1}} &= P(y_{2_{x_1}})\\
&.\\
&.\\
&.\\
\sum_{\substack{\{j_2,\ldots,j_n\}\\ \in\{1,\ldots,m\}^{n-1}}} \sum_{j_{n+1}=1}^{n} P_{m-1 j_2 \ldots j_n j_{n+1}} &= P(y_{m-1_{x_1}})\\
\sum_{\substack{\{j_1,j_3,\ldots,j_n\}\\ \in\{1,\ldots,m\}^{n-1}}} \sum_{j_{n+1}=1}^{n} P_{j_1 1 j_3 \ldots j_n j_{n+1}} &= P(y_{1_{x_2}})\\
&.\\
&.\\
&.\\
\sum_{\substack{\{j_1,j_3,\ldots,j_n\}\\ \in\{1,\ldots,m\}^{n-1}}} \sum_{j_{n+1}=1}^{n} P_{j_1 m-1 j_3 \ldots j_n j_{n+1}} &= P(y_{m-1_{x_2}})\\
&.\\
&.\\
&.\\
&.\\
&.\\
&.\\
\sum_{\substack{\{j_1,\ldots,j_{n-1}\}\\ \in\{1,\ldots,m\}^{n-1}}} \sum_{j_{n+1}=1}^{n} P_{j_1 j_2 \ldots j_{n-1} 1 j_{n+1}} &= P(y_{1_{x_n}})\\
&.\\
&.\\
&.
\end{aligned}$$

$$
\begin{aligned}
\sum_{\substack{\{j_1,\ldots,j_{n-1}\}\\ \in\{1,\ldots,m\}^{n-1}}} \sum_{j_{n+1}=1}^{n} P_{j_1 j_2 \ldots j_{n-1} m-1 j_{n+1}} &= P(y_{m-1_{x_n}}) \\
\sum_{\substack{\{j_2,\ldots j_n\}\\ \in\{1,\ldots,m\}^{n-1}}} P_{1 j_2 \ldots j_n 1} &= P(x_1, y_1) \\
\sum_{\substack{\{j_2,\ldots,j_n\}\\ \in\{1,\ldots,m\}^{n-1}}} P_{2 j_2 \ldots j_n 1} &= P(x_1, y_2) \\
&\;\;\vdots \\
\sum_{\substack{\{j_2,\ldots,j_n\}\\ \in\{1,\ldots,m\}^{n-1}}} P_{m j_2 \ldots j_n 1} &= P(x_1, y_m) \\
\sum_{\substack{\{j_1,j_3,\ldots,j_n\}\\ \in\{1,\ldots,m\}^{n-1}}} P_{j_1 1 j_3 \ldots j_n 2} &= P(x_2, y_1) \\
&\;\;\vdots \\
\sum_{\substack{\{j_1,j_3,\ldots,j_n\}\\ \in\{1,\ldots,m\}^{n-1}}} P_{j_1 m j_3 \ldots j_n 2} &= P(x_2, y_m) \\
&\;\;\vdots \\
&\;\;\vdots \\
\sum_{\substack{\{j_1,\ldots,j_{n-1}\}\\ \in\{1,\ldots,m\}^{n-1}}} P_{j_1 j_2 \ldots j_{n-1} 1 n} &= P(x_n, y_1) \\
&\;\;\vdots \\
\sum_{\substack{\{j_1,\ldots,j_{n-1}\}\\ \in\{1,\ldots,m\}^{n-1}}} P_{j_1 j_2 \ldots j_{n-1} m-1 n} &= P(x_n, y_{m-1})
\end{aligned}
$$

By setting

$$P(x_l) = 0, P(y_{j_{x_l}}) = 0, P(y_{m_{x_l}}) = 1$$

for $m+1 \leq l \leq n$ and $1 \leq j \leq m-1$ and keeping

$$P(y_{j_{x_l}}) = P(y_{j_{x'_l}}), P(x_l, y_j) = P(x'_l, y_j)$$

for $1 \leq l \leq m, 1 \leq j \leq m$, the two formulations are again identical.

The proofs of equivalence for the other three theorems (Psub(K,p), PRep(K,q), and PN(K,p,q)) can be derived using similar steps outlined above. □

A.1.6 Replaceability in Probability of Causation

Theorem 7 (Replaceability in probabilities of causation)**.** *Suppose variable X has n values $x_1, \ldots, x_n$ and Y has n values $y_1, \ldots, y_n$, then the bounds of the probability,*

$P(y_{1_{x_1}}, ..., y_{i-1_{x_{i-1}}}, y_{\hat{i}_{x_i}}, y_{i+1_{x_{i+1}}}, ..., y_{k_{x_k}})$, *can be obtained by replacing* $y_{i_{x_i}}$ *with* $y_{\hat{i}_{x_i}}$ *for any* i, *such that* $1 \leq i \leq n$, *in the bounds of the probability,* $P(y_{1_{x_1}}, ..., y_{k_{x_k}})$.

Proof. By replacing each term of $y_{i_{x_i}}$ with $y_{\hat{i}_{x_i}}$ in $P(y_{1_{x_1}}, ..., y_{k_{x_k}})$, and following the same steps used in the proof of Theorem 2 (see A.1.1), we obtain exactly the same upper and lower bounds as the bounds of $P(y_{1_{x_1}}, ..., y_{i-1_{x_{i-1}}}, y_{\hat{i}_{x_i}}, y_{i+1_{x_{i+1}}}, ..., y_{k_{x_k}})$.

The proofs of replaceability for the other three probabilities of causation (i.e., Psub(K, p), PRep(K, q), and PN(K, p, q)) can be derived by replacing the term $y_{i_{x_i}}$ with $y_{\hat{i}_{x_i}}$ first and then following the same steps (as in A.1.2, A.1.3, A.1.4) outlined above. $\square$

A.2 Calculation in the Examples

A.2.1 Marketing strategy

The experimental data provide the following estimates:

$$P(y_{1_{x_1}}) = 46/300, P(y_{2_{x_1}}) = 23/300, P(y_{3_{x_1}}) = 231/300,$$
$$P(y_{1_{x_2}}) = 270/300, P(y_{2_{x_2}}) = 8/300, P(y_{3_{x_2}}) = 22/300,$$
$$P(y_{1_{x_3}}) = 40/300, P(y_{2_{x_3}}) = 223/300, P(y_{3_{x_3}}) = 37/300.$$

The observational data provide the following estimates:

$$P(x_1, y_1) = 131/900, P(x_1, y_2) = 68/900, P(x_1, y_3) = 1/900,$$
$$P(x_2, y_1) = 45/900, P(x_2, y_2) = 22/900, P(x_2, y_3) = 51/900,$$
$$P(x_3, y_1) = 38/900, P(x_3, y_2) = 483/900, P(x_3, y_3) = 61/900.$$

By Theorem 2 and Theorem 7, we derive the following bounds of the target probability of causation $P(y_{3_{x_1}}, y_{2_{x_2}}, y_{3_{x_3}})$:

$$\max\left\{\begin{array}{c} 0, \\ P(y_{3_{x_1}}) + P(y_{1_{x_2}}) + P(y_{2_{x_3}}) - 2, \\ P(y_{3_{x_1}}) + P(x_1) - P(x_1, y_3) \\ +P(y_{1_{x_2}}) + P(x_2) - P(x_2, y_1) + P(x_3, y_2) - 2, \\ P(y_{3_{x_1}}) + P(x_1) - P(x_1, y_3) \\ +P(y_{2_{x_3}}) + P(x_3) - P(x_3, y_2) + P(x_2, y_1) - 2, \\ P(y_{1_{x_2}}) + P(x_2) - P(x_2, y_1) \\ +P(y_{2_{x_3}}) + P(x_3) - P(x_3, y_2) + P(x_1, y_3) - 2 \end{array}\right\} \leq P(y_{3_{x_1}}, y_{1_{x_2}}, y_{2_{x_3}})$$

$$\min\left\{\begin{array}{c} P(x_1, y_3) + P(x_2, y_1) + P(x_3, y_2), \\ P(y_{3_{x_1}}), \\ P(y_{1_{x_2}}), \\ P(y_{2_{x_3}}), \\ P(y_{3_{x_1}}) + P(y_{1_{x_2}}) - P(x_1, y_3) - P(x_2, y_1), \\ P(y_{3_{x_1}}) + P(y_{2_{x_3}}) - P(x_1, y_3) - P(x_3, y_2), \\ P(y_{1_{x_2}}) + P(y_{2_{x_3}}) - P(x_2, y_1) - P(x_3, y_2), \\ \frac{1}{2}\Big[P(y_{3_{x_1}}) + P(y_{1_{x_2}}) + P(y_{2_{x_3}}) \\ -P(x_1, y_3) - P(x_2, y_1) - P(x_3, y_2)\Big] \end{array}\right\} \geq P(y_{3_{x_1}}, y_{1_{x_2}}, y_{2_{x_3}})$$

Thus,

$$\max\left\{\begin{array}{c} 0, \\ (231 + 270 + 223)/300 - 2, \\ (231 + 270)/300 + (131 + 68 + 22 + 51 + 483)/900 - 2, \\ (231 + 223)/300 + (131 + 68 + 38 + 61 + 45)/900 - 2, \\ (270 + 223)/300 + (22 + 51 + 38 + 61 + 1)/900 - 2 \end{array}\right\} \leq P(y_{3_{x_1}}, y_{1_{x_2}}, y_{2_{x_3}})$$

$$\min\left\{\begin{array}{c}(1+45+483)/900,\\ 231/300,\\ 270/300,\\ 223/300,\\ (231+270)/300-(1+45)/900,\\ (231+223)/300-(1+483)/900,\\ (270+223)/300-(45+483)/900,\\ \frac{1}{2}\Big[(231+270+223)/300-(1+45+483)/900\Big]\end{array}\right\}\geq P(y_{3_{x_1}},y_{1_{x_2}},y_{2_{x_3}})$$

Overall,

$$0.509 \leq P(y_{3_{x_1}},y_{1_{x_2}},y_{2_{x_3}}) \leq 0.588$$

A.2.2 Personal Decision-Making on Supplement Use

The experimental data provide the estimates:

$$\begin{array}{l}P(y_{1_{x_1}})=195/300, P(y_{2_{x_1}})=51/300, P(y_{3_{x_1}})=54/300,\\ P(y_{1_{x_2}})=11/300, P(y_{2_{x_2}})=266/300, P(y_{3_{x_2}})=23/300,\\ P(y_{1_{x_3}})=80/300, P(y_{2_{x_3}})=198/300, P(y_{3_{x_3}})=22/300,\\ P(y_{1_{x_4}})=100/300, P(y_{2_{x_4}})=147/300, P(y_{3_{x_4}})=53/300\end{array}$$

The observational data provide the estimates:

$$\begin{array}{l}P(x_1,y_1)=67/1200, P(x_1,y_2)=129/1200, P(x_1,y_3)=193/1200,\\ P(x_2,y_1)=11/1200, P(x_2,y_2)=17/1200, P(x_2,y_3)=87/1200,\\ P(x_3,y_1)=53/1200, P(x_3,y_2)=53/1200, P(x_3,y_3)=70/1200,\\ P(x_4,y_1)=46/1200, P(x_4,y_2)=436/1200, P(x_4,y_3)=38/1200\end{array}$$

We plug the experimental and observational estimates into Theorem 5 and Theorem 7 to obtain the following bounds:

$$\max\left\{\begin{array}{c}0,\\ P(y_{1_{x_1}})+P(x_1)-P(x_1,y_1)+\\ +P(y_{2_{x_2}})+P(x_2)-P(x_2,y_2)+\\ +P(y_{2_{x_3}})+P(x_3)-P(x_3,y_2)+P(x_4,y_2)-3\end{array}\right\}\leq P(y_{1_{x_1}},y_{2_{x_2}},y_{2_{x_3}},x_4,y_2)$$

$$\min\left\{\begin{array}{c}P(x_4,y_2),\\ P(y_{1_{x_1}})-P(x_1,y_1),\\ P(y_{2_{x_2}})-P(x_2,y_2),\\ P(y_{2_{x_3}})-P(x_3,y_2)\end{array}\right\}\geq P(y_{1_{x_1}},y_{2_{x_2}},y_{2_{x_3}},x_4,y_2)$$

Thus,

$$\max\left\{\begin{array}{c}0,\\ (195+266+198)/300+\\ +(129+193+11+87+53+70+436)/1200-3\end{array}\right\}\leq P(y_{1_{x_1}},y_{2_{x_2}},y_{2_{x_3}},x_4,y_2)$$

$$\min\left\{\begin{array}{c}436/1200,\\ 195/300-67/1200\\ 266/300-17/1200\\ 198/300-53/1200\end{array}\right\}\geq P(y_{1_{x_1}},y_{2_{x_2}},y_{2_{x_3}},x_4,y_2)$$

Overall,

$$0.0125 \leq P(y_{1_{x_1}},y_{2_{x_2}},y_{2_{x_3}},x_4,y_2) \leq 0.363$$