Causal Network Learning from Multiple Interventions of Unknown Manipulated Targets

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Abstract

In this paper, we discuss structure learning of causal networks from multiple data sets obtained by external intervention experiments where we do not know what variables are manipulated. For example, the conditions in these experiments are changed by changing temperature or using drugs, but we do not know what target variables are manipulated by the external interventions. From such data sets, the structure learning becomes more difficult. For this case, we first discuss the identifiability of causal structures. Next we present a graph-merging method for learning causal networks for the case that the sample sizes are large for these interventions. Then for the case that the sample sizes of these interventions are relatively small, we propose a data-pooling method for learning causal networks in which we pool all data sets of these interventions together for the learning. Further we propose a re-sampling approach to evaluate the edges of the causal network learned by the data-pooling method. Finally we illustrate the proposed learning methods by simulations.

Keywords: directed acyclic graphs, intervention, manipulated targets

1. Introduction

Directed acyclic graphs (DAGs) can be used to represent causal networks among variables. Many methods have been developed to learn the structures of DAGs from observational and/or experimental data (Cooper and Yoo, 1999; Finegold and Drton, 2011; Friedman, 2004; Geng et al., 2004; Heckerman et al., 1999; Jansen et al., 2003; Maathuis et al., 2009; Pearl, 1995). Unlike an observational study, we can externally manipulate a few of target variables in an intervention experiment. Thereafter the variables which are manipulated in an experiment are simply called targets. The score-based and constraint-based methods are available to learn causal networks from interventional data when the targets in intervention experiments are known. For examples, Cooper and Yoo (1999) present a Bayesian method of causal discovery from a mixture of experimental and observational data. Eberhardt (2006) discusses independence test used in the constraint-based methods via the data from multiple interventions and shows that two data sets obtained from two interventions with different targets can be pooled to test the conditional independence of two variables $x_1$ and $x_2$ given a variable set $S$ if $S$ separates $(x_1, x_2)$ from all targets in the two interventions. Vincenzo et al. (2012) show that the data pooling is valid for testing independencies with
those interventions in which all targets except one are manipulated to the same value across the interventions. Hauser and Bühlmann (2012) discuss the graph representation of Markov equivalence class under interventions and causal structure learning from multiple intervention experiments.

In some applications, the statuses or values of variables are stable and even keep constant in the normal condition and environment. Thus to discover the causal relationships among these variables, we have to manipulate a few of variables or change the condition or environment such that these variables change their statuses and values and affect their effect variables. In some situations, we may not know what target variables are manipulated in intervention experiments. For examples, when experiments are implemented by changing temperature or by using some medicine, we may not know exactly the targets of these interventions. To deal these situations, Eaton and Murphy (2007) introduce a vertex for each intervention and use DAGs over the regular and intervention vertices to represent the causal relationships among regular vertices and the targets of the interventions. They apply the dynamic programming algorithm introduced in Mikko and Kismat (2004) to computes the exact posterior marginal edge probabilities of the DAGs. As they mentioned, their computation is limited to about 20 vertices due to the space and time limits. To our knowledge, there are still many unresolved issues left when the targets of intervention are unknown, such as the identification of causal structures and the learning methods for large causal networks.

In this paper, we focus on the constraint-based causal learning methods using data from multiple interventions with unknown manipulated targets. We first discuss the identifiability of causal structures. Then for the case that the sample size from each intervention is large, we propose to learn a network from each intervention data set and merge these learned networks. This method can learn more directed edges from intervention data sets than from an observational data set even if we do not know the targets of interventions. Next when the sample sizes are small, the statistical errors of tests for each small intervention data set cannot be neglected, and thus we pool all intervention data sets together to learn a network structure, and then we use re-sampling technique to evaluate the edges of the learned network. We discuss the identifiability of causal structures learned from the pooled data and show that the proposed data-pooling method can correctly learn some local structures of the underlying causal network.

The rest of the paper is arranged as follows. In Section 2, we introduce the notation of causal network model and discuss the causal structure learning with interventions. In Section 3, we propose two methods of causal network learning from multiple interventions with unknown targets. We evaluate the proposed methods via simulations in Section 4. Finally we discuss these methods in Section 5.

2. Causal network model and causal learning with interventions

In this section, we first introduce notation and assumptions of causal network models, and then discuss causal structural learning with interventions.
2.1 Causal network model

A directed acyclic graph (DAG) $G = (X, E)$ is used to represent the causal relationships of vertices, where $X = \{x_1, \cdots, x_p\}$ denotes a vertex set and $E$ denotes a set of directed edges. For a directed edge $x_i \rightarrow x_j$ in a DAG $G$, $x_j$ is a parent vertex of $x_j$ and $x_i$ is a child vertex of $x_j$; we also interpret $x_i$ as a cause of $x_j$ and the vertex $x_j$ as an effect of $x_i$. A directed path from $x_1$ to $x_k$ in $G$ is a sequence of directed edges that connect $x_i$ and $x_{i+1}$ ($x_i \rightarrow x_{i+1}$) for $i = 1, \cdots, k - 1$. A vertex $x_j$ is a descendant of $x_i$ if there is at least a directed path from $x_i$ to $x_j$ in $G$; otherwise, $x_j$ is non-descendant of $x_i$. We use $pa(x_i)$, $ch(x_i)$ and $nd(x_i)$ (or simply $pa_i$, $ch_i$ and $nd_i$) for the sets of parents, children, and non-descendants of a vertex $x_i$, respectively. A graph $G' = (X, E')$ is an edge-deleted subgraph of $G = (X, E)$ if $E' \subset E$. The skeleton of $G$ is an undirected graph obtained by replacing all directed edges in $G$ with the corresponding undirected edges. A three-vertex structure $x_i \rightarrow x_j \leftarrow x_k$ is called a $v$-structure if neither $x_i \rightarrow x_k$ nor $x_i \leftarrow x_k$ appears in $G$.

A causal graph $G$ is causally sufficient if no latent vertices affect two or more vertices contained in $G$ (Eberhardt and Scheines, 2007; Pearl, 2000). In this paper, we assume that the causal graphs under consideration satisfy the causal sufficiency. A causal network model contains a DAG $G = (X, E)$ and a joint distribution $P$ over $X$. Let $x_k$ and $x_l$ be two distinct vertices in $X$ and $S$ be a subset of $X \setminus \{x_k, x_l\}$. We use $(x_k \! 
abla \! x_l \mid S)_P$ to denote that $x_k$ and $x_l$ be conditionally independent given $S$ according to the joint distribution $P$. A causal network model $(G, P)$ satisfies causal Markov if a variable $x$ is conditionally independent of its non-descendants given all of its parents; that is, $(x \! 
abla \! nd(x) \mid pa(x))_P$ holds for the causal model $(G, P)$.

If a causal network model $(G, P)$ satisfies the causal Markov condition, then the joint distribution of $p$ variables $X$ can be factored as follows (Pearl, 1995; Spirtes et al., 2001)

$$P(X) = \prod_{i=1}^{p} P(x_i \mid pa_i), \quad (1)$$

where $P(x_i \mid pa_i)$ is the conditional probability of $x_i$ given its parent set $pa_i$.

From Equation (1), some conditional independencies for the joint distribution $P$ can be read from the DAG $G$. The concept of d-separation is used to describe the relation of vertices in a DAG $G$. For any pair of vertices $x_k$ and $x_l$ in $X$, and a subset $S \subseteq X \setminus \{x_k, x_l\}$, the set $S$ d-separates $x_k$ and $x_l$ in $G$ implies that the set $S$ blocks all connections of a certain type between $x_k$ and $x_l$ in $G$, denoted by $(x_k \! 
abla \! x_l \mid S)_G$. The exact definition of d-separation can be found in Pearl and Shafer (1988). To learn the causal DAG $G$ from an observed data set of the joint distribution $P$, one often assumes that the causal models under consideration satisfy the faithfulness assumption defined as follows.

**Assumption 1** The faithfulness assumption. We say that $P(x_1, \cdots, x_p)$ is faithful to the DAG $G$ if, for any pair of vertices $x_k$ and $x_l$ in $X$, and a subset $S \subseteq X \setminus \{x_k, x_l\}$, the set $S$ d-separates $x_k$ and $x_l$ in $G$ if $(x_k \! 
abla \! x_l \mid S)_P$ holds.

With the causal Markov condition and the faithfulness assumption, the set of all (conditional) independencies read from a causal sufficient graph $G$ is the same as that from the joint distribution $P$. A Markov equivalence class is a set of DAGs that encode the same set
of conditional independencies. Verma and Pearl (1990) shows that two DAGs are Markov equivalent if and only if they have the same skeleton and the same v-structures. Therefore, one can recover the Markov equivalence class of the underlying DAG from the corresponding joint distribution $P$, which can be represented by the skeleton and v-structures of $G$. A constraint-based learning algorithm tries to find a DAG using the conditional independency testing. The PC algorithm (Spirtes and Meek, 1995; Spirtes et al., 2001) is the most well-known constraint-based algorithm. In this paper, we propose a structural learning approach based on the PC algorithm, which learning a Markov equivalence class from the multiple intervention data sets with unknown manipulated targets, and we theoretically discuss the identifiability and the correctness of the local structures learned by our approach.

2.2 Causal learning with interventions

Suppose that in an intervention experiment, some vertices in $X$ may be the targets of the intervention which are manipulated externally. Several types of interventions have been studied in the literature (Pearl, 1995). A hard intervention cuts off the edges between its targets and their parents; and a soft intervention just changes the conditional probabilities of the targets given their parents. Let $M$ denote the set of targets in an intervention experiment, and the set $O = X \setminus M$ be the set of observational variables. When an intervention affects more than one targets (i.e. $|M| > 1$), we assume that the intervention changes the condition probability of each target separately. That is, the intervention may delete some of arrows pointing at these targets from the original DAG or may change the conditional probabilities of these targets. Therefore, the post-intervention joint distribution of $X$ for such an intervention can be factorized as

$$P'(x_1, \ldots, x_n) = \prod_{x_i \in O} P(x_i | pa_i) \times \prod_{x_i \in M} P'(x_i | pa'_i),$$

where $P(x_i | pa_i)$ is the same as the conditional probabilities of $X_i$ in Equation (1) if $X_i$ is not a target of intervention, and $P'(x_i | pa'_i)$ be the post-intervention conditional probability of $x_i$ given its revised parent set $pa'_i$ in the intervention experiment. We have that $pa'_i = \emptyset$ when the intervention on $x_i$ is hard, and $pa'_i = pa_i$ if the intervention on $x_i$ is null. Notice that $pa'_i \subseteq pa_i$ in Equation (2), that is, the intervention on $x_i$ might be partially soft and partially hard.

In general, interventions with known targets are informative to identify the causal network in a Markov equivalence class (Eberhardt et al., 2005; He and Geng, 2008). However, when we do not know the targets of the interventions, additional uncertainty is introduced and the interventions might be useless to identify the causal networks. Below we give an example that the causal structure is not identified if the manipulated target of intervention is unknown, while the structure is identified if the target is known.

**Example 1.** Consider the two causally sufficient graphs with two vertices: $x_1 \rightarrow x_2$ and $x_1 \leftarrow x_2$, which are Markov equivalent. If we know that $x_1$ is the target in a hard intervention, under the faithfulness assumption, $x_1 \rightarrow x_2$ is identified by $x_1 \perp \! \! \! \perp x_2$ from the intervention data. However, if we do not know which one of $x_1$ and $x_2$ is the target, then $x_1 \perp \! \! \! \perp x_2$ (or $x_1 \perp \! \! \! \perp x_2$) cannot be used to identify which of $x_1 \rightarrow x_2$ and $x_1 \leftarrow x_2$ is true.

In the next section, we will propose two methods for learning causal structures from multiple intervention data sets with unknown manipulated targets.
3. Causal structure learning from multiple interventions with unknown targets

Suppose that there are $m$ interventions. For the $j$th intervention, let $G_j$ be the DAG, $M_j$ the set of targets, $O_j = X \setminus M_j$ the set of observational variables. Let $E$ and $E_j$ be the edge sets of $G$ and $G_j$ respectively. By Equation (2), the post-intervention joint probability for the $j$th intervention can be formulated as, for $j = 1, \ldots, m$,

$$P_j(X) = \prod_{x_i \in O_j} P(x_i | pa_i) \times \prod_{x_i \in M_j} P_j(x_i | pa^j_i),$$

where $pa_i$ is the parent set of $x_i$ in $G$, $pa^j_i$ is the parent set of $x_i$ in $G_j$, and $pa^j_i \subseteq pa_i$.

In Section 3.1, a graph merging method is proposed for the case that each intervention has a large sample such that we can efficiently learn a DAG from each intervention data set. In Section 3.2, for the case that each intervention has a small sample, we pool all intervention data sets together to learn the causal network.

3.1 The graph merging method for causal structure learning

Let $D_j$ denote the data set from the $j$th intervention for $j \in \{1, \ldots, m\}$. When the sample size of $D_j$ is large enough to learn a graph efficiently, we learn the graph $G_j$ from $D_j$, and then we construct an overall graph merging the $m$ learned graphs, $G_j$ for $j \in \{1, \ldots, m\}$.

We give the details of this method in Algorithm 1.

**Algorithm 1:** Structural learning by combing the graphs learned from multiple experiments

```
Input: $D = \{D_j, j = 1, \ldots, m\}$, data sets from $m$ intervention experiments
Output: $G' = (X, E', V')$, a skeleton graph with v-structures.
1 for $j = 1$ to $m$ do
2   Learn a skeleton graph with v-structures $G'_j = (X, E'_j, V'_j)$ from $D_j$ via the PC algorithm.
3 Combine $\{G'_j, j = 1, \ldots, m\}$ to a graph $G' = (X, E', V')$ where $E' = \cup_{j=1}^m E_j$ and $V' = \cup_{j=1}^m V_j$. That is, an edge (v-structure) appears in $E'(V')$ if and only if it is in $E_j(V_j)$ for some $j \in \{1, \ldots, m\}$.
4 return $G'$
```

Let $P_j$ be the underlying joint probability for the $j$th intervention, which can be formalized by Equation (3). Before showing the correctness of Algorithm 1, we describe the following faithfulness assumption.

**Assumption 2** The joint probability $P_j(x_1, \ldots, x_p)$ is faithful to the DAG $G_j$ for any $j = 1, \ldots, m$.

Let $G = (X, E, V)$ denote the skeleton and v-structures of a DAG with an undirected edge set $E$ and a v-structure set $V$, $G_j(X, E_j, V_j)$ denote the skeleton and v-structures of the post-intervention graph for the $j$th intervention, and $P_j(x_1, \ldots, x_p)$ denote the post-intervention joint distribution for the $j$th intervention. Let $G' = (X, E', V')$ and $G'_j = (X, E'_j, V'_j)$ denote the skeleton and v-structures of the corresponding graphs learned by Algorithm 1.
Theorem 1 Let $P_j(x_1, \cdots, x_p)$ be defined by Equation (3), and Assumption 2 holds. If there are no statistical errors for testing conditional independencies, then we have

1. $E'_j = E_j$ and $V'_j = V_j$ for $j = 1, \ldots, m$,

2. $E' \subseteq E$, and

3. all directed edges in $G'$ appear in the underlying graph $G$.

Proof Because $P_j(x_1, \cdots, x_p)$ follows Equation (3) and faithfulness defined in Assumption 2 holds for $j = 1, \cdots, m$. The joint probabilities and the underlying causal graph of $j$th intervention, $P_j$ and $G_j$, satisfy the conditions of Markov properties and the assumption of faithfulness, and further encode the same conditional independencies. According to the general results of constraint-based causal learning, we can recover the Markov equivalence class of $G_j$. That is, we can identify the skeleton and v-structures of $G_j$ correctly. It leads to $E'_j = E_j$ and $V'_j = V_j$ for any $j \in \{1, \cdots, m\}$.

According to the Equation (3), $E_j$ is a subset of $E$, that is $E_j \subseteq E$. We have that $E' \subseteq E$ since $E' = \bigcup E'_j$ and $E'_j = E_j$.

Because $V'_j = V_j$ and all directed edges in $V_j$ also appear in the underlying graph $G$, we have that all directed edges in $V' (= \bigcup V'_j)$, also appear in $G$.

Theorem 2 shows that we can learn the skeleton and v-structures $(E_j, V_j)$ for $G_j, j = 1, \cdots, m$} correctly and all edges and all directions of the learned graph $G'$ are true, but some edges and some v-structures in $G$ may be lost by the interventions. Clearly, if an edge is cut off in every intervention, we cannot recover it in $G'$. Similarly, a v-structure might be missed in $G'$ if it is removed by all interventions.

We say that a set of interventions is conservative if for every vertex, there is at least one intervention which does not affect the vertex (Hauser and Bühlmann (2012)).

Assumption 3 The set of $m$ interventions is conservative.

Proposition 2 Let $P_j(x_1, \cdots, x_p)$ be defined by Equation (3), and Assumptions 2 and 3 hold. Then the skeleton and v-structures of the underlying DAG $G$ can be recovered correctly by Algorithm 1 if there are no statistical testing errors for conditional independencies.

Proof For any edge in $G$, say $x_l \rightarrow x_h$, suppose that $x_h$ is not a target in the $j$–th intervention, and then we have that the post intervention graph $G_j$ contains the edge $x_l \rightarrow x_h$. Algorithm 1 can learn the edge between $x_l$ and $x_h$ from Theorem 2. Similarly, for any v-structure $x_l \rightarrow x_h \leftarrow x_r$, suppose that $x_h$ is not a target in $j$–th intervention, and then we have that the post intervention graph $G_j$ contains the v-structure $x_l \rightarrow x_h \leftarrow x_r$. According to Theorem 2, the set of learned v-structures $V'$ obtained by Algorithm 1 contains v-structure $x_l \rightarrow x_h \leftarrow x_r$. Therefore, we have that the skeleton and v-structures of the underlying graph $G$ can be recovered via Algorithm 1.

Several papers discuss the learning of graphical models from multiple data sets. Danks (2002) and Tillman et al. (2009) propose some methods to learn a minimal equivalence class using the local independence information from distributed databases. Vincenzo et al. (2012)
propose to learn a causal network from multiple interventions by multiple independence tests. Comparing to our proposed Algorithm 1, their methods do not learn a graph for each experiment, so these methods might miss some specific causal structures in the individual interventions.

### 3.2 The data-pooling method for causal structure learning

When the sample size of each intervention is small, the conditional independence test by a single intervention data set becomes less powerful. In this section, we pool all intervention data sets together to learn a causal structure.

Let $D_j$ denote the data set of the $j$th intervention whose joint distribution is $P_j(X)$ in Equation (3). The data set $D$ contains all $D_j$ for $j = 1, \ldots, m$. Below we present a data-pooling learning method and its evaluation in Algorithm 2.

**Algorithm 2:** Structural learning by pooling all intervention data sets

**Input:** $D = \{D_j, j = 1, \ldots, m\}$, data from all $m$ interventions

**Output:** $G'$, a graph with v-structures and edge set; and the frequencies of edges learned by re-sampling.

1. **begin Meta Learning**
   2. Learn a skeleton graph $G' = (X, E', V')$ with v-structures using the conditional independence tests in which the pooled data set $D$ is used via the PC algorithm.

3. **begin Evaluation**
   4. for $i = 1$ to $K$ do
   5. Draw a subset $I_i$ randomly from $\{1, \ldots, m\}$ without replacement.
   6. Pooling the data together from the drawn data sets: $D_{I_i} = \bigcup_{j \in I_i} D_j$.
   7. Learn a skeleton graph $G'_i = (X, E'_i)$ from the pooled data set $D_{I_i}$.
   8. Let $E^* = \bigcup_{i=1}^{K} E'_i$ and $\tilde{E}' = E^* \setminus E'$.
   9. For any edge in $E'$ and $\tilde{E}'$, calculate the frequency of the edge appearing in $\{G'_i, i = 1, \ldots, K\}$.

10. **return** $G'$, the frequencies of edges in $E'$ and $\tilde{E}'$

In Algorithm 2, we first give a meta learning of the underlying graph from the pooled data in Step 1, and then evaluate it with an intervention sampling technique. We will show the correction of the meta learning in Theorem 3, and then we discuss the evaluation of edges according to their frequencies.

Let $I$ be a categorical variable with $m$ values $\{1, \ldots, m\}$ to indicate $m$ interventions, and the probability distribution $P(I = j) = p_j$, $p_j > 0$ and $\sum_{j=1}^{m} p_j = 1$. Suppose that the data set $D$ is generated as follows: (1) generate the frequencies $(n_1, \ldots, n_m)$ of $I$ from the probabilities and $N = \sum_{j=1}^{m} n_j$ and (2) draw a data set $D_j$ of $X$ with the sample size $n_j$ from the joint distribution $P_j$ defined in Equation (3). Clearly, the data in $D = \bigcup_{j=1}^{m} D_j$ are independently and identically distributed (iid) from the mixture joint distribution

$$P_M(X) = \sum_{j=1}^{m} P(X|I = j)P(I = j) = \sum_{j=1}^{m} p_j P_j(X). \quad (4)$$
Define \( M = \bigcup_{j=1}^{m} M_j \) and \( O = \bigcap_{j=1}^{m} O_j = X \setminus M \), that is, \( M \) is the set of all manipulated targets, and \( O \) is the common observational variables in all interventions. We give the Markov properties of \( P_M \) with respect to the underlying graph \( G \) as follows.

**Lemma 1** For any \( x_i \in O \), the vertex \( x_i \) is independent of the vertex set \( \text{nd}(x_i) \) given the parent set \( \text{pa}_i \) under the mixture distribution \( P_M \), denoted as \( (x_i \not\perp \!\!\!\perp \text{nd}(x_i) | \text{pa}_i)_{P_M} \).

**Proof** For any \( x_i \in O \), we first obtain an order as \( (x_{i_1}, \ldots, x_i) \) in which all non-descendants of \( x_i \) are ranked before \( x_i \) and every vertex is behind of its parents in the sequence as follows

1. let \( L = X, Y = () \);
2. if there exists non-descendant \( x \) of \( x_i \) and there is no parents of \( x \) in \( L \), add \( x \) to the end of \( Y \) and \( L = L \setminus \{x\} \);
3. repeat 2, until \( L \) only contains \( x_i \) and its descendants;
4. add \( x_i \) to the end of \( Y \).

Denoting \( Y = (x_{i_1}, \ldots, x_i) \), we have \( \text{nd}(x_i) \subseteq Y \) and

\[
P(Y, I = j) = P(Y|I = j)P(I = j) = P(Y|I = j)p_j
= \prod_{x_k \in O\cap Y} P(x_k|\text{pa}(x_k)) \prod_{x_k \in M\cap Y} P_j(x_k|\text{pa}(x_k))p_j
= P(x_i|\text{pa}(x_i)) \prod_{x_k \in \{O\cap Y}\setminus x_i} P(x_k|\text{pa}(x_k)) \prod_{x_k \in M\cap Y} P_j(x_k|\text{pa}(x_k))p_j
= P(x_i|\text{pa}(x_i))f(Y\setminus x_i, I = j),
\]

where \( f(Y\setminus x_i, I) = \prod_{x_k \in \{O\cap Y\setminus x_i} P(x_k|\text{pa}(x_k)) \prod_{x_k \in M\cap Y} P_j(x_k|\text{pa}(x_k))p_j \).

Let \( Z = \{x_i, \text{nd}(x_i)|\text{pa}(x_i), \text{pa}(x_i)\} \). From the construction of \( Y \), we have \( Z \subseteq Y \) and

\[
P_M(Z) = \sum_{j=1}^{m} \sum_{x_k \notin \{x_i, \text{nd}(x_i), \text{pa}(x_i)\}} P(Y, I = j)
= \sum_{j=1}^{m} \sum_{x_k \notin \{x_i, \text{nd}(x_i), \text{pa}(x_i)\}} P(x_i| \text{pa}(x_i))f(Y\setminus x_i, I = j)
= P(x_i| \text{pa}(x_i))g(\text{nd}(x_i)|\text{pa}(x_i), \text{pa}(x_i)),
\]

where \( g(\text{nd}(x_i)|\text{pa}(x_i), \text{pa}(x_i)) = \sum_{j=1}^{m} \sum_{x_k \notin \{x_i, \text{nd}(x_i), \text{pa}(x_i)\}} f(Y\setminus x_i, I = j) \). Therefore,

\[
P_M(\text{nd}(x_i), \text{pa}(x_i)) = \sum_{x_i} P_M(Z) = g(\text{nd}(x_i)|\text{pa}(x_i), \text{pa}(x_i)).
\]

We have

\[
P_M(Z) = P(x_i|\text{pa}(x_i)) P_M(\text{nd}(x_i)|\text{pa}(x_i), \text{pa}(x_i)) = P(x_i|\text{pa}(x_i)) P_M(\text{nd}(x_i)|\text{pa}(x_i)) P_M(\text{pa}(x_i)).
\]

Thus we get,

\[
P_M(\text{nd}(x_i), x_i|\text{pa}(x_i)) = \frac{P_M(Z)}{P_M(\text{pa}(x_i))} = P(x_i|\text{pa}(x_i)) P_M(\text{nd}(x_i)|\text{pa}(x_i)).
\]

That is, we have \((v \not\perp \!\!\!\perp \text{nd}(x_i) | \text{pa}(x_i)\)\). \(\blacksquare\)
Eberhardt (2008) shows that two data sets from two interventions with different targets can be pooled to test \( x_i \perp x_j \mid S \) if \( S \) can separate \((x_i, x_j)\) from the targets in each intervention. Below we give an example to show the difference between Eberhardt’s condition and Lemma 1.

**Example 2.** Consider a DAG with edges \( x_1 \rightarrow x_2 \rightarrow x_3 \rightarrow x_4 \rightarrow x_5 \) and \( x_1 \rightarrow x_5 \). We implement two interventions, one on \( x_1 \) and the other on \( x_5 \). \( x_4 \perp x_2 \mid x_3 \) can be confirmed by the pooling data set \( \mathcal{D} \) of two interventions. From Lemma 1, we have \( x_4 \perp x_2 \mid x_3 \) by \( P_M \). However, this does not satisfy the condition required by Eberhardt since \( x_3 \) does not separate \((x_2, x_4)\) from \( x_1 \).

We introduce another Markov property of the mixture joint distribution with respect to a DAG \( G \).

**Lemma 2** For any non-adjacent pair \( \{x_i, x_j\} \) which is contained in \( O \), there is a subset \( S \) of \( X \) such that \((x_i \perp x_j \mid S)_{P_M}\).

**Proof** For any pair \((x_i, x_j)\) of non-adjacent vertices belong to \( O \) in causal graph \( G \), without of generality, we suppose that \( x_j \) is non-descendant of \( x_i \), and then \( x_j \in nd(x_i) \). Letting \( S = pa(x_i) \), we have \( x_j \notin S \) and \((x_i \perp x_j \mid S)_{P_M}\) according to Lemma 1.

This result means that the mixture distribution \( P_M \) has the pairwise Markov property for any pair of non-adjacent vertices in the observational set \( O \). According to this lemma, there is an edge connecting vertices \( x_i \) and \( x_j \) in \( O \) if \((x_i \perp x_j \mid S)_{P_M}\) for any subset \( S \) of \( X \). Similar to the traditional constraint-based methods, we also need the concept of faithfulness assumption to show the correctness of a causal learning method.

**Assumption 4** The faithfulness assumption of \( P_M \) to \( G \) over the observational set \( O \). We say under Assumption 3 of the conservative interventions that \( P_M \) is faithful to the network \( G \) over the observation set \( O \) if, for any pair of vertices \( x_i \) and \( x_j \) in \( O \), there is a set \( S \) which \( d \)-separates the vertices \( x_i \) and \( x_j \) (denoted as \((x_i \perp x_j \mid S)_{G}\)) when the conditional independence \((x_i \perp x_j \mid S)_{P_M}\) holds, where \( S \) is a subset of \( X \setminus \{x_i, x_j\} \).

Unlike Assumption 1, we do not require that the faithfulness assumption holds for vertices in the target set \( M \) since spurious independencies among these vertices may be introduced due to the interventions. Under Assumption 4, we present the following two results which ensure that edges and v-structures contained in the observational set \( O \) can be discovered correctly.

**Lemma 3** For a pair of vertices \( x_i \) and \( x_j \) contained in \( O \), under Assumption 4, \( x_i \) and \( x_j \) are adjacent in a DAG \( G \) if and only if \((x_i \perp x_j \mid S)_{P_M}\) holds for any subset \( S \) of \( X \).

**Proof** For any \( x_i \in O \), and \( x_j \in O \), if \( x_i \) and \( x_j \) are not adjacent in \( G \), from Lemma 2, we can get a subset \( S \) such that \((x_i \perp x_j \mid S)_{P_M}\). If there is no subset \( S \subseteq X \) such that \((x_i \perp x_j \mid S)_{P_M}\), then \( x_i \) and \( x_j \) are adjacent in \( G \). Because \( P_M \) is faithful to \( G \) over \( O \) according to Assumption 4, if there is a subset \( S \) such that \((x_i \perp x_j \mid S)_{P_M}\) then \((x_i \perp x_j \mid S)_{G}\), that is \( x_i \) and \( x_j \) is not adjacent in \( G \). So if \( x_i \) and \( x_j \) are adjacent in \( G \), then there is no
subset $S \subseteq X$ such that $(x_i \perp \perp x_j | S)_{P_M}$. 

Lemma 4 Suppose that vertices $x_i$ and $x_k$ are adjacent and $x_j$, $x_k$ are adjacent, but $x_i$ and $x_j$ are not adjacent in $G$ where $x_i$, $x_j$ and $x_k$ are contained in $O$. Under Assumption 4, $x_i \rightarrow x_k \leftarrow x_j$ is a subgraph of $G$ if and only if $x_k \in S$ implies $(x_i \perp \perp x_j | S)_{P_M}$ for any subset $S$ of $X$.

Proof For any $x_i \in O$, $x_j \in O$, if there is a subset $S$, where $x_k \in S$, such that $(x_i \perp \perp x_j | S)_{P_M}$, then $(x_i \perp \perp x_j | S)_G$ according to Assumption 4. From the definition of d-separation, we can get that $x_i, x_k, x_j$ must not be head to head, since $x_i \rightarrow x_k \leftarrow x_j$ is subgraph of $G$ and $x_k \in S$ implies $(x_i \perp \perp x_j | S)_{P_M}$. On the other hand, because $x_i$ and $x_k$, $x_k$ and $x_j$ are adjacent and $x_i$ and $x_j$ are not adjacent in $G$, if $x_i \rightarrow x_k \leftarrow x_j$ is not subgraph of $G$, then the structure of $x_i, x_k$ and $x_j$ should be $x_i \rightarrow x_k \rightarrow j, x_i \leftarrow x_k \leftarrow x_j$ or $x_i \leftarrow x_k \rightarrow x_j$, and thus all d-separation set of $x_i$ and $x_j$ must be including $x_k$. Since $x_i$ and $x_j$ are not adjacent, there is a set $S$ such that $(x_i \perp \perp x_j | S)_{P_M}$, and then $(x_i \perp \perp x_j | S)_G$, thus we can get that $x_k \in S$. It means that if $x_k \in S$ implies $(x_i \perp \perp x_j | S)_{P_M}$, then $x_i \rightarrow x_k \leftarrow x_j$ is a subgraph of $G$.

Let $G_O$ be the induced subgraph of $G$ over the observational set $O$. With Lemmas 1, 3 and 4, we obtain the following main result of this section.

Theorem 3 Let $G' = (E', V')$ denote the graph obtained by the meta learning of Algorithm 2. If Assumption 4 holds and there is no statistical errors in independence tests, then all of edges and v-structure in $G'_O$ are exactly the same as those in $G_O$.

Proof Under Assumption 4, we have that Lemma 3 and Lemma 4 hold. That is, $G_O$ can be learned correctly using the conditional independencies encoded in the underlying joint probabilities. Therefore, if there is no statistical errors in independency tests, the learned $G'_O$ is the same as $G_O$.

Theorem 3 means that all edges and v-structures that are contained in the set $O$ can be discovered correctly from the mixture distribution $P_M$. However, between the vertices which are not contained in the set $O$, the mixture distribution $P_M$ may lead to spurious independencies and dependencies that do not encoded in the underlying joint distribution $P_M$. This is a cost of Algorithm 2 for the cases in which the sample size of each intervention is small. Moreover, whether a spurious dependence (or independence) appears in the mixture joint distribution $P_M$ depends on how much it is distorted by the interventions. In general, if only a small number of interventions “contaminate” the underlying independence (or dependence) of two vertices, it will keep in $P_M$. Therefore, many causal structures out of $O$ can be learned correctly.

Below, we give two remarks about how to use the frequencies of edges obtained by the re-sampling method to evaluate and improve the network learned by the meta learning of Algorithm 2.

Remark. The edges in $\bar{E}'$ are those which are not discovered from the original sample data set of all interventions but are discovered from some re-sampling data sets. If the
frequency of such an edge $e$ is large, it means that the edge $e$ may be missed by the spurious independency due to manipulating the relevant vertices in the interventions. Thus we add the edge $e$ to $E'$ if its frequency appearing in $E_i'$'s is larger than a threshold. We shall evaluate the re-sampling learning approach using simulations in Section 4.

4. Experimental study

In this section, we conduct three simulations to evaluate the proposed causal structure learning methods using the 37-vertex Alarm network (Beinlich et al., 1989). We denote its causal graph as $G = (X, E)$, where $X = \{X_1, \ldots, X_{37}\}$. We illustrate and compare Algorithms 1 and 2 in the first experiment, then we study the performance of the different number of manipulated targets in the second one, and finally we discuss the re-sampling in Algorithm 2 in the third one.

In each simulation, we generate artificial data as follows. We first generate $m$ interventions. In each intervention, we randomly choose some vertices as targets to be manipulated, and the probability that an edge between a target and its parents is cut off is set to 0.5. The post-intervention conditional probabilities of each target are then generated from an uninformative Dirichlet distribution. We finally generate a sample of size $n$ in each intervention, so there are $mn$ individuals in all interventions. The conditional probabilities for the underlying ALARM network are from Beinlich et al. (1989)

We learn the skeleton and v-structures from the artificial data generated from an underlying graph using Algorithm 1 or Algorithm 2, in which the PC algorithm is used and the conditional independencies are checked by $\chi^2$ testing at a significance level $\alpha = 1\%$. Let $TP$ be the number of true positive edges, $FN$ the number of false negative edges, and $FP$ the false positive edges regardless of the edge directions; and let $TP_1$ be the number of true positive directed edges or arrows, $FN_1$ the number of false negative directed edges, and $FP_1$ the false positive directed edges, where directed edges are limited only to those in v-structures. The true positive rate (TPR) and the true discovery rate (TDR) are defined as $TP/(TP + FP)$ and $TP/(TP + FN)$, respectively; and the true positive rate D-TPR and the true discovery rate D-TDR of directed edges in v-structures are defined as $TP_1/(TP_1 + FP_1)$ and $TP_1/(TP_1 + FN_1)$, respectively.

In the first experiment, for each intervention, we first generate randomly an integer $k$ from $\{1, 2, 3, 4, 5\}$ with the same probabilities, and we choose randomly $k$ vertices from the vertex set of ALARM as the targets to be manipulated in the intervention. Next we generate a sample of size $m \times n = 5000$ for the multiple interventions for each of four cases of $(n = 2500, m = 2), (n = 500, m = 10), (n = 200, m = 25)$ and $(n = 100, m = 50)$. Then, we learn the skeleton and v-structures from each generated data set using Algorithm 1 and the meta learning of Algorithm 2. We repeat 100 simulations for each case, and give TPR, TDR, D-TPR and D-TDR in Figure 1. We can see that Algorithm 1 works well when the sample sizes are large for all interventions, and that it works worse for small samples. Algorithm 2 works better than Algorithm 1 when the sample sizes are relative small.

From Figure 1, we can also see that with the increasing of the number $m$ of intervention data sets from 2 to 50, Algorithm 2 has larger true discovery rate TDR. It coincides with our discussion about the interventions with unknown target below Theorem 3 in Section 3.2. Since targets are chosen randomly, the distribution of the manipulated targets are more
uniform over all vertices for the case of \((n = 100, m = 50)\) than those for other cases, and thus each target is manipulated fewer times. So the distortion of the dependencies relevant to a manipulated vertex is much weaker than that for the case of \((n = 2500, m = 2)\), in which the chosen target is manipulated in at least a half of samples (2500).

In the second experiment, we generate the data sets only for \((n = 100, m = 50)\). We set the numbers of manipulated targets in all interventions to be a constant \(C\) for a case, and we use four constants \(C = 2, 5, 10, 20\) as four cases. We apply the meta learning of Algorithm 2 to the generated data sets. We repeat 100 simulations for each case and report the means of TPR, TDR, D-TPR and D-TDR in Figure 2. We can see that the performance of Algorithm 2 becomes worse for the case of a larger constant \(C\). It means that the larger the number of manipulated variables is, the worse the learning performance is.

In the third experiment, we apply the re-sampling technique to the interventions but not to the individuals in the original sample. Since an intervention deletes some of edges, it may make some of spurious independencies. Making use of the re-sampling of the interventions, we can see which edges are frequently found from the re-sampling data sets and which are infrequently found. Especially we should add these edges to the graph which are frequently found but are not found from the original data set of all interventions. In this experiment, we use the case of \((n = 100, m = 50)\) to illustrate the performance of the re-sampling learning approach. Let \(G' = (X, E')\) denote the graph learned from the original data set of
Number of targets in each intervention
Rates
TPR
TDR
D−TPR
D−TDR
2 5 10 20
0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0

Figure 2: TPR, TDR, D-TPR and D-TDR of causal learning with Algorithm 2 with different numbers of manipulated targets.

all interventions by Algorithm 2. We repeat $K = 100$ re-samplings, and we randomly draws 30 interventions from $m = 50$ interventions as the $i$th re-sampling data set for $i = 1, \ldots, K$. From the $i$th re-sampling data set, we learn the $i$th graph $G'_i = (X, E'_i)$. Let $E^* = \bigcup_{i=1}^{100} E'_i$, the union of the edge sets $E'_i$; and $\bar{E}' = E^* \setminus E'$, the set of edges that appear in $E^*$ but not in $E'$. For each edge $e$ in $E' \cup E^*$, we count the frequency $f(e)$ of each edge $e$ appearing in all $E'_i$’s, that is, $f(e) = \sum_{i=1}^{K} I_{e \in E'_i}$, where $I(\cdot)$ is an indicator function. Intuitively, for an edge $e \notin E'$, we should add $e$ to $E'$ if $f(e)$ is larger; but for an edge $e \in E'$, we may or may not remove $e$ from $E'$ even if $f(e)$ is smaller. In Table 1, we show the frequencies of some edges in $E^*$. In the upper part of Table 1, for these edges in $\bar{E}'$, we give 10 edges which have the largest frequencies among all edges in $E^*$, these edges labelled ‘True’ are the true edges, and these labelled ‘False’ are the false edges. We can see that the top 3 edges with frequencies $\geq 68$ should be added to $E'$, and other edges have frequencies $\leq 35$. In the lower part of Table 1, for these edges in $E'$, we show 10 edges which have the smallest frequencies. We can see that the top 4 edges with frequencies $\leq 50$ have 2 false edges.

We repeat the above process for 100 times in which we first generate a sample of the underlying ALARM network for the case $(n = 100, m = 50)$, next apply the re-sampling technique to the sample, and then obtain a frequency table like Table 1. From the 100 frequency tables obtained from the 100 repetitions, we calculate the frequencies of ‘True’ edges in the corresponding orders, and we give the results in Table 2. From the upper part of Table 2, we can see that an edge $e \in \bar{E}'$ with a larger $f(e)$ has a larger frequencies to be a true edge. From the lower part of Table 2, we can see that an edge $e \in E'$ with a smaller $f(e)$ has a smaller frequencies to be a true edge.

Our goal of the re-sampling is to find the spurious independencies due to the interventions, we consider only to ‘add edges to $E''$ but not to ‘remove edges from $E'$. Now we consider the threshold $\theta$ of the frequencies $f(e)$’s for adding edges to $E'$. After obtaining
\(G' = (X, E')\) learned by Algorithm 2, we add an edge \(e\) in \(\tilde{E}'\) to \(E'\) if \(f(e) > \theta\). Below we show the simulation results for various thresholds. Let FN denote the average number of false negative edges and FP the average number of false positive edges in the 100 learned graphs. We give FNs and FPs for different \(\theta\) in Table 3. For the simulation results, the best threshold is \(\theta = 20\) since the sum of FN=3.37 and FP=1.32 is the least. A suitable threshold may be between 20 and 50, for which not so many edges are added to the learned graph.

Table 1: The 10 edges having the largest frequencies in the \(f(e)\) descending (\(\downarrow\)) order, and the 10 edges having the smallest frequencies in the \(f(e)\) ascending (\(\uparrow\)) order. \(i\)-\(j\) denotes a skeleton edge \(e\) between vertices \(i\) and \(j\).

| \(f(e)\downarrow\) | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|-----------------|---|---|---|---|---|---|---|---|---|----|
| \(e \in \tilde{E}'\) | 25-30 | 17-23 | 2-4 | 30-31 | 21-32 | 15-16 | 34-37 | 9-34 | 1-27 | 11-16 |
| \(f(e)\) | 79 | 77 | 68 | 35 | 10 | 2 | 2 | 1 | 1 |     |
| \(e \in E\) \(\uparrow\) | True | True | True | False | False | True | False | False | True | True |
| \(f(e)\uparrow\) | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
| \(e \in E'\) | 4-27 | 9-17 | 24-25 | 17-34 | 16-17 | 2-3 | 18-19 | 21-22 | 25-31 | 14-15 |
| \(f(e)\) | 23 | 24 | 31 | 44 | 61 | 89 | 90 | 90 | 90 | 96 |
| \(e \in E\) True | True | True | False | True | True | True | True | True | True | True |

Table 2: The frequencies of an edge at a top order to be a true edge in 100 repetitions

| \(f(e)(\downarrow)\) order for \(e \in \tilde{E}'\) | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---------------------------------|---|---|---|---|---|---|---|---|---|----|
| Freq. to be a true edge in \(E\) | 95 | 76 | 64 | 41 | 30 | 24 | 13 | 8 | 7 | 7 |

| \(f(e)(\uparrow)\) order for \(e \in E'\) | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---------------------------------|---|---|---|---|---|---|---|---|---|----|
| Freq. to be a true edge in \(E\) | 55 | 77 | 91 | 96 | 99 | 100 | 100 | 100 | 100 | 100 |

Finally we give the simulation results of learning the ALARM network from an observational data set without interventions. In each simulation, we first generate an observed data

Table 3: The simulation results of FN and PF for different thresholds in the re-sampling learning

| \(\theta\) | 0 | 5 | 10 | 15 | 20 | 25 | 30 | 35 | 50 | 100 |
|----------|---|---|----|----|----|----|----|----|----|-----|
| FN       | 1.8 | 2.64 | 3.03 | 3.26 | 3.37 | 3.53 | 3.73 | 3.9 | 4.09 | 5.13 |
| FP       | 9.82 | 3.25 | 2.08 | 1.58 | 1.32 | 1.18 | 1.11 | 1.05 | 0.97 | 0.96 |
| Sum      | 11.62 | 5.89 | 5.11 | 4.84 | 4.69 | 4.71 | 4.84 | 4.95 | 5.06 | 6.09 |

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set of the same sample size 5000 from the distribution without interventions, and then we apply the PC algorithm to learn a graph. We repeat 100 simulations and obtain \(\text{FN}=5.51\) and \(\text{FP}=0.22\). According to the sum of \(\text{FN}\) and \(\text{FP}\), this result \((5.51+0.22)\) of learning from an observational data set is better than that \((5.13+0.96)\) for \(\theta = 100\) of learning from a multiple intervention data set and worse than that \((3.37+1.32)\) for \(\theta = 20\) of learning from the re-sampling learning approach.

5. Discussion

In this paper, we study how to learn causal structures from a data set with multiple interventions of unknown targets. Two approaches are presented to learn causal structures from large or small samples in each intervention. We show that the graph merging method works well when each intervention has a large enough sample to learn a graph efficiently, while the pooling data method is preferable when the sample size in each intervention is small.

Algorithm 1 assumes that there are no statistical errors for testing conditional independencies. However, in a real scenario, two v-structures in two graphs learned by Algorithm 1 may contain the same edge oriented in different ways because of statistical errors. This conflicting problem due to statistical errors may also appear in the constrain-based algorithms even without interventions. As treated in most algorithms, we can simply remove some v-structures inducing the conflicting constrains. Triantafillou and Tsamardinos (2014) propose an approach in which a function of their corresponding p-values is used to sort the constrains in order of confidence.

In Algorithm 2, we output the frequencies of edges appearing in the graphs learned by re-sampling method to evaluate the skeleton of meta learning graph. Additionally, we also can evaluate directed edges in v-structures learned in Algorithm 2 in a similar way.

Moreover, we use R to implement algorithms and experiments in this paper and the R package can be found at http://www.math.pku.edu.cn/teachers/heyb/

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