

## A Characterization of Interventional Distributions in Semi-Markovian Causal Models

**Jin Tian and Changsung Kang**

Department of Computer Science  
Iowa State University  
Ames, IA 50011  
{jtian, cskang}@cs.iastate.edu

**Judea Pearl**

Cognitive Systems Laboratory  
Computer Science Department  
University of California, Los Angeles, CA 90024  
judea@cs.ucla.edu

### Abstract

We offer a complete characterization of the set of distributions that could be induced by local interventions on variables governed by a causal Bayesian network of unknown structure, in which some of the variables remain unmeasured. We show that such distributions are constrained by a simply formulated set of inequalities, from which bounds can be derived on causal effects that are not directly measured in randomized experiments.

### Introduction

The use of graphical models for encoding distributional and causal information is now fairly standard (Pearl 1988; Spirtes, Glymour, & Scheines 1993; Heckerman & Shachter 1995; Lauritzen 2000; Pearl 2000; Dawid 2002). The most common such representation involves a *causal Bayesian network (BN)*, namely, a directed acyclic graph (DAG)  $G$  which, in addition to the usual conditional independence interpretation, is also given a causal interpretation. This additional feature permits one to infer the effects of interventions or actions, called causal effects, such as those encountered in policy analysis, treatment management, or planning. Specifically, if an external intervention fixes any set  $T$  of variables to some constants  $t$ , the DAG permits us to infer the resulting post-intervention distribution, denoted by  $P_t(v)$ ,<sup>1</sup> from the pre-intervention distribution  $P(v)$ . A complete characterization of the set of interventional distributions induced by a causal BN of a known structure has been given in (Pearl 2000, pp.23-4) when all variables are observed.

If we do not possess the structure of the underlying causal BN, can we still reason about causal effects? One approach is to identify a set of properties or axioms that characterize causal relations in general, and use those properties as symbolic inferential rules. Assuming deterministic functional relationships between variables, complete axiomatizations of causal relations using counterfactuals are given in (Galles & Pearl 1998; Halpern 2000). The resulting axioms, however, cannot be directly applied to probabilistic domains in

their deterministic setting, prior to deriving their probabilistic implications. Additionally, statisticians and philosophers have expressed suspicion of deterministic models as a basis for causal analysis (Dawid 2002), partly because such models stand contrary to statistical tradition and partly because they do not apply to quantum mechanical systems. The causal models treated in this paper are purely stochastic.

We seek a characterization for the set of interventional distributions,  $P_t(v)$ , that could be induced by some causal BN of unknown structure. The motivation is two-fold. Assume that we have obtained a collection of experimental distributions by manipulating various sets of variables and observing others. We may ask several questions: (1) Is this collection compatible with the predictions of some underlying causal BN? That is, can this collection indeed be generated by some causal BN? (2) If we assume that the collection was generated by some underlying causal BN (even if we do not know its structure), what can we predict about new interventions that were not tried experimentally? (that is, about interventional distributions that are not in the given collection.)

These questions can be answered by an axiomatization of interventional distributions generated by causal BNs. When all variables are observed, a complete characterization of the set of interventional distributions inducible by some causal BN is given in (Tian & Pearl 2002). In this paper, we will seek a characterization of interventional distributions inducible by Semi-Markovian BNs, a class of Bayesian networks in which some of the variables are unobserved. We identify four properties that are both necessary and sufficient for the existence of a semi-Markovian BN capable of generating any given set of interventional distributions.

### Causal Bayesian Networks and Interventions

A causal Bayesian network, also known as a *Markovian model*, consists of two mathematical objects: (i) a DAG  $G$ , called a *causal graph*, over a set  $V = \{V_1, \dots, V_n\}$  of vertices, and (ii) a probability distribution  $P(v)$ , over the set  $V$  of discrete variables that correspond to the vertices in  $G$ .<sup>2</sup> The interpretation of such a graph has two

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<sup>1</sup>(Pearl 1995; 2000) used the notation  $P(v|set(t))$ ,  $P(v|do(t))$ , or  $P(v|\hat{t})$  for the post-intervention distribution, while (Lauritzen 2000) used  $P(v||t)$ .

<sup>2</sup>We only consider discrete random variables in this paper.

components, probabilistic and causal.<sup>3</sup> The probabilistic interpretation views  $G$  as representing conditional independence restrictions on  $P$ : Each variable is independent of all its non-descendants given its direct parents in the graph. These restrictions imply that the joint probability function  $P(v) = P(v_1, \dots, v_n)$  factorizes according to the product

$$P(v) = \prod_i P(v_i | pa_i) \quad (1)$$

where  $pa_i$  are (values of) the parents of variable  $V_i$  in  $G$ .

The causal interpretation views the arrows in  $G$  as representing causal influences between the corresponding variables. In this interpretation, the factorization of (1) still holds, but the factors are further assumed to represent autonomous data-generation processes, that is, each conditional probability  $P(v_i | pa_i)$  represents a stochastic process by which the values of  $V_i$  are assigned<sup>4</sup> in response to the values  $pa_i$  (previously chosen for  $V_i$ 's parents), and the stochastic variation of this assignment is assumed independent of the variations in all other assignments in the model. Moreover, each assignment process remains invariant to possible changes in the assignment processes that govern other variables in the system. This modularity assumption enables us to predict the effects of interventions, whenever interventions are described as specific modifications of some factors in the product of (1). The simplest such intervention, called *atomic*, involves fixing a set  $T$  of variables to some constants  $T = t$ , which yields the post-intervention distribution

$$P_t(v) = \begin{cases} \prod_{\{i|V_i \notin T\}} P(v_i | pa_i) & v \text{ consistent with } t. \\ 0 & v \text{ inconsistent with } t. \end{cases} \quad (2)$$

Eq. (2) represents a truncated factorization of (1), with factors corresponding to the manipulated variables removed. This truncation follows immediately from (1) since, assuming modularity, the post-intervention probabilities  $P(v_i | pa_i)$  corresponding to variables in  $T$  are either 1 or 0, while those corresponding to unmanipulated variables remain unaltered. If  $T$  stands for a set of treatment variables and  $Y$  for an outcome variable in  $V \setminus T$ , then Eq. (2) permits us to calculate the probability  $P_t(y)$  that event  $Y = y$  would occur if treatment condition  $T = t$  were enforced uniformly over the population. This quantity, often called the ‘‘causal effect’’ of  $T$  on  $Y$ , is what we normally assess in a controlled experiment with  $T$  randomized, in which the distribution of  $Y$  is estimated for each level  $t$  of  $T$ .

When some variables in a Markovian model are unobserved, the probability distribution over the observed variables may no longer be decomposed as in Eq. (1). Let

<sup>3</sup>A more refined interpretation, called *functional*, is also common (Pearl 2000), which, in addition to interventions, supports counterfactual readings. The functional interpretation assumes strictly deterministic, functional relationships between variables in the model, some of which may be unobserved.

<sup>4</sup>In contrast with functional models, here the probability of each  $V_i$ , not its precise value, is determined by the other variables in the model.

$V = \{V_1, \dots, V_n\}$  and  $U = \{U_1, \dots, U_{n'}\}$  stand for the sets of observed and unobserved variables respectively. If no  $U$  variable is a descendant of any  $V$  variable, then the corresponding model is called a *semi-Markovian model*. In a semi-Markovian model, the observed probability distribution,  $P(v)$ , becomes a mixture of products:

$$P(v) = \sum_u \prod_i P(v_i | pa_i, u^i) P(u) \quad (3)$$

where  $PA_i$  and  $U^i$  stand for the sets of the observed and unobserved parents of  $V_i$ , and the summation ranges over all the  $U$  variables. The post-intervention distribution, likewise, will be given as a mixture of truncated products

$$P_t(v) = \begin{cases} \sum_u \prod_{\{i|V_i \notin T\}} P(v_i | pa_i, u^i) P(u) & v \text{ consistent with } t. \\ 0 & v \text{ inconsistent with } t. \end{cases} \quad (4)$$

## Characterizing Interventional Distributions

Let  $\mathbf{P}_*$  denote the set of all interventional distributions

$$\mathbf{P}_* = \{P_t(v) | T \subseteq V, t \in Dm(T), v \in Dm(V)\} \quad (5)$$

where  $Dm(T)$  represents the domain of  $T$ . The set of interventional distributions induced by a given causal BN must satisfy some properties. For example the following property

$$P_{pa_i}(v_i) = P(v_i | pa_i), \text{ for all } i, \quad (6)$$

must hold in all Markovian models, but may not hold in semi-Markovian models. A complete characterization of the set of interventional distributions induced by a given Markovian model is given in (Pearl 2000, pp.23-4).

Now assume that we are given a collection of interventional distributions, but the underlying causal BN, if such exists, is unknown. We ask whether the collection is compatible with the predictions of some underlying causal BN. As an example, assume that  $V$  consists of two binary variables  $X$  and  $Y$  with the domain of  $X$  being  $\{x_0, x_1\}$  and the domain of  $Y$  being  $\{y_0, y_1\}$ . Then  $\mathbf{P}_*$  consists of the following distributions

$$\mathbf{P}_* = \{P(x, y), P_{x_0}(x, y), P_{x_1}(x, y), P_{y_0}(x, y), P_{y_1}(x, y), P_{x_0, y_0}(x, y), P_{x_0, y_1}(x, y), P_{x_1, y_0}(x, y), P_{x_1, y_1}(x, y)\},$$

where each  $P_t(x, y)$  is an *arbitrary* probability distribution over  $X, Y$  with an index  $t$ . For this set of distributions to be induced by some underlying causal BN such that each  $P_t(x, y)$  corresponds to the distribution of  $X, Y$  under the intervention  $do(T = t)$  to the causal BN, they have to satisfy some norms of coherence. For example, it must be true that  $P_{x_0}(x_0) = 1$ . For another example, if the causal graph is  $X \rightarrow Y$  then  $P_{y_0}(x_0) = P(x_0)$ , and if the causal graph is  $X \leftarrow Y$  then  $P_{x_0}(y_0) = P(y_0)$ , therefore, it must be true that either  $P_{y_0}(x_0) = P(x_0)$  or  $P_{x_0}(y_0) = P(y_0)$ , which reflects the constraints that we are considering acyclic models.

Assume that each  $P_t(v)$  in  $\mathbf{P}_*$  is a (indexed) probability distribution over  $V$ . We would like to know what properties the set of distributions in  $\mathbf{P}_*$  must satisfy such that  $\mathbf{P}_*$  is compatible with some underlying causal BN in the sense that each  $P_t(v)$  corresponds to the post-intervention distribution of  $V$  under the intervention  $do(T = t)$  to the causal BN. (Tian & Pearl 2002) has shown that the following three properties: effectiveness, Markov, and recursiveness, are both necessary and sufficient for a  $\mathbf{P}_*$  set to be induced from a Markovian causal model.

**Property 1 (Effectiveness)** For any set of variables  $T$ ,

$$P_t(t) = 1. \quad (7)$$

**Property 2 (Markov)** For any two disjoint sets of variables  $S_1$  and  $S_2$ ,

$$P_{v \setminus (s_1 \cup s_2)}(s_1, s_2) = P_{v \setminus s_1}(s_1)P_{v \setminus s_2}(s_2). \quad (8)$$

**Definition 1** For two single variables  $X$  and  $Y$ , define “ $X$  affects  $Y$ ”, denoted by  $X \rightsquigarrow Y$ , as  $\exists W \subset V, w, x, y$ , such that  $P_{x,w}(y) \neq P_w(y)$ . That is,  $X$  affects  $Y$  if, under some setting  $w$ , intervening on  $X$  changes the distribution of  $Y$ .

**Property 3 (Recursiveness)** For any set of variables  $\{X_0, \dots, X_k\} \subseteq V$ ,

$$(X_0 \rightsquigarrow X_1) \wedge \dots \wedge (X_{k-1} \rightsquigarrow X_k) \Rightarrow \neg(X_k \rightsquigarrow X_0). \quad (9)$$

These three properties impose constraints on the interventional space  $\mathbf{P}_*$  such that this vast space can be encoded succinctly, in the form of a single Markovian model. In this paper, we seek a characterization of  $\mathbf{P}_*$  set induced from semi-Markovian causal models. The effectiveness and recursiveness properties still hold in semi-Markovian models but the Markov property does not. First some discussions about the effectiveness and recursiveness properties.

Effectiveness states that, if we force a set of variables  $T$  to have the value  $t$ , then the probability of  $T$  taking that value  $t$  is one. We give some corollaries of effectiveness that are very useful during future discussions. For any set of variables  $S$  disjoint with  $T$ , an immediate corollary of effectiveness reads:

$$P_{t,s}(t) = 1, \quad (10)$$

which follows from

$$P_{t,s}(t) \geq P_{t,s}(t, s) = 1. \quad (11)$$

Equivalently, if  $T_1 \subseteq T$ , then

$$P_t(t_1) = \begin{cases} 1 & \text{if } t_1 \text{ is consistent with } t. \\ 0 & \text{if } t_1 \text{ is inconsistent with } t. \end{cases} \quad (12)$$

We further have that, for  $T_1 \subseteq T$  and  $S$  disjoint of  $T$ ,

$$P_t(s, t_1) = \begin{cases} P_t(s) & \text{if } t_1 \text{ is consistent with } t. \\ 0 & \text{if } t_1 \text{ is inconsistent with } t. \end{cases} \quad (13)$$

Recursiveness is a stochastic version of the (deterministic) recursiveness axiom given in (Halpern 2000). It comes from restricting the causal models under study to those having acyclic causal graphs. For example, for  $k = 1$  we have  $X \rightsquigarrow Y \Rightarrow \neg(Y \rightsquigarrow X)$ , saying that for any two variables  $X$  and  $Y$ , either  $X$  does not affect  $Y$  or  $Y$  does not affect

$X$ . (Halpern 2000) pointed out that, recursiveness can be viewed as a collection of axioms, one for each  $k$ , and that the case of  $k = 1$  alone is not enough to characterize a recursive model.

Recursiveness defines an order over the set of variables. Define a relation “ $\prec$ ” as:  $X \prec Y$  if  $X \rightsquigarrow Y$ . The transitive closure of  $\prec$ ,  $\prec^*$ , is a partial order over the set of variables  $V$  from the recursiveness property. Then the following property holds in semi-Markovian models. (Note that since a Markovian model is a special type of semi-Markovian model, all properties that hold in semi-Markovian models also hold in Markovian models.)

**Property 4 (Directionality)** There exists a total order, “ $<$ ”, consistent with  $\prec^*$ , such that

$$P_{v_i,w}(s) = P_w(s) \quad \text{if } \forall X \in S, X < V_i, \quad (14)$$

for any set of variables  $W$  disjoint of  $S$ .

Intuitively, directionality implies that an intervention on any variable  $V_i$  cannot affect earlier variables. If  $S$  contains a single variable  $X$ , this property is implied by the recursiveness property, because if  $P_{v_i,w}(x) \neq P_w(x)$ , then  $V_i \rightsquigarrow X$ , and therefore  $V_i \prec X$ , which contradicts the fact that  $X < V_i$  is consistent with  $\prec^*$ . In Markovian models, the directionality property can be derived from the recursiveness and Markov properties.

**Property 5 (Inclusion-Exclusion Inequalities)** For any subset  $S_1 \subseteq V$ ,

$$\sum_{S_2 \subseteq V \setminus S_1} (-1)^{|S_2|} P_{v \setminus (s_1 \cup s_2)}(v) \geq 0, \quad \forall v \in Dm(V), \quad (15)$$

where  $|S_2|$  represents the number of variables in  $S_2$ .

The inclusion-exclusion inequalities specify  $2^{|V|}$  number of inequalities (including the trivial one  $P(v) \geq 0$ ), each hold for all possible instantiations of  $V$ . For example, if  $V = \{X, Y, Z\}$ , then the inclusion-exclusion inequalities specify the following: for all  $x \in Dm(X)$ ,  $y \in Dm(Y)$ ,  $z \in Dm(Z)$ ,

$$1 - P_{yz}(x) - P_{xz}(y) - P_{xy}(z) + P_z(xy) + P_y(xz) + P_x(yz) - P(xyz) \geq 0 \quad (16)$$

$$P_{yz}(x) - P_z(xy) - P_y(xz) + P(xyz) \geq 0 \quad (17)$$

$$P_{xz}(y) - P_z(xy) - P_x(yz) + P(xyz) \geq 0 \quad (18)$$

$$P_{xy}(z) - P_y(xz) - P_x(yz) + P(xyz) \geq 0 \quad (19)$$

$$P_z(xy) - P(xyz) \geq 0 \quad (20)$$

$$P_y(xz) - P(xyz) \geq 0 \quad (21)$$

$$P_x(yz) - P(xyz) \geq 0 \quad (22)$$

If we assume that a causal order  $V_1 < V_2 \dots < V_n$  is given such that Eq. (14) is satisfied, then some of the inequalities in Eq. (15) can be derived from others. More exactly, we only need the following set of inequalities.

**Property 6 (Inclusion-Exclusion Inequalities with Order)**

Let  $V' = V \setminus \{V_n\}$ . For any subset  $S_1 \subseteq V'$ ,

$$\sum_{S_2 \subseteq V' \setminus S_1} (-1)^{|S_2|} P_{v' \setminus (s_1 \cup s_2)}(s_1, s_2, v_n) \geq 0, \quad \forall v \in Dm(V), \quad (23)$$

Eq. (23) specifies  $2^{|V|-1}$  number of inequalities. The other half of the inequalities in Eq. (15) can be derived from Eq. (23) and the following equation

$$P_{v_n s}(v' \setminus s) = P_s(v' \setminus s) \quad (24)$$

which follows from Eq. (14). Summing the left hand side of Eq. (23) over all the instantiation of  $V_n$  except  $v'_n$ , we have

$$\begin{aligned} & \sum_{S_2 \subseteq V' \setminus S_1} (-1)^{|S_2|} [P_{v' \setminus (s_1 \cup s_2)}(s_1, s_2) \\ & \quad - P_{v' \setminus (s_1 \cup s_2)}(s_1, s_2, v'_n)] \\ = & \sum_{S_2 \subseteq V' \setminus S_1} (-1)^{|S_2|} [P_{v' \setminus (s_1 \cup s_2), v'_n}(s_1, s_2) \\ & \quad - P_{v' \setminus (s_1 \cup s_2)}(s_1, s_2, v'_n)] \text{ (from Eq. (24))} \\ = & \sum_{S_2 \subseteq V \setminus S_1} (-1)^{|S_2|} P_{v \setminus (s_1 \cup s_2)}(s_1, s_2). \end{aligned} \quad (25)$$

Therefore, we obtain that, for any subset  $S_1 \subseteq V'$ ,

$$\sum_{S_2 \subseteq V \setminus S_1} (-1)^{|S_2|} P_{v \setminus (s_1 \cup s_2)}(v) \geq 0, \quad (26)$$

which are the other half of the inequalities in Eq. (15) besides those in Eq. (23).

As an example, assuming that  $V = \{X, Y, Z\}$ , and we are given a causal order  $X < Y < Z$ , then Directionality and inclusion-exclusion inequalities specify the following

$$P_y(x) = P(x) \quad (27)$$

$$P_z(x, y) = P(x, y) \quad (28)$$

$$P_{zx}(y) = P_x(y) \quad (29)$$

$$P_{zy}(x) = P_y(x) \quad (30)$$

$$P_{xy}(z) - P_y(xz) - P_x(yz) + P(xyz) \geq 0 \quad (31)$$

$$P_y(xz) - P(xyz) \geq 0 \quad (32)$$

$$P_x(yz) - P(xyz) \geq 0 \quad (33)$$

**Theorem 1 (Soundness)** *Effectiveness, recursiveness, directionality, and inclusion-exclusion inequalities hold in all semi-Markovian models.*

See the Appendix A for the proof of soundness.

**Theorem 2 (Completeness)** *If a  $\mathbf{P}_*$  set satisfies effectiveness, recursiveness, directionality, and inclusion-exclusion inequalities, then there exists a semi-Markovian model that can generate this  $\mathbf{P}_*$  set.*

See the Appendix B for the proof sketch of completeness. The full proof is given in (Tian, Kang, & Pearl 2006).

## Conclusion

We have shown that the experimental implications of an underlying semi-Markovian causal model with unknown structure are fully characterized by four properties. The key element in our characterization is the set of inclusion-exclusion inequalities Eq. (15). One practical application of this characterization is that any empirical violation of the inequalities in Eq. (15) would permit us to conclude that the underlying model is not semi-Markovian; this means that feedback

loops may operate in data generating process, or that the interventions in the experiments are not conducted properly. (e.g., the intervention may not be properly randomized or they may have side effects). Another application permits us to bound the effects of untried interventions from experiments involving auxiliary interventions that are easier or cheaper to implement. For example, if we have performed experiments in which  $X$  and  $Y$  are randomized separately, yielding the distributions  $P_y(xz)$  and  $P_x(yz)$  respectively, then Eq. (19) bounds the experimental distribution  $P_{xy}(z)$  that would obtain under a new experimental design where  $X$  and  $Y$  are randomized simultaneously. The resulting bound, given by  $P_{xy}(z) \geq P_y(xz) + P_x(yz) - P(xyz)$ , makes no assumption on the structure of the underlying model, or the temporal order of the variable, or the absence of confounding variables in the domain.

The fact that our proof constructs a complete graph does not mean, of course, that one cannot attempt to extract a more informative graph from  $\mathbf{P}_*$ . For example, the set of directed edges can be reduced noting that, in every semi-Markovian model, the parents of each  $V_i$  are a minimal set  $S_i$  satisfying  $P_{s_i}(v_i) = P_{v \setminus v_i}(v_i)$ . In words, once we hold fixed the parents of  $V_i$ , no additional intervention may influence the probability of  $V_i$ . Likewise, the set of bidirected arcs can be reduced by removing all arcs between a node  $V_i$  and a maximal set  $T_i$  of non-descendants of  $V_i$  satisfying

$$P_{v \setminus v_i}(v_i) = P_{(v \setminus v_i) \setminus t_i}(v_i | t_i). \quad (34)$$

Indeed, intervening on variables to which  $V_i$  is not connected by an arc or observing those variables gives us the same information on  $V_i$  (once we hold fixed all other variables). The question remains however whether the removal of these edges from the complete graph induces additional inequalities and equalities that need be checked against  $\mathbf{P}_*$ . We leave this question for future work.

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## Appendix A: Proof of Soundness

**Theorem (Soundness)** *Effectiveness, recursiveness, directionality, and inclusion-exclusion inequalities hold in all semi-Markovian models.*

*Proof:* All four properties follow from Eq. (4).

**Effectiveness** From Eq. (4), we have

$$P_t(T = t') = 0 \quad \text{for } t' \neq t, \quad (35)$$

and since

$$\sum_{t' \in Dm(T)} P_t(t') = 1, \quad (36)$$

we obtain the effectiveness property of Eq. (7).

**Recursiveness** Assume that a total order over  $V$  that is consistent with the causal graph is  $V_1 < \dots < V_n$ , such that

$V_i$  is a nondescendant of  $V_j$  if  $V_i < V_j$ . Consider a variable  $V_j$  and any set of variables  $S \subseteq V$  which does not contain  $V_j$ . Let  $B_j = \{V_i | V_i < V_j, V_i \in V \setminus S\}$  be the set of variables not in  $S$  and ordered before  $V_j$ , and let  $A_j = \{V_i | V_j < V_i, V_i \in V \setminus S\}$  be the set of variables not in  $S$  and ordered after  $V_j$ . Then

$$P_s(b_j, v_j, a_j) = \sum_u \prod_{\{i | V_i \in B_j\}} P(v_i | pa_i, u^i) P(v_j | pa_j, u^j) \cdot \prod_{\{i | V_i \in A_j\}} P(v_i | pa_i, u^i) P(u) \quad (37)$$

and

$$P_{v_j, s}(b_j, a_j) = \sum_u \prod_{\{i | V_i \in B_j\}} P(v_i | pa_i, u^i) \cdot \prod_{\{i | V_i \in A_j\}} P(v_i | pa_i, u^i) P(u) \quad (38)$$

Summing both sides of Eq. (37) over all the instantiations of variables in  $A_j$  and  $V_j$ , such that the variable ordered last is summed first, we obtain

$$P_s(b_j) = \sum_u \prod_{\{i | V_i \in B_j\}} P(v_i | pa_i, u^i) P(u). \quad (39)$$

Similarly, summing both sides of Eq. (38) over all the instantiations of variables in  $A_j$ , we obtain that

$$P_{v_j, s}(b_j) = P_s(b_j). \quad (40)$$

Since  $B_j$  is the set of variables ordered before  $V_j$ , we have that, for any two variables  $V_i < V_j$  and any set of variables  $S$ ,

$$P_{v_j, s}(v_i) = P_s(v_i), \quad (41)$$

which states that if  $V_i$  is ordered before  $V_j$  then  $V_j$  does not affect  $V_i$ , based on our definition of “ $X$  affects  $Y$ ”. Therefore, we have that if  $V_j$  affects  $V_i$  then  $V_j$  is ordered before  $V_i$ , or

$$V_j \rightsquigarrow V_i \Rightarrow V_j < V_i. \quad (42)$$

Recursive property (9) then follows from (42) because the relation “ $<$ ” is a total order.

**Directionality** Let  $<$  be a total order consistent with the causal graph. In the above proof for recursiveness, we have shown that Eq. (40) and (42) hold. (42) means that the total order  $<$  is consistent with  $\prec^*$ . And Eq. (14) follows immediately from Eq. (40).

**Inclusion-Exclusion Inequalities** We use the following equation

$$\prod_{i=1}^k (1 - a_i) = 1 - \sum_i a_i + \sum_{i,j} a_i a_j - \dots + (-1)^k a_1 \dots a_k. \quad (43)$$

Take  $a_j = P(v_j | pa_j, u^j)$ , we have that

$$\sum_u \prod_{\{i | V_i \in S_1\}} P(v_i | pa_i, u^i) \cdot \prod_{\{j | V_j \in V \setminus S_1\}} (1 - P(v_j | pa_j, u^j)) P(u) = \sum_{S_2 \subseteq V \setminus S_1} (-1)^{|S_2|} P_{v \setminus (S_1 \cup S_2)}(s_1, s_2) \geq 0 \quad (44)$$

since for all  $V_i \in V$

$$0 \leq P(v_i | pa_i, u^i) \leq 1. \quad (45)$$

□

## Appendix B: Proof Sketch of Completeness

From directionality property, there exists a total order on  $V$ ,  $V_1 < V_2 < \dots < V_n$ , such that

$$P_{v_i, w}(s) = P_w(s) \text{ if } \forall X \in S, X < V_i, \quad (46)$$

We will construct a causal model consistent with this order. Let the domain of each variable  $V_j$  be

$$Dm(V_j) = \{v_j^1, \dots, v_j^{d_j}\}$$

where  $d_j$  is the number of values  $V_j$  can take. We will construct a functional model in the form of

$$v_j = f_j(v_1, \dots, v_{j-1}, r_j), \quad j = 1, \dots, n. \quad (47)$$

For discrete variables, the number of possible functions is finite. We will use the “response” variable representation (Balke & Pearl 1994b; 1994a) (called “mapping” variable in (Heckerman & Shachter 1995)). Let the domain of  $r_j$  be

$$Dm(r_j) = \{1, 2, \dots, |Dm(r_j)|\}$$

where  $|Dm(r_j)| = d_j^{d_1 \dots d_{j-1}}$ .

We will construct a model of the form

$$P(v) = \sum_{r_1, \dots, r_n} \prod_j P(v_j | v_1, \dots, v_{j-1}, r_j) P(r_1, \dots, r_n) \quad (48)$$

For a functional model, each of the probabilities  $P(v_j | v_1, \dots, v_{j-1}, r_j)$  would be either 0 or 1, and only non-zero values contribute to the summation in Eq. (48). For a fixed value of  $v_1, \dots, v_j$ , let  $D_j(v_j | v_1, \dots, v_{j-1}) \subset Dm(r_j)$  be the set of values of  $r_j$  such that  $P(v_j | v_1, \dots, v_{j-1}, r_j) = 1$ . Then

$$P(v) = \sum_{r_1 \in D_1} \dots \sum_{r_n \in D_n} P(r_1, \dots, r_n), \quad (49)$$

and for any  $T \subseteq V$

$$P_{v \setminus T}(v) = \sum_{\substack{r_i \in Dm(r_i) \\ \{i | V_i \notin T\}}} \sum_{\substack{r_i \in D_i \\ \{i | V_i \in T\}}} P(r_1, \dots, r_n). \quad (50)$$

If we can construct a distribution  $P(r_1, \dots, r_n)$  such that Eq. (50) holds for any  $T \subseteq V$  and  $v \in Dm(V)$ , then we have a semi-Markovian model that can induce the  $\mathbf{P}_*$  set.

Given a distribution  $P(r_1, \dots, r_n)$ , we will define an event  $A_j^{i_j|i_1, \dots, i_{j-1}}$  as the event that  $r_j$  is in  $D_j(v_j^{i_j}|v_1^{i_1}, \dots, v_{j-1}^{i_{j-1}})$ , and we will think of the event  $A_j^{i_j|i_1, \dots, i_{j-1}}$  as a set in the space  $Dm(r_1) \times \dots \times Dm(r_n)$ . Then Eqs. (49) and (50) become

$$P(v_1^{i_1}, \dots, v_n^{i_n}) = P(A_1^{i_1} \cap A_2^{i_2|i_1} \cap \dots \cap A_n^{i_n|i_1, \dots, i_{n-1}}), \quad (51)$$

and

$$P_{v \setminus t}(v) = P\left(\bigcap_{\{k|V_k \in T\}} A_k^{i_k|i_1, \dots, i_{k-1}}\right). \quad (52)$$

For a fixed  $i_1, \dots, i_{n-1}$ , the set of events  $A_n^{j_n|i_1, \dots, i_{n-1}}, j_n = 1, \dots, d_n$  are mutually exclusive and exhaustive. For a fixed  $i_1, \dots, i_{n-1}$ , letting  $A_k$  be a shorthand notation for  $A_k^{i_k|i_1, \dots, i_{k-1}}$  and letting  $\overline{A_k}$  represent the event not  $A_k$ , the set of events

$$\bigcap_{k \in I} A_k \bigcap_{k \notin I} \overline{A_k} \bigcap A_n^{j_n}, \forall I \subseteq \{1, \dots, n-1\}, j_n = 1, \dots, d_n \quad (53)$$

are mutually exclusive and exhaustive, and thus form a partition of the space  $Dm(r_1) \times \dots \times Dm(r_n)$ . The probabilities of these events can be computed from Eq. (52) using the inclusion-exclusion principle, and we obtain

$$\begin{aligned} & P\left(\bigcap_{k \in I} A_k \bigcap_{k \notin I} \overline{A_k} \bigcap A_n^{j_n}\right) \\ &= \sum_{S_2 \subseteq V' \setminus S_1} (-1)^{|S_2|} P_{v \setminus (s_1 \cup s_2)}(s_1, s_2, v_n), \end{aligned} \quad (54)$$

where  $V' = V \setminus \{V_n\}$ , and  $S_1 = \{V_i | i \in I\}$ . From the Inclusion-Exclusion Inequalities with Order given in Eq. (23), we have a valid assignment of probabilities to each of the mutually exclusive and exhaustive events in (53).

It is not hard to see that the equations (52) for  $V_n \in V \setminus T$  lead to constraints in the form of, for each  $S \subset V'$ ,

$$P_{v_n s}(v' \setminus s) = P_s(v' \setminus s). \quad (55)$$

These constraints are satisfied by the  $\mathbf{P}_*$  set since Eq.(46) holds.

For each fixed value  $i_1, \dots, i_{n-1}$ , we have a probability assignment to the set of mutually exclusive and exhaustive events  $\bigcap_{k \in I} A_k \bigcap_{k \notin I} \overline{A_k} \bigcap A_n^{j_n}$  given by Eq.(54). Are these assignments consistent for different values of  $i_1, \dots, i_{n-1}$ ? In other words, does there exist a distribution  $P(r_1, \dots, r_n)$  that satisfies the assignments in Eq.(54) for  $i_1 = 1, \dots, d_1, \dots, i_{n-1} = 1, \dots, d_{n-1}$ ? If the answer is yes, then there exists a distribution  $P(r_1, \dots, r_n)$  such that Eq. (52) holds for any  $T \subseteq V$  and  $v \in Dm(V)$ , and therefore there exists a semi-Markovian model that can induce the  $\mathbf{P}_*$  set.

For a fixed value  $i_1, \dots, i_{n-1}$ , we consider another (finer) partition of the space  $Dm(r_1) \times \dots \times Dm(r_n)$ , denoted by  $K_{i_1, \dots, i_{n-1}}$ ,

$$\begin{aligned} & A_1^{j_1} \cap A_2^{j_2|i_1} \cap \dots \cap A_n^{j_n|i_1, \dots, i_{n-1}}, \\ & j_1 = 1, \dots, d_1, \dots, j_n = 1, \dots, d_n. \end{aligned} \quad (56)$$

We use  $P(K_{i_1, \dots, i_{n-1}})$  to denote a probability assignment that assigns a probability value to each set in  $K_{i_1, \dots, i_{n-1}}$ . We can show the following

**Lemma 1** *Given the probability assignments in Eq. (54), there exist probability assignments  $P(K_{i_1, \dots, i_{n-1}})$  for  $i_1 = 1, \dots, d_1, \dots, i_{n-1} = 1, \dots, d_{n-1}$ , such that, for two different partitions  $K_{i_1, \dots, i_{n-1}}$  and  $K_{i'_1, \dots, i'_{n-1}}$ , if  $i_1 = i'_1, \dots, i_k = i'_k$ , then  $P(K_{i_1, \dots, i_{n-1}})$  and  $P(K_{i'_1, \dots, i'_{n-1}})$  induce the same probabilities  $P(A_1^{j_1} \cap A_2^{j_2|i_1} \cap \dots \cap A_{k+1}^{j_{k+1}|i_1, \dots, i_k})$ .*

Then we can show that

**Lemma 2** *There exists a distribution  $P(r_1, \dots, r_n)$  such that all the probability assignments  $P(K_{i_1, \dots, i_{n-1}})$  in Lemma 1 are satisfied for  $i_1 = 1, \dots, d_1, \dots, i_{n-1} = 1, \dots, d_{n-1}$ .*

The completeness Theorem 2 follows from Lemma 2.

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