Learning causal Bayes networks using interventional path queries in polynomial time and sample complexity

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Abstract

Causal discovery from empirical data is a fundamental problem in many scientific domains. Observational data allows for identifiability only up to Markov equivalence class. In this paper, we propose a polynomial time algorithm for learning the exact correctly-oriented structure of the transitive reduction of any causal Bayesian networks with high probability, by using interventional path queries. Each path query takes as input an origin node and a target node, and answers whether there is a directed path from the origin to the target. This is done by intervening the origin node and observing samples from the target node. We theoretically show the logarithmic sample complexity for the size of interventional data per path query, for continuous and discrete networks. We extend our work by presenting how to learn the transitive edges using logarithmic sample complexity (albeit in time exponential in the maximum number of parents for discrete networks) and by providing an analysis of imperfect interventions.

1 Introduction

Motivation. Scientists in diverse areas (e.g., epidemiology, economics, etc.) aim to unveil causal relationships within variables from collected data. For instance, biologists try to discover the causal relationships between genes. By providing a specific treatment to a particular gene (origin), one can observe whether there is an effect in another gene (target). This effect can be either direct (if the two genes are connected with a directed edge) or indirect (if there is a directed path from the origin to the target gene).

Bayesian networks (BNs) are a powerful representation of joint probability distributions. BNs are also used to describe causal relationships among variables [13]. The structure of a causal BN (CBN) is represented by a directed acyclic graph (DAG), where nodes represent random variables, and an edge between two nodes $X$ and $Y$ (i.e., $X \rightarrow Y$) represents that the former ($X$) is a direct cause of the latter ($Y$). Learning the DAG structure of a CBN is of much relevance in several domains, and is a problem that has long been studied during the last decades.

From observational data alone (i.e., passively observed data from an undisturbed system), DAGs are only identifiable up to Markov equivalence. However, since our goal is causal discovery, this is inadequate as two BNs might be Markov equivalent and yet make different predictions about the consequences of interventions (e.g., $X \leftarrow Y$ and $X \rightarrow Y$ are Markov equivalent, but make very different assertions about the effect on $Y$ by changing $X$). In general, the only way to distinguish DAGs from the same Markov equivalence class is to use interventional data [10, 11, 18]. This data is produced after performing an experiment (intervention) [20], in which one or several random variables are forced to take some specific values, irrespective of their causal parents.

Related work. Several methods have been proposed for learning the structure of Bayesian networks from observational data. Approaches ranging from score-maximizing heuristics, exact exponential-time score-maximizing, ordering-based search methods using MCMC, and test-based methods have been developed to name a few. The umbrella of tools for structure learning of Bayesian networks go from exact methods (exponential-time with convergence/consistency guarantees) to heuristics methods (polynomial-time without any convergence/consistency guarantee). [12] provide a score-maximizing algorithm that is likelihood consistent, but that needs super-exponential time. [20, 8] provide polynomial-time test-based methods that are structure consistent, but results hold only in the infinite-sample limit (i.e., when given an infinite number of samples). [5] show that greedy hill-climbing is structure consistent in the infinite sample limit, with unbounded

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1. Two graphs are Markov equivalent if they imply the same set of (conditional) independencies. In general, two graphs are Markov equivalent iff they have the same structure ignoring arc directions, and have the same v-structures [30]. (A v-structure consists of converging directed edges into the same node, such as $X \rightarrow Y \leftarrow Z$.)
We show that for a CBN of discrete random variables, the sample complexity is \( \tilde{O}(\log(nr)) \) whereas for CBNs of sub-Gaussian random variables, the sample complexity is \( \tilde{O}(\sigma_{ub}^2 \log n) \) where \( \sigma_{ub} \) is an upper bound of the variable variances (marginally as well as after interventions). We also present two extensions: an algorithm to learn the transitive edges (i.e., the edges that are part of the true network but not of the transitive reduction), albeit not in polynomial-time for discrete CBNs (exponential in the maximum number of parents). We also analyze imperfect interventions, where the sample complexity for discrete CBNs is scaled by \( \alpha^{-1} \), where \( \alpha \) accounts for the degree of uncertainty in the intervention; whereas for CBNs of sub-Gaussian random variables, the sample complexity remains unchanged. Finally, we validate our theoretical results in synthetic and benchmark networks.

2 Preliminaries

In this section, we introduce our formal definitions and notations. Vectors and matrices are denoted by lowercase italicized letters. Random variables are denoted by italicized uppercase letters. Vector \( \ell_p \)-norms are denoted by \( \| \cdot \|_p \). For matrices, \( \| \cdot \|_{p,q} \) denotes the entrywise \( \ell_{p,q} \) norm, i.e., for \( \| A \|_{p,q} = \| \| (|A_{1,1}|, \ldots, |A_{m,1}|) \|_p, \ldots, \| (|A_{1,n}|, \ldots, |A_{m,n}|) \|_q \).

Let \( G = (V, E) \) be directed acyclic graph (DAG) with vertex set \( V = \{1, \ldots, n\} \) and edge set \( E \subset V \times V \), where \( (i, j) \in E \) implies the edge \( i \rightarrow j \). For a node \( i \in V \), we denote \( \pi_G(i) \) as the parent set of the node \( i \). In addition, a directed path of length \( k \) from node \( i \) to node \( j \) is a sequence of nodes \( (i, v_1, v_2, \ldots, v_{k-1}, j) \) such that \( \{(i, v_1), (v_1, v_2), \ldots, (v_{k-2}, v_{k-1}), (v_{k-1}, j)\} \) is a subset of the edge set \( E \).

Let \( X = \{X_1, \ldots, X_n\} \) be a set of random variables, with each variable \( X_i \) taking values in some domain \( \text{Dom}[X_i] \). A Bayesian network (BN) over \( X \) is a pair \( \mathcal{B} = (G, \mathcal{P}_G) \) that represents a distribution over the joint space of \( X \). Here, \( G \) is a DAG, whose nodes correspond to the random variables in \( X \) and whose structure encodes conditional independence properties about the joint distribution, while \( \mathcal{P}_G \) quantifies the network by specifying the conditional probability distributions (CPDs) \( P(X_i | X_{\pi_G(i)}) \). We use \( X_{\pi_G(i)} \) to denote the set of random variables which are parents of \( X_i \). A Bayesian network represents a joint probability distribution over the set of variables \( X \), i.e., \( P(X_1, \ldots, X_n) = \prod_{i=1}^n P(X_i | X_{\pi_G(i)}) \).

Viewed as a probabilistic model, a BN can answer any “conditioning” query of the form \( P(Z|E = e) \)
where $Z$ and $E$ are sets of variables and $e$ is an assignment of values to $E$. Nonetheless, a BN can also be viewed as a causal model or causal BN (CBN) [20]. Under this perspective, the CBN can also be used to answer interventional queries, which specify probabilities after we intervene in the model, forcibly setting one or more variables to take on particular values. The manipulation theorem [26, 20] states that one can compute the consequences of such interventions (perfect interventions) by “cutting” all the arcs coming into the nodes which have been clamped by intervention, and then doing typical probabilistic inference in the “mutilated” graph (see Figure 1 as an example). We follow the standard notation [20] for denoting the probability of the CBN after the intervention, thus, the new joint is the “mutilated” graph, and then doing typical probabilistic inference in the nodes which have been clamped by intervention, thus, the new joint is the “mutilated” graph, and then doing typical probabilistic inference in the “mutilated” graph (see Figure 1 as an example).

We follow the standard notation [20] for denoting the probability distribution of a variable $X_j$ after intervening $X_i$, that is, $P(X_j|do(X_i = x_i))$. In this case, the joint distribution after intervention is given by $P(X_1, \ldots, X_{i-1}, X_i, X_{i+1}, \ldots, X_n|do(X_i = x_i)) = \mathbb{1}[X_i = x_i] \prod_{j \neq i} P(X_j|X_{\pi_G(j)})$.

We refer to CBNs in which all random variables $X_i$ have finite domain, $Dom[X_i]$, as discrete CBNs. In this case, we will denote the probability mass function (PMF) of a random variable as a vector. That is, a PMF, $P(Y)$, can be described as a vector $p(Y) \in [0, 1]^{Dom[Y]}$ indexed by the elements of $Dom[Y]$, i.e., $p_j(Y) = P(Y = j), \forall j \in Dom[Y]$. We refer to networks with variables that have continuous domains as continuous CBNs.

Next, we formally define transitive edges.

**Definition 1** (Transitive edge). Let $G = (V, E)$ be a DAG. We say that an edge $(i, j) \in E$ is transitive if there exists a directed path from $i$ to $j$ of length greater than 1.

The algorithm for removing transitive edges from a DAG is called transitive reduction and it was introduced by Aho, Garey and Ullman [1]. The transitive reduction of a DAG $G$, TR($G$), is then $G$ without any of its transitive edges. Our proposed methods also make use of path queries, which we define as follows:

**Definition 2** (Path query). Let $G = (V, E)$ be a DAG. A path query is a function $Q_G : V \times V \to \{0, 1\}$ such that $Q_G(i, j) = 1$ if there exists a directed path in $G$ from $i$ to $j$, and $Q_G(i, j) = 0$ otherwise.

General DAGs are identifiable only up to their transitive reduction by using path queries. In general, DAGs can be non-identifiable by using path queries. We will use $Q(i, j)$ to denote $Q_G(i, j)$ since for our problem, the DAG $G$ is fixed (but unknown). For instance, consider the two graphs shown in Figure 2. In both cases, we have that $Q(1, 2) = Q(1, 3) = Q(2, 3) = 1$. Thus, by using path queries, it is impossible to discern whether the edge $(1, 3)$ exists or not. Later in Subsection 4.1 we focus on the recovery of transitive edges, which requires a different type of query.

**Definition 3** ($\delta$-noisy partially-correct path query). Let $G = (V, E)$ be a DAG, and let $Q_G$ be a path query. Let $\delta \in (0, 1)$ be a probability of error. A $\delta$-noisy partially-correct path query is a function $Q_{\delta-G} : V \times V \to \{0, 1\}$ such that $Q_{\delta-G}(i, j) = Q_G(i, j)$ with probability at least $1 - \delta$ if $i \in \pi_G(j)$ or if there is no directed path from $i$ to $j$.

We will use the term noisy path query to refer to $\delta$-noisy partially-correct path query. Note that Definition 3 requires a noisy path query to be correct only in certain cases, when one variable is parent of the other, or when there is no directed path between both variables. We do not require correctness when there is a directed path of length greater than 1 between both variables. Additionally, note that the uncertainty of the exact recovery of the transitive reduction of a CBN relies on answering multiple noisy path queries.

**2.1 Assumptions**

Before diving into our technical contributions, we state the main set of assumptions used throughout our paper.

**Assumption 1.** Let $G = (V, E)$ be a DAG. All nodes in $G$ are observable, furthermore, we can perform interventions on any node $i \in V$. 

Figure 1: (Left) A CBN of 6 variables, where the joint distribution, $P(X)$, is factorized as $\prod_i P(X_i|X_{\pi_G(i)})$. (Right) The mutilated CBN after intervening $X_1$ with value $x_4$. Note that the edges $\{(1, 4), (2, 4)\}$ are not part of the CBN after the intervention, thus, the new joint is $P(X|do(X_1 = x_4)) = \mathbb{1}[X_4 = x_4] \prod_{i \neq 4} P(X_i|X_{\pi_G(i)})$.

Figure 2: Two directed acyclic graphs that produce the same answers when using path queries.

How to answer path queries is a key step in this work. Since we answer path queries by using a finite number of interventional samples, we require a noisy path query, which is defined below.

We will use the term noisy path query to refer to $\delta$-noisy partially-correct path query. Note that Definition 3 requires a noisy path query to be correct only in certain cases, when one variable is parent of the other, or when there is no directed path between both variables. We do not require correctness when there is a directed path of length greater than 1 between both variables. Additionally, note that the uncertainty of the exact recovery of the transitive reduction of a CBN relies on answering multiple noisy path queries.

Next, we formally define transitive edges.

**Definition 1** (Transitive edge). Let $G = (V, E)$ be a DAG. We say that an edge $(i, j) \in E$ is transitive if there exists a directed path from $i$ to $j$ of length greater than 1.
Assumption 2 (Causal Markov). The data is generated from an underlying CBN \((G, P_G)\) over \(X\).

Assumption 3 (Faithfulness). The distribution \(P\) over \(X\) induced by \((G, P_G)\) satisfies no independencies beyond those implied by the structure of \(G\).

Assumption 2 implies the availability of purely interventional data, and has been widely used in the active learning literature \([13, 27, 11, 10, 25]\). We consider only observed variables because we perform interventions on each node, thus, latent variables do not present any additional challenge (see Appendix A for more details). By assuming that a causal graph is causally Markov (Assumption 2), we assume that any population produced by a causal graph has the independence relations obtained by applying d-separation to it, while with the faithfulness condition (Assumption 3), we ensure that the population has exactly these and no additional challenge (see Appendix A for more details).

### 3 Algorithms and Sample Complexity

In this section we present our first set of results and provide a formal analysis on the sample complexity of noisy path queries.

#### 3.1 Algorithm for Learning the Transitive Reduction of CBNs

We now present a simple algorithm for learning the structure of the transitive reduction of any CBN exactly. Algorithm 1 performs \(O(n^2)\) path queries for all possible node pairs, and then calls the transitive reduction algorithm. As proved in 1, the time complexity of the best algorithm for finding the transitive reduction of a DAG is the same as the time to compute the transitive closure of a graph or to perform Boolean matrix multiplication. Therefore, we can use any exact algorithm for fast matrix multiplication, such as 14, which has \(O(n^{2.3729})\) time complexity. As a result, the time complexity of Algorithm 1 is dominated by the computation of the transitive reduction since answering a query \(\hat{Q}(i, j)\) is in \(O(\log n)\). Finally, note that performing \(n^2\) queries (one per each node pair) is equivalent to performing \(n\) single-vertex interventions, in which we intervene one node and observe the remaining \(n - 1\) nodes, as discussed in 8.

While Algorithm 1 is a simple algorithm, we briefly present some negative results which show that \(\Omega(n^2)\) path queries are necessary in the worst case for reconstructing a DAG. (Please see Appendix B).

Assuming that we have correct answers for all path queries, Algorithm 1 will indeed exactly recover the TR of any DAG \(G\). However, this is not necessary. We can recover the true transitive reduction, \(\text{TR}(G)\), if we have correct answers for queries \(Q_G(i, j)\) when \(i \in \pi_G(j)\), and when there is no directed path from \(i\) to \(j\), and arbitrary answers when there is a directed path from \(i\) to \(j\). This is because the transitive reduction step will remove every transitive edge. It is the previous observation that motivated our characterization of noisy queries given in Definition 3.

We now present the following lemma which in turn is a very useful property for our methods.

**Lemma 1.** Let \(B = (G, P_G)\) be a CBN with \(X_i, X_j \in X\) being any two random variables in \(G\). If there is no directed path from \(i\) to \(j\) in \(G\), then \(P(X_j|\text{do}(X_i = x_i)) = P(X_j)\).

Please see Appendix D for details of all proofs. As described later in our results, Lemma 1 is a key property that will help us to determine the answer for a noisy path query. Next, we show an important lemma.

**Lemma 2.** Let \(B = (G, P_G)\) be a CBN and let \(X_i\) and \(X_j\) be two random variables in \(G\), such that \(i \in \pi_G(j)\). Then, the following propositions hold:

1. \(\exists x_i \text{ s.t. } P(X_j) \neq P(X_j|\text{do}(X_i = x_i))\)

2. \(\exists x_i, x'_i \text{ s.t. } P(X_j|\text{do}(X_i = x_i)) \neq P(X_j|\text{do}(X_i = x'_i))\)

Lemma 2 while simple, motivates the idea that we can search for two different values of \(X_i\) to determine the causal dependence on \(X_j\) (Claim 2), which is arguably useful for discrete CBNs. Alternatively, we can use the expected value of \(X_j\), since \(E[X_j] \neq E[X_j|\text{do}(X_i = x_i)]\) implies that \(P(X_j) \neq P(X_j|\text{do}(X_i = x_i))\) (Claim 1).
3.2 Noisy Path Query Algorithm

Next, we propose a polynomial time algorithm for answering a noisy path query. Algorithms 2 and 3 present our algorithms for answering a noisy path query $\hat{Q}(i,j)$ motivated by Theorems 1 and 2 respectively. For discrete CBNs, we first create a list $\mathcal{L}$ of size $d = |\text{Dom}[X_j]|$, containing the empirical probability mass functions (PMFs) of $X_j$ after intervening $X_i$ with all the possible values from its domain $\text{Dom}[X_i]$. Next, if the $\ell_\infty$-norm of the difference of any pair of PMFs in $\mathcal{L}$ is greater than a constant $\gamma$, then we answer the query with 1, and 0 otherwise. For continuous CBNs, we intervene $X_i$ with a constant value $z$ and compute the empirical expected value of $X_j$. We then output 1 if the expected value is greater than $1/2$, and 0 otherwise.

The threshold of $1/2$ is set in a clever way, motivated by the conditions in Theorem 1 and explained in detail in its proof in Appendix D.4.

Algorithm 2 Noisy path query algorithm for discrete variables

Input: Nodes $i$ and $j$, number of interventional samples $m$, and constant $\gamma$.
Output: $\hat{Q}(i,j)$
1: $\mathcal{L} \leftarrow \text{emptyList}()$
2: for $x_i \in \text{Dom}[X_i]$ do
3: Intervene $X_i$ by setting its value to $x_i$, and obtain $m$ samples $x_j^{(1)}, \ldots, x_j^{(m)}$ of $X_j$
4: $\hat{p}_k = \frac{1}{m} \sum_{i=1}^{m} \mathbb{1}[x_j^{(j)} = k], \forall k \in \text{Dom}[X_j]$
5: Add $\hat{p}$ to the list $\mathcal{L}$
6: $\hat{Q}(i,j) \leftarrow \mathbb{1}[\exists \hat{p}, \hat{q} \in \mathcal{L} \| \hat{p} - \hat{q} \|_\infty > \gamma]$

Algorithm 3 Noisy path query algorithm for continuous variables

Input: Nodes $i$ and $j$, number of interventional samples $m$, and constant $z$
Output: $\hat{Q}(i,j)$
1: Intervene $X_i$ by setting its value to $z$, and obtain $m$ samples $x_j^{(1)}, \ldots, x_j^{(m)}$ of $X_j$
2: $\hat{\mu} \leftarrow \frac{1}{m} \sum_{k=1}^{m} x_j^{(k)}$
3: $\hat{Q}(i,j) \leftarrow \mathbb{1}[\hat{\mu} > 1/2]$

Discrete random variables. In this paper we use conditional probability tables (CPTs) as the representation of the CPDs for discrete CBNs. Next, we present a theorem that provides the sample complexity of a noisy path query.

Theorem 1. Let $\mathcal{B} = (G, \mathcal{P}_G)$ be a discrete CBN, such that each random variable $X_j$ has a finite domain $\text{Dom}[X_j]$, with $|\text{Dom}[X_j]| \leq r$. Furthermore, let

$$
\gamma = \min_{j \in V} \min_{x_i, x'_i \in \text{Dom}[X_i]} \frac{\min_{x_i, x'_i \in \text{Dom}[X_i]} \mathbb{P}(X_j | \text{do}(X_i = x_i)) - \mathbb{P}(X_j | \text{do}(X_i = x'_i))}{\mathbb{E}(X_j | \text{do}(X_i = x_i)) - \mathbb{E}(X_j | \text{do}(X_i = x'_i))},
$$

and let $\hat{G} = (V, \hat{E})$ be the learned graph by using Algorithm 4. Then for $\gamma > 0$ and a fixed probability of error $\delta \in (0, 1)$, we have

$$
P\left(\mathcal{E}(G) = \hat{G}\right) \geq 1 - \delta,
$$

provided that $m \in O\left(\frac{1}{\gamma^2} \ln \left(n + \ln \frac{rz}{\delta}\right)\right)$ interventional samples are used per $\delta$-noisy partially-correct path query in Algorithm 4.

In the theorem above, $\gamma = 0$ would mean that there exists two random variables $X_i$ and $X_j$, such that they are statistically independent, which would violate Assumption 3 (faithfulness), therefore, it is safe to assume that $\gamma > 0$. The constant $\gamma$ is used for deciding whether two empirical PMFs are equal or not in our path query algorithm, which implements Claim 2 in Lemma 3. Finally, in practice, the value of $\gamma$ is unknown. Fortunately, knowing a lower bound of $\gamma$ suffices for structure recovery.

Continuous random variables. For continuous CBNs, our algorithm compares two empirical expected values for answering a path query. This is related to Claim 1 in Lemma 3 since $E[X_j] \neq E[X_j | \text{do}(X_i = x_i)]$ implies $P(X_j) \neq P(X_j | \text{do}(X_i = x_i))$. We analyze continuous CBNs where every random variable is sub-Gaussian. The class of sub-Gaussian variables includes for instance Gaussian variables, any bounded random variable (e.g., uniform), any random variable with strictly log-concave density, and any finite mixture of sub-Gaussian variables. Note that sample complexity using sub-Gaussian variables has been studied in the past for other models, such as Markov random fields. Next, we present a theorem that formally characterizes the class of continuous CBNs that our algorithm can learn, and provides the sample complexity for each noisy path query.

Theorem 2. Let $\mathcal{B} = (G, \mathcal{P}_G)$ be a continuous CBN such that each random variable $X_j$ is a sub-Gaussian random variable with full support on $\mathbb{R}$, with mean $\mu_j = 0$ and variance $\sigma_j^2$. Let $\mu_{j \mid \text{do}(X_i = z)}$ and $\sigma_{j \mid \text{do}(X_i = z)}^2$ denote the expected value and variance of $X_j$ after intervening $X_i$.
Algorithm 3. If there exist an upper bound with value \( z \)

\[
\mu(B, z) = \min_{i \in \pi_G(j)} \left| \mu_{j|do(X_i = z)} \right|
\]

\[
\sigma^2(B, z) = \max \left( \max_{j \in V} \sigma^2_{j|do(X_i = z)}, \max_{j \in V} \sigma^2_{j} \right)
\]

and let \( \hat{G} = (V, \hat{E}) \) be the learned graph by using Algorithm 4. If there exist an upper bound \( \sigma^2_{ab} \) and a finite value \( z \) such that \( \sigma^2(B, z) \leq \sigma^2_{ab} \) and \( \mu(B, z) \geq 1 \), then for a fixed probability of error \( \delta \in (0, 1) \), we have

\[
P\left( TR(G) = \hat{G} \right) \geq 1 - \delta,
\]

provided that \( m \in \mathcal{O}(\sigma^2_{ab} \log \frac{1}{\delta}) \) interventional samples are used per \( \delta \)-noisy partially-correct path query in Algorithm 3.

It is worth noting that the conditions \( \mu_j = 0, \forall j \in V \), and \( \mu(B, z) \geq 1 \) are set to offer clarity in the derivations. One could for instance set an upper bound for the magnitude of \( \mu_j \), assume \( \mu(B, z) \) to be greater than this upper bound plus 1, and still have the same sample complexity. Finally, our motivation for giving such conditions is that of guaranteeing a proper separation of the expected values in cases where there is effect of a variable \( X_i \) over another variable \( X_j \), versus cases where there is no effect at all.

Next, we define the additive sub-Gaussian noise model (ASGN).

**Definition 4.** Let \( G = (V, E) \) be a DAG, let \( W \in \mathbb{R}^{n \times n} \) be the matrix of edge weights and let \( S = \{ \sigma^2_i \in \mathbb{R}_+ \mid i \in V \} \) be the set of noise variances. An additive sub-Gaussian noise network is a tuple \( (G, P(W, S)) \) where each variable \( X_i \) can be written as follows:

\[ X_i = \sum_{j \in \pi_G(i)} W_{ij} X_j + N_i, \quad \forall i \in V, \]

with \( N_i \) being an independent sub-Gaussian noise with full support on \( \mathbb{R} \), with zero mean and variance \( \sigma^2_i \) for all \( i \in V \), and \( W_{ij} \neq 0 \) iff \( (i, j) \in E \).

**Remark 1.** Let \( B = (G, P(W, S)) \) be an ASGN network. We can rewrite the model in vector form as: \( X = WX + N \) or equivalently \( X = (I - W)^{-1}N \), where \( X = (X_1, \ldots, X_n) \) and \( N = (N_1, \ldots, N_n) \) are the vector of variables and the noise vector respectively. Additionally, we denote \( \odot W \) as the weight matrix \( W \) with its \( i \)-th row set to 0. This means that we can interpret \( \odot W \) as the weight matrix after performing and intervention on node \( i \) (mutilated graph).

We now present a corollary that fulfills the conditions presented in Theorem 2.

**Corollary 1** (Additive sub-Gaussian noise model). Let \( B = (G, P(W, S)) \) be an ASGN network as in Definition 4 such that \( \sigma^2_i \leq \sigma^2_{max}, \forall j \in V \). Also, let \( w_{min} = \min_{(i,j) \in E} \{(I - \odot W)^{-1}\}_{ji} \), and \( w_{max} = \max \| (I - W)^{-1} \|_2^2, \max_{i \in V} \| (I - \odot W)^{-1} \|_2^2 \). If \( z = \frac{1}{w_{min}} \) and \( \sigma^2_{ab} = \sigma^2_{max}w_{max} \), then for a fixed probability of error \( \delta \in (0, 1) \), we have \( P( TR(G) = \hat{G} ) \geq 1 - \delta \). Where \( \hat{G} = (V, \hat{E}) \) is the learned graph by using Algorithm 4 and provided that \( m \in \mathcal{O}(\sigma^2_{ab} \log \frac{1}{\delta}) \) interventional samples are used per \( \delta \)-noisy partially-correct path query in Algorithm 3.

The values of \( w_{min} \) and \( w_{max} \) follow the specifications of Theorem 2. In addition, the value of \( w_{min} \) is guaranteed to be greater than 0 because of the faithfulness assumption (see Assumption 3). For instance, consider the following ASGN network in Figure 3 assume that \( X_1 \) is intervened, then we have that the expected value of \( X_3 \) is 0 regardless of the value of the intervention. This occurs because the effect is canceled via the directed paths \( \{(1,2),(2,3)\} \) and \( \{(1,3)\} \). This motivated us to use the faithfulness assumption and rule out such “pathological” parameterizations. Finally, in practice, the values of \( w_{min} \) and \( \sigma^2_{ab} \) are unknown. Fortunately, knowing a lower bound of \( w_{min} \) and an upper bound of \( \sigma^2_{ab} \) suffices for structure recovery.

**Figure 3:** An ASGN network in which the effect of \( X_1 \) on \( X_3 \) is none.

### 4 Extensions

#### 4.1 On the Recovery of Transitive Edges

In this section, we show a method to recover the transitive edges by using multiple-vertex interventions. Next, we present a new query defined as follows.

**Definition 5** (\( \delta \)-noisy transitive query). Let \( G = (V, E) \) be a DAG, and let \( \delta \in (0, 1) \) be a probability of error. A \( \delta \)-noisy transitive query is a function \( T_G : V \times V \times 2^V \rightarrow \{0, 1\} \) such that \( T_G(i, j, S) = 1 \) with probability at least \( 1 - \delta \) if \( (i, j) \in E \) is a transitive edge, and 0 otherwise. Here \( S \subseteq \pi_G(j) \) is an auxiliary set necessary to answer the query, in order to block any influence from \( i \) to \( S \), and to unveil the direct effect from \( i \) to \( j \).

Algorithms 4 and 5 show how to answer a transitive query for discrete and continuous CBNs respectively. Both algorithms are motivated on a property of CBNs, that is, \( \forall i \in V \) and for every set \( S \) disjoint of \( \{i, \pi_G(i)\} \),
we have $P(X_i|do(X_{πG(i)} = x_{πG(i)}), do(X_S = x_S)) = P(X_i|do(X_{πG(i)} = x_{πG(i)}))$. Thus, both algorithms intervene the set $S$, if $S$ is the parent set of $i$, then $i$ will have no effect on $j$ and they return 0, and 1 otherwise.

**Algorithm 4** Noisy transitive query algorithm for discrete variables

**Input:** Nodes $i$ and $j$, set of nodes $S$, number of interventional samples $m$, and constant $γ$.

**Output:** $T(i, j, S)$

1: $L ←$ emptyList()
2: for $x_s ∈ \times_{s ∈ S} Dom[X_s]$ do
3: Intervene set $X_S$ by setting its value to $x_s$
4: for $x_i ∈ Dom[X_i]$ do
5: Intervene $X_i$ by setting its value to $x_i$, and obtain $m$ samples $x_j^{(1)}, ..., x_j^{(m)}$ of $X_j$
6: $\tilde{p}_k = \frac{1}{m} \sum_{j^{(m)}} 1[x_j^{(k)} = k], \forall k ∈ Dom[X_j]$
7: Add $\tilde{p}$ to the list $L$
8: $T(i, j, S) ← 1[∃ p, q ∈ L \parallel p - q∥_∞ > γ]$
9: if $T(i, j, S) = 1$ then STOP

**Algorithm 5** Noisy transitive query algorithm for continuous variables

**Input:** Nodes $i$ and $j$, set of nodes $S$, number of interventional samples $m$, and constants $z_1, z_2$

**Output:** $T(i, j, S)$

1: Intervene all variables $X_S$ by setting their values to $z_1$
2: Intervene $X_i$ by setting its value to $z_2$, and obtain $m$ samples $x_j^{(1)}, ..., x_j^{(m)}$ of $X_j$
3: $\hat{μ} ← \frac{1}{m} \sum_{j^{(m)}} x_j^{(k)}$
4: $\tilde{T}(i, j, S) ← 1[|μ - 1/2|]$

Recall that by using Algorithm 1 we obtain the transitive reduction of the CBN, thus, we have the true topological ordering of the CBN, and also for each node $i ∈ V$, we know its parent set or a subset of it. Using these observations, we can cleverly set the input $i$, $j$, and $S$ of a noisy transitive query, as done in Algorithm 6. It is clear that Algorithm 6 makes $O(n^2)$ noisy transitive queries in total. The time complexity to answer a transitive query for a discrete CBN can be exponential in the maximum number of parents. However, the sample complexity for queries in discrete and continuous CBNs remains polynomial in $n$ as prescribed in the following theorems.

**Theorem 3.** Let $B = (G, PG)$ be a discrete CBN, such that each random variable $X_j$ has a finite domain $Dom[X_j]$, with $|Dom[X_j]| ≤ r$. Furthermore, let

$$γ = \min_{j \in V} \min_{S ⊆ πG(j), |S| ≥ 1} \min_{x_S, x_{j}' ∈ \times_{s ∈ S} Dom[X_s]} p(X_j|do(X_S = x_S), πG(j)|do(X_S = x_S))$$

$$\|p(X_j|do(X_S = x_S)) - p(X_j|do(X_S = x_S'))\|_∞,$$

and let $\tilde{G} = (V, \tilde{E})$ be the output of Algorithm 6. Then for $γ > 0$ and a fixed probability of error $δ ∈ (0, 1)$, we have

$$P(G = \tilde{G}) ≥ 1 - δ,$$

provided that $m ∈ O(\frac{1}{γ} \ln n + \ln \frac{1}{δ})$ interventional samples are used per $δ$-noisy transitive query in Algorithm 6.

**Theorem 4.** Let $B = (G, PG)$ be a continuous CBN such that each variable $X_j$ is a sub-Gaussian random variable with full support on $R$, with mean $μ_j = 0$ and variance $σ_j^2$. Let $μ_{j|do(X_S = 1)}$ and $σ_{j|do(X_S = 1)}^2$ denote the expected value and variance of $X_j$ after intervening each node of $X_S$ with value $z$. Furthermore, let

$$μ(B, z_1, z_2) = \min_{S ⊆ πG(j), |S| ≥ 1} \min_{x_S \in Dom[X_S]} |μ_{j|do(X_S = 1)}|$$

$$σ_j^2(B, z_1, z_2) = \max_{j \in V} \max_{S ⊆ πG(j), |S| ≥ 1} σ_{j|do(X_S = 1)}^2,$$

and let $\tilde{G} = (V, \tilde{E})$ be the output of Algorithm 6. If there exist an upper bound $σ_{ab}^2$ and finite values $z_1, z_2$ such that $σ_j^2(B, z_1, z_2) ≤ σ_{ab}^2$ and $μ(B, z_1, z_2) ≥ 1$, then for a fixed probability of error $δ ∈ (0, 1)$, we have

$$P\left(G = \tilde{G}\right) ≥ 1 - δ,$$

provided that $m ∈ O(\frac{σ_{ab}^2}{δ} \ln n)$ interventional samples are used per $δ$-noisy transitive query in Algorithm 6.

Next, we show that ASGN networks can fulfill the conditions in Theorem 4.

**Corollary 2.** Let $B = (G, P(W, S))$, and $σ_{max}$ follow the same definition as in Corollary 1. Let

$$w_{min} = \min_{ij} |W_{ij}|, \quad w_{max} = \max(||(I -$$
of Algorithm 1. Then for query in Algorithm 5.

Let \( \mu_j \) follow the same definition as in Theorem 2. Let \( \sigma_{j|do(X_i = z)} \) denote the expected value and variance of \( X_i \) after perfectly intervening \( X_i \) with value \( z \). Furthermore, let \( \mu(B, z) = \min_{(i, j) \in E} \mathbb{E}_{X_i} [\mu_{j|do(X_i, z = z)}] \), and \( \sigma^2(B, z) = \max_{(i, j) \in E} \mathbb{E}_{X_i} [\sigma_{j|do(X_i, z = z)}^2] \). Let \( \tilde{G} = (V, \tilde{E}) \) be the output of Algorithm 4. If there exist an upper bound \( \sigma_{ab}^2 \) and a finite value \( z \) such that \( \sigma^2(B, z) \leq \sigma_{ab}^2 \) and \( \mu(B, z) \geq 1 \), then for a fixed probability of error \( \delta \in (0, 1) \), we have \( \mathbb{P}(\text{TR}(G) = \tilde{G}) \geq 1 - \delta \), provided that \( m \in \mathcal{O}(\sigma_{ab}^2 \log \frac{1}{\delta}) \) interventional samples are used per \( \delta \)-noisy partially-correct path query in Algorithm 3.

The motivation of the conditions in Theorem 6 are similar to Theorem 2. Next, we show that ASGN models can fulfill the conditions above.

**Corollary 3.** Under the settings given in Corollary 2. If for all \( j \in V \), \( \nu_j^2 \leq \sigma_{\max}^2 \) in terms of imperfect interventions. Then, for a fixed probability of error \( \delta \in (0, 1) \), we have \( \mathbb{P}(\text{TR}(G) = \tilde{G}) \geq 1 - \delta \), provided that \( m \in \mathcal{O}(\sigma_{ab}^2 \log \frac{1}{\delta}) \) interventional samples are used per \( \delta \)-noisy partially-correct path query in Algorithm 3.

**Experiments.** In Appendix E, we provide several experiments. In Section E.1, we tested our algorithms for perfect and imperfect interventions in synthetic networks, in order to empirically prove the logarithmic phase transition of the number of interventional samples. Section E.2 shows that in several benchmark BNs, most of the graph belongs to its transitive reduction, meaning that one can learn most of the network in polynomial time. Section E.3 shows experiments on some of these benchmark networks, using the aforementioned algorithms and also our algorithm for learning transitive edges. Finally, in Section E.4, as an illustration of the availability of interventional data, we show experimental evidence using a genetics dataset.

**Concluding remarks.** There are several ways of extending this work. For instance, it would be interesting to analyze more general modifications to perfect interventions as in [7], which also deals uncertain interventions. For continuous CBNs, we opted to use expected values and not to compare continuous distributions directly. The fact that the conditioning is with respect to a continuous random variable makes this task more complex than the typical comparison of continuous distributions. Still, it would be interesting to see whether kernel density estimators [15] could be beneficial.
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Appendix A  On Latent Variables

It is well-known that the existence of confounders imposes the most crucial problem for inferring causal relationships from observational data [16, 21]. However, since we perform single-vertex interventions for every node in the CBN, the existence of hidden confounders does not impose a problem. In the leftmost graph of Figure 4, X and Y are associated observationally due to a hidden common cause, but neither of them is a cause of the other. By intervening X or Y, we remove the “hidden edges”. As a consequence, we are able to infer that neither X nor Y is a cause. The middle graph shows an association between X and Y, and the need to intervene X in order to discover that X is a cause of Y. Finally, the rightmost graph shows that even in more complex latent configurations, by intervening X we are removing any association between X and Y due to confounders.

Figure 4: Examples of a latent configurations that associate the variables X and Y.

Appendix B  Negative Results in Learning DAGs by Using Path Queries

Theorem 7. In order to reconstruct a sparse disconnected or a sparse connected DAG of n nodes, any deterministic algorithm requires at least \( \Omega(n^2) \) queries in the worst case.

Proof. For sparse disconnected DAGs, the proof relies on constructing a family of graphs with a single edge. Assume two fixed nodes \( i, j \in V \), unknown to a graph reconstruction algorithm. The directed graph to be reconstructed is \( G = (V, E) \) where \( E = \{(i, j)\} \). Note that \( Q(i, j) = 1 \). Furthermore \( Q(k, l) = 0 \) for every node pair \( (k, l) \neq (i, j) \). That is, only one query returns 1, while \( n^2 - 1 \) queries return 0. Thus, a deterministic algorithm does not obtain any information from the \( n^2 - 1 \) queries in order to guess the edge \( (i, j) \), and therefore it requires at least \( n^2 \) path queries in the worst case.

Figure 5: A “v-structured two-layered” directed acyclic graph.

For sparse connected DAGs, the proof relies on constructing a family of “v-structured two-layered” graphs. Assume the node set \( V \) is partitioned into two fixed sets \( V_1 \) and \( V_2 \), unknown to a graph reconstruction algorithm. For simplicity assume that there is an odd number of nodes, and that \( |V_2| = |V_1| + 1 \). We then create the graph \( G = (V, E) \) with \( n - 1 \) edges such that each node in \( V_1 \) is the source of at most 2 edges, and each node in \( V_2 \) is the target of at most 2 edges. This creates a “v-structured two-layered” graph as shown in Figure 5. Note that \( Q(i, j) = 1 \) for \( (i, j) \in E \), while \( Q(i, j) = 0 \) for \( (i, j) \notin E \). That is only \( n - 1 \) queries return 1, while \( n^2 - n + 1 \) queries return 0. Thus, a deterministic algorithm does not obtain any information from the \( n^2 - n + 1 \) queries in order to guess the edge set \( E \), and therefore it requires at least \( n^2 - n + 2 \) queries in the worst case. (Since the algorithm knows that there are \( n - 1 \) edges, it can stop asking queries as soon as the first bit 1 is returned.)
Appendix C  Query Algorithm for Discrete Networks Under Imperfect Interventions

Algorithm 7 shows how to answer a noisy query for discrete CBNs under imperfect interventions.

**Algorithm 7** Noisy path query algorithm for discrete variables under imperfect interventions.

**Input:** Nodes $i$ and $j$, number of interventional samples $m$, and constant $\gamma$

**Output:** $\hat{Q}(i,j)$

1. $\mathcal{L} \leftarrow \text{emptyList}()$
2. for $x_i \in \text{Dom}[X_i]$ do
3. Try to intervene $X_i$ with value $x_i$, and obtain $m$ pair samples $(x_i^{(1)}, x_j^{(1)}), \ldots, (x_i^{(m)}, x_j^{(m)})$ of $X_i$ and $X_j$
4. $\hat{p}_k = \frac{1}{\sum_{\ell=1}^{m} 1[x_i^{(\ell)} = x_j^{(\ell)}]} \sum_{l=1}^{m} 1[x_j^{(l)} = k \land x_i^{(l)} = x_i], \forall k \in \text{Dom}[X_j]$
5. Add $p$ to the list $\mathcal{L}$
6. $\hat{Q}(i,j) \leftarrow 1[(\exists \hat{p}, \hat{q} \in \mathcal{L}) \|\hat{p} - \hat{q}\|_{\infty} > \gamma]

Appendix D  Detailed Proofs

We now present the proofs of Lemmas, Theorems and Corollaries from our main text.

**D.1 Proof of Lemma 1**

*Proof.* The proof follows a d-separation argument. Let $\bar{B}$ be the network after we perform an intervention on $X_i$ with value $x_i$, i.e., $\bar{B}$ has the edge set $E \setminus \{(p_i, i) | p_i \in \pi_G(i)\}$. Let $\text{anc}_G(i)$ and $\text{anc}_G(j)$ be the ancestor set of $i$ and $j$ respectively. Now, if there is no directed path from $i$ to $j$ in $\bar{B}$ then there is no directed path in $\bar{B}$ either, therefore, $i \notin \text{anc}_G(j)$. Also, $\text{anc}_G(i) = \emptyset$ as a consequence of intervening $X_i$. Next, we follow the d-separation procedure to determine if $X_i$ and $X_j$ are marginally independent in $\bar{B}$. Since $\text{anc}_G(i) = \emptyset$, the ancestral graph of $i$ consists of just $i$ itself in isolation, moralizing and disorienting the edges of the ancestral graph of $j$ will not create a path from $i$ to $j$. Thus, guaranteeing the independence of $X_i$ and $X_j$, i.e., $P(X_j|\text{do}(X_i = x_i)) = P(X_j)$. Finally, since $P(X_j|X_{\pi_G(j)})$ is fully specified by the parents of $j$ and these parents are not affected by $i$, we have that the marginal of $X_j$ in $\bar{B}$ remains unchanged in $\bar{B}$, i.e., $P(X_j|\text{do}(X_i = x_i)) = P(X_j)$.

**D.2 Proof of Lemma 2**

*Proof.* Both claims follow a proof by contradiction. For Claim 1, if for all $x_i \in \text{Dom}[X_i]$ we have that $P(X_j) = P(X_j|\text{do}(X_i = x_i))$ then $X_i$ would not be a cause of $X_j$ which contradicts the fact that $i \in \pi_G(j)$. For Claim 2, if for all $x_i, x_i' \in \text{Dom}[X_j]$ we have that $P(X_j|\text{do}(X_i = x_i)) = P(X_j|\text{do}(X_i = x_i'))$ then in the mutilated graph we have that $P(X_j) = P(X_j|X_i = x_i)$ for all $x_i$, which implies that $X_i$ would not be a cause of $X_j$, thus contradicting the fact that $i \in \pi_G(j)$.

**D.3 Proof of Theorem 1**

To answer a path query in a discrete CBN, our algorithm compares two empirical PMFs, therefore, we need a good estimation of these PMFs. The following lemma shows the sample complexity to estimate several PMFs simultaneously by using maximum likelihood estimation.

**Lemma 3.** Let $Y_1, \ldots, Y_L$ be L random variables, such that w.l.o.g. the domain of each variable, $\text{Dom}[Y_i]$, is a finite subset of $\mathbb{Z}^+$. Also, let $y_i^{(1)}, \ldots, y_i^{(m)}$ be $m$ independent samples of $Y_i$. The maximum likelihood estimator, $\hat{p}(Y_i)$, is obtained as follows:

$$\hat{p}_j(Y_i) = \frac{1}{m} \sum_{k=1}^{m} 1[y_i^{(k)} = j], \quad j \in \text{Dom}[Y_i].$$

Then, for fixed values of $t > 0$ and $\delta \in (0, 1)$, and provided that $m \geq \frac{2}{\delta^2} \ln \frac{2L}{\delta}$, we have

$$P \left( \forall i \in \{1 \ldots L\} \left\| \hat{p}(Y_i) - p(Y_i) \right\|_{\infty} \leq t \right) \geq 1 - \delta.$$
Proof. We use the Dvoretzky-Kiefer-Wolfowitz inequality [17, 6]:

\[ P \left( \sup_{j \in \text{Dom}[Y_i]} \left| \hat{F}_j(Y_i) - F_j(Y_i) \right| > t \right) \leq 2e^{-2mt^2}, \quad t > 0, \]

where \( \hat{F}_j(Y_i) = \sum_{k \leq j} \hat{p}_k(Y_i) \) and \( F_j(Y_i) = \sum_{k \leq j} p_k(Y_i) \). Since \( \hat{p}_j(Y_i) = \hat{F}_j(Y_i) - \hat{F}_{j-1}(Y_i) \) and \( p_j(Y_i) = F_j(Y_i) - F_{j-1}(Y_i) \), we have

\[ |\hat{p}_j(Y_i) - p_j(Y_i)| = \left| (\hat{F}_j(Y_i) - \hat{F}_{j-1}(Y_i)) - (F_j(Y_i) - F_{j-1}(Y_i)) \right| \leq |\hat{F}_j(Y_i) - F_j(Y_i)| + |\hat{F}_{j-1}(Y_i) - F_{j-1}(Y_i)| \]

therefore, for a specific \( i \), we have

\[ P \left( \|\hat{p}(Y_i) - p(Y_i)\|_\infty > t \right) \leq 2e^{-mt^2/2}, \quad t > 0. \]

Then by the union bound, we have

\[ P \left( \exists i \in \{1 \ldots L\} \right) \|\hat{p}(Y_i) - p(Y_i)\|_\infty > t \right) \leq 2Le^{-mt^2/2}, \quad t > 0. \]

Let \( \delta = 2Le^{-mt^2/2} \), then for \( m \geq \frac{2}{\delta} \log \frac{2L}{\delta} \), we have

\[ P \left( \forall i \in \{1 \ldots L\} \right) \|\hat{p}(Y_i) - p(Y_i)\|_\infty \leq t \right) \geq 1 - \delta, \quad \delta \in (0, 1), \quad t > 0. \]

Which concludes the proof of Lemma 3.

Lemma 3 states that simultaneously for all \( L \) PMFs, the maximum likelihood estimator \( \hat{p}(Y_i) \) is at most \( t \)-away of \( p(Y_i) \) in \( \ell_\infty \)-norm with probability at least \( 1 - \delta \). Next, we provide the proof of Theorem 1.

Proof. We analyze a path query \( \hat{Q}(i, j) \) for nodes \( i, j \in V \). From the contrapositive of Lemma 1, we have that if \( P(X_j|do(X_i = x_i)) \neq P(X_j) \) then there exists a directed path from \( i \) to \( j \). To detect the latter, we opt to use Claim 2 from Lemma 2.

Let \( \hat{p}^{(k)}_{ij} = P(X_j|do(X_i = x_k)) \) for all \( i, j \in V \) and \( x_k \in \text{Dom}[X_i] \), and let \( \hat{p}^{(k)}_{ij} \) be the maximum likelihood estimation of \( \hat{p}^{(k)}_{ij} \). Also, let \( \tau = \frac{\tau}{2} \) for convenience. Next, using Lemma 3 with \( t = \tau/4 \) and \( L = rn^2 \), we have

\[ P \left( \forall i \in V, \forall x_k \in \text{Dom}[X_i] \right) \|\hat{p}^{(k)}_{ij} - \hat{p}^{(k)}_{ij}\|_\infty \leq \tau/4 \right) \geq 1 - \delta. \]

That is, with probability at least \( 1 - \delta \), simultaneously for all \( i, j, k \), the estimators \( \hat{p}^{(k)}_{ij} \) are at most \( \tau/4 \)-away from the true distributions \( \hat{p}^{(k)}_{ij} \) in \( \ell_\infty \) norm, provided that \( m \geq \frac{2}{\tau^2} (2\ln n + \ln \frac{2L}{\delta}) \) samples are used in the estimation.

Now, we analyze the two cases that we are interested to answer with high probability. First, let \( i \in \pi_G(j) \). We have that for any two distributions \( p^{(u)}_{ij}, p^{(v)}_{ij} \) where \( x_u, x_v \in \text{Dom}[X_i] \), either \( p^{(u)}_{ij} = p^{(v)}_{ij} \) or \( \|p^{(u)}_{ij} - p^{(v)}_{ij}\|_\infty > \tau \) (recall the definition of \( \gamma \) and \( \tau \)). Next, for a specific \( i, j \), we show how to test if two distributions \( p^{(u)}_{ij}, p^{(v)}_{ij} \) are equal or not. Let us assume \( p^{(u)}_{ij} = p^{(v)}_{ij} \), then we have

\[ \|p^{(u)}_{ij} - p^{(v)}_{ij}\|_\infty = \|p^{(u)}_{ij} - p^{(u)}_{ij} - (p^{(v)}_{ij} - p^{(v)}_{ij})\|_\infty \leq \|p^{(u)}_{ij} - p^{(u)}_{ij}\|_\infty + \|p^{(v)}_{ij} - p^{(v)}_{ij}\|_\infty \leq \tau/2. \]
Therefore, if \( \|p_{ij}^{(u)} - \hat{p}_{ij}^{(v)}\|_\infty > \tau/2 \) then w.h.p. \( p_{ij}^{(u)} \neq \hat{p}_{ij}^{(v)} \). On the other hand, if \( \|p_{ij}^{(u)} - \hat{p}_{ij}^{(v)}\|_\infty \leq \tau/2 \) then w.h.p. we have:

\[
\|p_{ij}^{(u)} - \hat{p}_{ij}^{(v)}\|_\infty = \|p_{ij}^{(u)} - p_{ij}^{(v)} - (\hat{p}_{ij}^{(v)} - \hat{p}_{ij}^{(v)}) + (\hat{p}_{ij}^{(v)} - \hat{p}_{ij}^{(v)})\|_\infty \\
\leq \|p_{ij}^{(u)} - p_{ij}^{(v)}\|_\infty + \|\hat{p}_{ij}^{(v)} - \hat{p}_{ij}^{(v)}\|_\infty + \|\hat{p}_{ij}^{(v)} - \hat{p}_{ij}^{(v)}\|_\infty \\
\leq \tau.
\]

From the definition of \( \gamma \) and \( \tau \), we have \( \|p_{ij}^{(u)} - \hat{p}_{ij}^{(v)}\|_\infty > \tau \) for any pair \( p_{ij}^{(u)} \neq \hat{p}_{ij}^{(v)} \), then w.h.p. we have that \( \hat{p}_{ij}^{(u)} = \hat{p}_{ij}^{(v)} \).

Second, let be the case that there is no directed path from \( i \) to \( j \). Then, following Lemma 1 we have that all the distributions \( p_{ij}^{(k)}, \forall x_k \in \text{Dom}[X_i] \), are equal. Similarly as in the first case, we have that if \( \|p_{ij}^{(u)} - \hat{p}_{ij}^{(v)}\|_\infty > \tau/2 \) then w.h.p. \( p_{ij}^{(u)} \neq p_{ij}^{(v)} \), and equal otherwise.

Next, note that since Algorithm 2 compares pair of distributions, the provable guarantee of all queries (after eliminating the transitive edges) is directly related to the estimation of all PMFs with probability of error at most \( \delta \), i.e., we have that

\[
P\left( (\forall j = 1, \ldots, n \land (i \in \pi_G(j) \lor j \notin \text{desc}_G(i))) \hat{Q}(i, j) = Q_G(i, j) \right) \geq 1 - \delta,
\]

where \( \text{desc}_G(i) \) denotes the descendants of \( i \). Finally, note that we are estimating each distribution by using \( m \geq 2\delta/(2\ln n + \ln \frac{2\tau}{\delta}) \) samples, i.e., \( m \in \mathcal{O}(\frac{1}{\delta}(\ln n + \ln \frac{\tau}{\delta})) \). However, for each query \( \hat{Q}(i, j) \) in Algorithm 2 we estimate a maximum of \( r \) distributions, as a result, we use \( \frac{32\tau^2}{r}(2\ln n + \ln \frac{2\tau}{\delta}) \) interventional samples in total per query.

**D.4 Proof of Theorem 2**

*Proof.* From the contrapositive of Lemma 1 we have that if \( P(X_j | \text{do}(X_i = x_i)) \neq P(X_j) \) then there exists a directed path from \( i \) to \( j \). To detect the latter, we opt to use Claim 1 from Lemma 2 i.e., using expected values. Recall from the characterization of the BN that there exist a finite value \( z \) and upper bound \( \sigma_{ab}^2 \), such that \( \mu(B, z) \geq 1 \) and \( \sigma^2(B, z) \leq \sigma_{ab}^2 \). Let \( x_j^{(1)}, \ldots, x_j^{(m)} \) be \( m \) i.i.d. samples of \( X_j \) after intervening \( X_i \) with \( z \), and let \( \mu_{j|\text{do}(X_i = z)} \) and \( \sigma_{j|\text{do}(X_i = z)}^2 \) be the mean and variance of \( X_j \) respectively. Also, let \( \hat{\mu}_{j|\text{do}(X_i = z)} = \frac{1}{m} \sum_{k=1}^{m} x_j^{(k)} \) be the empirical expected value of \( X_j \).

Now, we analyze the two cases that we are interested to answer with high probability. First, let \( i \in \pi_G(j) \). Clearly, \( \mu_{j|\text{do}(X_i = z)} \) has expected value \( \mathbb{E}[\hat{\mu}_{j|\text{do}(X_i = z)}] = \mu_{j|\text{do}(X_i = z)} \geq 1 \), and variance \( \hat{\sigma}_{j|\text{do}(X_i = z)}^2 = \frac{\sigma_{j|\text{do}(X_i = z)}^2}{m} \leq \sigma_{ab}^2/m \). Then, using Hoeffding’s inequality we have

\[
P\left( |\hat{\mu}_{j|\text{do}(X_i = z)} - \mu_{j|\text{do}(X_i = z)}| \geq t \right) \leq 2e^{-t^2/(2\sigma_{j|\text{do}(X_i = z)}^2)} \\
\leq 2e^{-mt^2/(2\sigma_{ab}^2)}. \tag{7.1}
\]

Second, if there is no directed path from \( i \) to \( j \), then by using Lemma 1 we have \( \mu_{j|\text{do}(X_i = z)} = \mu_j = 0 \) and \( \sigma_{j|\text{do}(X_i = z)}^2 = \sigma_j^2 \leq \sigma_{ab}^2 \).

As we can observe from both cases described above, the true mean \( \mu_{j|\text{do}(X_i = z)} \) when \( i \in \pi_G(j) \) is at least separated by 1 from the true mean when there is no directed path. Therefore, to estimate the mean, a suitable value for \( t \) in inequality (7.1) is \( t \leq 1/2 \). The latter allows us to state that if \( |\hat{\mu}_{j|\text{do}(X_i = z)}| > 1/2 \) then \( \hat{Q}(i, j) = 1 \), and \( \hat{Q}(i, j) = 0 \) otherwise. Replacing \( t = 1/2 \) and restating inequality (7.1), we have that for a specific pair of nodes \((i, j)\), if \( i \in \pi_G(j) \) or if \( j \notin \text{desc}_G(i) \) (\( \text{desc}_G(i) \) denotes the descendants of \( i \)), then

\[
P\left( \hat{Q}(i, j) \neq \hat{Q}(i, j) \right) \leq 2e^{-m/(8\sigma_{ab}^2)}.
\]
The latter inequality is for a single query. Using the union bound we have
\[ P \left( \exists j = 1, \ldots, n \land (i \in \pi_G(j) \lor j \notin \text{desc}_G(i)) \mid \hat{Q}(i, j) \neq Q_G(i, j) \right) \leq 2n^2 e^{-m/(8\sigma^2_{ub})}. \]
Now, let \( \delta = 2n^2 e^{-m/(8\sigma^2_{ub})} \), if \( m \geq 8\sigma^2_{ub} \log \frac{2n^2}{\delta} \) then
\[ P \left( \forall j = 1, \ldots, n \land (i \in \pi_G(j) \lor j \notin \text{desc}_G(i)) \mid \hat{Q}(i, j) = Q_G(i, j) \right) \geq 1 - \delta. \]
That is, with probability of at least \( 1 - \delta \), the path query \( \hat{Q}(i, j) \) (in Algorithm 3) is equal to \( Q_G(i, j) \) for all \( n^2 \) performed queries in which either \( i \in \pi_G(j) \), or there is no directed path from \( i \) to \( j \). Note also that the probability at least \( 1 - \delta \) is guaranteed after we remove the transitive edges in the network. Therefore, we obtain \( m \geq 8\sigma^2_{ub}(2\log n + \log \frac{2}{\delta}) \), i.e., \( m \in \mathcal{O}(\sigma^2_{ub} \log \frac{2}{\delta}) \).

**D.5 Proof of Theorem 3**

The proof follows the same arguments given in the proof of Theorem 1. For a pair of nodes \( i, j \), Algorithm 6 sets \( S = \pi_G(j) \). If \( S \) is already the true parent set of \( j \), then \( X_j \) will only have effect on \( X_j \) if \( i \in S \). If \( S \) is a subset of the true parent set, then \( X_i \) will only have effect on \( X_j \) if there exists a transitive edge \( (i, j) \). This is because by intervening \( S \) we are blocking any possible effect of \( X_i \) on \( X_j \) through any node in \( S \), and since non-transitive edges are already recovered then \( (i, j) \) must be a transitive edge if there exists some effect. This effect is detected as in Theorem 1 i.e., through the \( \ell_\infty \)-norm of difference of empirical marginals of \( X_j \).

**D.6 Proof of Theorem 4**

The proof follows the same arguments given in the proof of Theorem 2. For a pair of nodes \( i, j \), Algorithm 6 sets \( S = \pi_G(j) \). If \( S \) is already the true parent set of \( j \), then \( X_j \) will only have effect on \( X_j \) if \( i \in S \). If \( S \) is a subset of the true parent set, then \( X_i \) will only have effect on \( X_j \) if there exists a transitive edge \( (i, j) \). This is because by intervening \( S \) we are blocking any possible effect of \( X_i \) on \( X_j \) through any node in \( S \), and since non-transitive edges are already recovered then \( (i, j) \) must be a transitive edge if there exists some effect. This effect is detected as in Theorem 2 i.e., through the absolute value of the difference of the empirical means of \( X_j \).

**D.7 Proof of Theorem 5**

To prove Theorem 5 we first derive a lemma that specifies the number of samples to obtain a good approximation with guarantees of conditional PMFs.

**Lemma 4.** Let \( Y_1, \ldots, Y_L \) be \( L \) discrete random variables, such that w.l.o.g. the domain of each variable, \( \text{Dom}[Y_i] \), is a finite subset of \( \mathbb{Z}_+ \). Let \( Z_1, \ldots, Z_L \) be \( L \) Bernoulli random variables, such that each variable fulfills \( P(Z_i = 1) \geq \alpha \geq 1/2 \). Also, let \( (z_i^{(1)}, y_i^{(1)}), \ldots, (z_i^{(m)}, y_i^{(m)}) \) be \( m \) pair of independent samples of \( Z_i \) and \( Y_i \). The conditional maximum likelihood estimator, \( \hat{p}(Y_i|Z_i = 1) \), is obtained as follows:
\[
\hat{p}_j(Y_i|Z_i = 1) = \frac{1}{\sum_{k=1}^{m} z_i^{(k)}} \sum_{k=1}^{m} 1[y_i^{(k)} = j \land z_i^{(k)}], \quad j \in \text{Dom}[Y_i].
\]
Then, for fixed values of \( t, \delta \in (0, 1) \), and provided that \( m \geq \frac{4}{\alpha \delta^2} \ln \frac{4L}{\delta} \), we have
\[
P \left( \forall i \in \{1 \ldots L\} \mid \|\hat{p}(Y_i|Z_i = 1) - p(Y_i|Z_i = 1)\|_\infty \leq t \right) \geq 1 - \delta.
\]

**Proof.** First, we analyze a pair of variables \( Z_i, Y_i \). Let \( \mathcal{E}_1 = \{\frac{1}{m} \sum_{k=1}^{m} z_i^{(k)} \geq \alpha - \epsilon\} \). Next, using the one-sided Hoeffding’s inequality, we have
\[
P(\mathcal{E}_1) \geq 1 - e^{-2m \epsilon^2}.
\]
Now, let the event \( \mathcal{E}_2 = \{\|\hat{p}(Y_i|Z_i = 1) - p(Y_i|Z_i = 1)\|_\infty \leq t\} \). Using Lemma 3 (see Proof D.3), we obtain
\[
P(\mathcal{E}_2|\mathcal{E}_1) \geq 1 - 2e^{-m(\alpha - \epsilon)t^2 / 2}.
\]
Then, by the law of total probability, we have
\[ P(\mathcal{E}_2) \geq P(\mathcal{E}_2|\mathcal{E}_1)P(\mathcal{E}_1) \geq 1 - e^{-2\epsilon^2m} - 2e^{-m(\alpha - \epsilon)t^2/2}. \]
Let \( \frac{\epsilon}{2} = e^{-2\epsilon^2m} \), and \( \delta = 2e^{-m(\alpha - \epsilon)t^2/2} \). Then provided that \( m \geq \max(\frac{2}{\alpha \epsilon^2}, \frac{2}{\alpha - \epsilon} \ln \frac{4}{\delta}) \),
\[ P(\mathcal{E}_2) \geq 1 - \delta. \]

For \( \epsilon = \frac{2}{\alpha \epsilon^2} \), and \( t \in (0, 1) \), we can simplify the bound on \( m \) to be \( m \geq \frac{4}{\alpha^2} \ln \frac{4}{\delta} \). Finally, using union bound and provided that \( m \geq \frac{4}{\alpha^2} \ln \frac{4}{\delta} \), we have
\[ P \left( \forall i \in \{1 \ldots L\} \right) \| \hat{p}(Y_i|Z_i = 1) - p(Y_i|Z_i = 1) \|_\infty \leq t \right) \geq 1 - \delta. \]

Which concludes the proof. \( \square \)

Now follows the proof of Theorem 6.

**Proof of Theorem 6**
The proof follows the same steps as in the proof of Theorem 1 (Appendix D.3). The difference is that we now use the sample complexity given by Lemma 4 instead of Lemma 3. Therefore, for a query \( \tilde{Q}(i, j) \) we obtain a sample complexity of \( m \in O(\frac{1}{\alpha \epsilon^2} (\ln n + \ln \frac{4}{\delta})) \).

**D.8 Proof of Theorem 6**

**Proof.** Recall from the characterization of the BN that there exist a finite value \( z \) and upper bound \( \sigma_{ub}^2 \), such that \( \mu(B, z) \geq 1 \) and \( \sigma^2(B, z) \leq \sigma_{ub}^2 \). Let \( x_j^{(1)}, \ldots, x_j^{(m)} \) be \( m \) i.i.d. samples of \( X_j \) after trying to intervene \( X_i \) with value \( z \). Let \( \mu_j|do(X_i = z) \) and \( \sigma_j^2|do(X_i = z) \) be the mean and variance of \( X_j \) respectively, after perfectly intervening \( X_i \) with value \( z \). Also, let \( \hat{\mu} = \frac{1}{m} \sum_{k=1}^{m} x_j^{(k)} \) be the empirical expected value of \( X_j \).

Now, we analyze the two cases that we are interested to answer with high probability. First, let \( i \in \pi_G(j) \). Clearly, \( \hat{\mu} \) has expected value \( |E[\hat{\mu}]| = |E_{X_i}[\mu_j|do(X_i = z)]| \geq 1 \), and variance \( \hat{\sigma}^2 = E_{X_i}[\sigma_j^2|do(X_i = z)] \leq \frac{1}{m} \sigma_{ub}^2 / m \). Then, using Hoeffding’s inequality we have
\[ P \left( | \hat{\mu} - E[\hat{\mu}] | \geq t \right) \leq 2e^{-t^2/(2\hat{\sigma}^2)} \leq 2e^{-mt^2/(2\sigma_{ub}^2)} \quad (\text{7.2}) \]

Second, if there is no directed path from \( i \) to \( j \), then by using Lemma 1, we have \( E_{X_i}[\mu_j|do(X_i = z)] = E_{X_i}[\mu_j] = 0 \) and \( E_{X_i}[\sigma_j^2|do(X_i = z)] = E_{X_i}[\sigma_j^2] \leq \sigma_{ub}^2 \).

As we can observe from both cases described above, the true mean \( E_{X_i}[\mu_j|do(X_i = z)] \) when \( i \in \pi_G(j) \) is at least separated by 1 from the true mean when there is no directed path. Therefore, to estimate the mean, a suitable value for \( t \) in inequality (7.2) is \( t \leq \frac{1}{2} \). The latter allows us to state that if \( |\hat{\mu}| > \frac{1}{2} \) then \( \hat{Q}(i, j) = 1 \), and \( \hat{Q}(i, j) = 0 \) otherwise. Replacing \( t = \frac{1}{2} \) and restating inequality (7.2), we have that for a specific pair of nodes \( (i, j) \), if \( i \in \pi_G(j) \) or if \( j \notin desc_G(i) \) (\( desc_G(i) \) denotes the descendants of \( i \)), then
\[ P \left( Q_G(i, j) \neq \hat{Q}(i, j) \right) \leq 2e^{-m/(8\sigma_{ub}^2)} \]

The latter inequality is for a single query. Using the union bound we have
\[ P \left( \exists j = 1, \ldots, n \land (i \in \pi_G(j) \lor j \notin desc_G(i)) \right) \hat{Q}(i, j) \neq Q_G(i, j) \leq 2n^2e^{-m/(8\sigma_{ub}^2)}. \]

Now, let \( \delta = 8n^2e^{-m/(8\sigma_{ub}^2)} \), if \( m \geq 8\sigma_{ub}^2 \log \frac{2\sigma_{ub}^2}{\delta} \) then
\[ P \left( \forall j = 1, \ldots, n \land (i \in \pi_G(j) \lor j \notin desc_G(i)) \hat{Q}(i, j) = Q_G(i, j) \right) \geq 1 - \delta. \]

That is, with probability of at least \( 1 - \delta \), the path query \( \hat{Q}(i, j) \) (in Algorithm 3) is equal to \( Q_G(i, j) \) for all \( n^2 \) performed queries in which either \( i \in \pi_G(j) \), or there is no directed path from \( i \) to \( j \). Note also that the probability at least \( 1 - \delta \) is guaranteed after we remove the transitive edges in the network. Therefore, we obtain
\[ m \geq 8\sigma_{ub}^2 (2 \log n + \log \frac{2}{\delta}) \], i.e., \( m \in O(\sigma_{ub}^2 \log \frac{4}{\delta}) \). \( \square \)
As shown above, for these values of \( \nu \), which concludes our proof.

Recall from Remark 1 that we can write the model as: \( X = W X + N \), which is equivalent to \( X = (I - W)^{-1} N \).

Let \( B = (I - W)^{-1} \), then \( B_{ij} \) denotes the total weight effect of the noise \( N \) on the node \( j \). Furthermore, let \( \odot_i B = (I - \odot_i W)^{-1} \) and similarly \( \{ \odot_i B \}_{jk} \) denotes the total weight effect of the noise \( N_k \) on the node \( j \) after intervening the node \( i \).

Next, we analyze if \( z = 1/w_{min} \), and \( \sigma_{ub}^2 = \sigma_{max}^2 w_{max} \) fulfill the conditions given in Theorem 2. First, let \( i \in \pi_G(j) \), i.e., \((i, j) \in E \). Since \( w_{min} = \min_{(i, j) \in E} \{|\odot_i B\}_{ji}| \), we have \( |\mu_{j,do(X_i=z)}| = |\{\odot_i B\}_{ji}| \times |z| = |\{\odot_i B\}_{ji}|/w_{min} \).

Since \( w_{min} \leq |\{\odot_i B\}_{ji}| \) for any \((i, j) \in E \), we have that \( \mu(B, z) \geq 1 \). Let \( v_{j,do(X_i=z)}^2 \) be the variance of \( X_j \) after intervening \( X_i \), then we have that \( v_{j,do(X_i=z)}^2 = \sum_{p \in V \setminus \{j\}} (\{\odot_i B\}_{jp})^2 \sigma_{ji}^2 \). Similarly, the variance of \( j \) without any intervention is \( v_{j}^2 = \sum_{p \in V \setminus \{j\}} (\{\odot_i B\}_{jp})^2 \sigma_{ji}^2 \). Then \( \max_{(i, j) \in E} v_{j,do(X_i=z)}^2 \leq \max_{i \in V} v_{j}^2 \leq \sigma_{max}^2 \|B\|^2_{\infty,2}, \) which results in \( \sigma_{ub}^2 = \sigma_{max}^2 w_{max} \).

Second, let be the case that there is no directed path from \( i \) to \( j \). Then from Lemma 1, \( X_i \) and \( X_j \) are independent after intervening \( X_i \), i.e., \( \mu_{j,do(X_i=z)} = \mu_j = 0 \), and \( v_{j,do(X_i=z)}^2 = v_{j}^2 \leq \sigma_{ub}^2 \).

As shown above, for these values of \( z = 1/w_{min} \) and \( \sigma_{ub}^2 = \sigma_{max}^2 w_{max} \), we fulfill the conditions given in Theorem 2 which concludes our proof.

### D.10 Proof of Corollary 2

For a pair of nodes \( i, j \), Algorithm 6 sets \( S = \tilde{\pi}_G(j) \). If \( S \) is already the true parent set of \( j \), then \( X_i \) will only have effect on \( X_j \) if \( i \in S \). If \( S \) is a subset of the true parent set, then \( X_i \) will only have effect on \( X_j \) if there exists a transitive edge \((i, j)\). This is because by intervening \( S \) we are blocking any possible effect of \( X_i \) on \( X_j \) through any node in \( S \), and since non-transitive edges are already recovered then \((i, j)\) must be a transitive edge if there exists some effect. Thus, \( w_{min} = \min_{j \in S} |W_{ij}| \) is enough to ensure a mean of at least 1 for \( X_j \), since only \( X_i \) is intervened with value \( z_2 = 1/w_{min} \) while the other nodes in \( S \) are intervened with value \( z_1 = 0 \). Finally, because the value of \( w_{max} \) takes the maximum across all possible interventions of subsets of the parent set of \( j \), then \( \sigma_{ub}^2 \) is an upper bound and similar arguments as in Corollary 1 hold.

### D.11 Proof of Corollary 3

Proof. To prove the corollary we need to show that for \( z = 1/w_{min} \) and \( \sigma_{ub}^2 = \sigma_{max}^2 w_{max} \), the conditions \( \mu(B, z) \geq 1 \) and \( \sigma_{B, z}^2 \leq \sigma_{ub}^2 \) hold, similarly to Proof D.9

For the case when \( i \in \pi_G(j) \), now \( X_i \) (the intervened variable) is a sub-Gaussian variable with mean \( z \) and variance \( \nu_i^2 \), we clearly have that the same upper bound \( \sigma_{ub} = \sigma_{max}^2 w_{max} \) works since \( \nu_i^2 \leq \sigma_{max}^2 \). Likewise, the value \( z \) is properly set since the value of \( w_{min} \) is \( w_{min} = \min_{(i, j) \in E} |\{\odot_i B\}_{ji}| \).

For the case when there is no directed path from \( i \) to \( j \), we have that \( X_i \) and \( X_j \) are independent after intervening \( X_i \), i.e., \( E[X_j] = \mu_j = 0 \), and \( \text{Var}[X_j] = v_j^2 \leq \sigma_{ub}^2 \).

From these analyses we conclude that the ASGN model fulfills the conditions given in Theorem 6. Which concludes our proof.

### Appendix E Experiments

#### E.1 Experiments on synthetic CBNs

In this section, we validate our theoretical results on synthetic data for perfect and imperfect interventions by using Algorithms 1, 2, and 3. Our objective is to characterize the number of interventional samples per query needed by our algorithm for learning the transitive reduction of a CBN exactly.
Our experimental setup is as follows. We sample a random transitively reduced DAG structure $G$ over $n$ nodes. We then generate a CBN as follows: for a discrete CBN, the domain of a variable $X_i$ is $\text{Dom}[X_i] = \{1, \ldots, d\}$, where $d$ is the size of the domain, which is selected uniformly at random from $\{2, \ldots, 5\}$, i.e., $r = 5$ in terms of Theorem 1. Then, each row of a CPT is generated uniformly at random. Finally, we ensure that the generated CBN fulfills $\gamma \geq 0.01$. For a continuous CBN, we use Gaussian noises following the ASGN model as described in Definition 4, where each noise variable $N_i$ is Gaussian with mean 0 and variance selected uniformly at random from $[1, 5]$, i.e., $\sigma^2_{\text{max}} = 5$, in terms of Corollary 1. The edge weights $W_{ij}$ are selected uniformly at random from $[-1.25, -0.01] \cup [0.01, 1.25]$ for all $(i, j) \in E$. We ensure that $W$ fulfills $\| (I - W) \|_{2, \infty} \leq 20$. After generating a CBN, one can now intervene a variable, and sample accordingly to a given query. Finally, we set $\delta = 0.01$, and estimate the probability $P(G = \hat{G})$ by computing the fraction of times that the learned DAG structure $\hat{G}$ matched the true DAG structure $G$ exactly, across 40 randomly sampled BNs. We repeated this process for $n \in \{20, 40, 60\}$. The number of samples per query was set to $e^{C \log nr}$ for discrete BNs, and $e^{C \log n}$ for continuous BNs, where $C$ was the control parameter, chosen to be in $[0, 16]$. Figure 6 shows the results of the structure learning experiments. We can observe that there is a sharp phase transition from recovery failure to success in all cases, and that the $\log n$ scaling holds in practice, as prescribed by Theorems 1 and 2.

Similarly, for imperfect interventions we work under the same experimental settings described above. For a discrete BN, we additionally set $\alpha = 0.9$ in terms of Theorem 5. Whereas for a continuous BN, we set $\nu^2 = \sigma^2_i$ for all $i \in V$, in terms of 5. Figure 6 shows the results of the structure learning experiments. We can observe that the sharp phase transition from recovery failure to success and the $\log n$ scaling is also preserved, as prescribed by Theorems 5 and 6.

![Figure 6: (Left, Top) Probability of correct structure recovery of the transitive reduction of a discrete BN vs. number of samples per query, where the latter was set to $e^{C \log nr}$, with all BNs having $r = 5$ and $\gamma \geq 0.01$. (Right, Top) Similarly, for continuous BNs, the number of samples per query was set to $e^{C \log n}$, with all BNs having $\| (I - W) \|_{2, \infty} \leq 20$. (Left, Bottom) Results for imperfect interventions for discrete BNs under same settings as in perfect interventions and $\alpha = 0.9$. (Right, Bottom) Results for imperfect interventions for continuous BNs under same settings as in perfect interventions and $\nu^2 = \sigma^2_i$, $\forall i \in V$. Finally, we observe that there is a sharp phase transition from recovery failure to success in all cases, and the $\log n$ scaling holds in practice, as prescribed by Theorems 1, 2, 5, and 6.](image)

E.2 Most benchmark BNs have few transitive edges

In this section we compute some attributes of 21 benchmark networks, which are publicly available at [http://compbio.cs.huji.ac.il/Repository/networks.html](http://compbio.cs.huji.ac.il/Repository/networks.html) and [http://www.bnlearn.com/bnrepository/](http://www.bnlearn.com/bnrepository/). These benchmark BNs contain the DAG structure and the conditional probability tables. Several prior works also
used these BNs and evaluated DAG recovery by sampling data observationally by using the joint probability distribution [2, 29].

Table 1 reports the number of vertices, $|V|$, the number of edges, $|E|$, the number of transitive edges, $|RE|$, and the ratio, $|RE|/|E|$. Finally, the mean and median of the ratios is presented. A median of 0.48% indicates that more than half of these networks have a number of transitive edges less than 0.50% of the total number of edges. In other words, our methods provide guarantees for exact learning of at least 99.5% of the true structure for many of these benchmark networks.

Table 1: For each network we show the number of vertices, $|V|$, the number of edges, $|E|$, the number of transitive edges, $|RE|$, and the ratio, $|RE|/|E|$.

| Network   | $|V|$ | $|E|$ | $|RE|$ | $|RE|/|E|$ |
|-----------|------|------|-------|----------|
| Alarm     | 37   | 46   | 4     | 8.70%    |
| Andes     | 223  | 338  | 45    | 13.31%   |
| Asia      | 8    | 8    | 0     | 0.00%    |
| Barley    | 48   | 84   | 14    | 16.67%   |
| Cancer    | 5    | 4    | 0     | 0.00%    |
| Carpo     | 60   | 74   | 0     | 0.00%    |
| Child     | 20   | 25   | 1     | 4.00%    |
| Diabetes  | 413  | 602  | 48    | 7.97%    |
| Earthquake| 5    | 4    | 0     | 0.00%    |
| Hailfinder| 56   | 66   | 4     | 6.06%    |
| Hepar2    | 70   | 123  | 16    | 13.01%   |
| Insurance | 27   | 52   | 12    | 23.08%   |
| Link      | 724  | 1125 | 0     | 0.00%    |
| Mildew    | 35   | 46   | 6     | 13.04%   |
| Munin1    | 186  | 273  | 1     | 0.37%    |
| Munin2    | 1003 | 1244 | 6     | 0.48%    |
| Munin3    | 1041 | 1306 | 6     | 0.46%    |
| Munin4    | 1038 | 1388 | 6     | 0.43%    |
| Pigs      | 441  | 592  | 0     | 0.00%    |
| Water     | 32   | 66   | 0     | 0.00%    |
| Win95pts  | 76   | 112  | 8     | 7.14%    |
| Average   |      |      |       | 5.46%    |
| Median    |      |      |       | 0.48%    |

E.3 DAG recovery on benchmark BNs

In this section we test Algorithms 1, 2, 3, 4, 5, and 6 on benchmark networks that may contain transitive edges. The networks are publicly available at [http://www.bnlearn.com/bnrepository/](http://www.bnlearn.com/bnrepository/) These standard benchmark BNs contain the DAG structure and the conditional probability distributions. We sample data interventionally by using the manipulation theorem [20]. We then compare the learned DAG versus the true DAG. Several prior works used these BNs and also evaluated DAG recovery by sampling data observationally by using the joint probability distribution [2, 29].

**Discrete networks.** We first present experiments on discrete BNs. For each network we set the number of samples $m = e^{12 \log nr}$, and ran Algorithm 1 once. After learning the transitive reduction, we ran Algorithm 6 to learn the missing transitive edges. For the true edge set $E$ and recovered edge set $\hat{E}$, we define the edge precision as $|E \cap \hat{E}|/|E|$, and the edge recall as $|E \cap \hat{E}|/|E|$. The F1 score was computed from the previously defined precision and recall. As we can observe in Table 2 all of the networks achieved an edge precision of 1.0, which indicates that all the edges that our algorithm learned are indeed part of the true network. Finally, all networks also achieved an edge recall of 1.0, which indicates that all edges (including the transitive edges) were correctly recovered.
Table 2: Results on real-world discrete networks. For each network, we show the number of nodes, \( n \), the number of edges, \(|E|\), the number of transitive edges, \(|RE|\), the maximum domain size, \( r \), the edge precision, \(|\hat{E} \cap E|/|\hat{E}|\), the edge recall, \(|\hat{E} \cap E|/|E|\), and the F1 score.

| Network    | \( n \) | \(|E|\) | \(|RE|\) | \( r \) | Edge precision | Edge recall | F1 score |
|------------|---------|--------|---------|-------|----------------|-------------|---------|
| Carpo      | 60      | 74     | 0       | 4     | 1.00           | 1.00        | 1.00    |
| Child      | 20      | 25     | 1       | 6     | 1.00           | 1.00        | 1.00    |
| Hailfinder | 56      | 66     | 4       | 11    | 1.00           | 1.00        | 1.00    |
| Win95pts   | 76      | 112    | 8       | 2     | 1.00           | 1.00        | 1.00    |

Additive Gaussian networks. Next, we present experiments on continuous BNs. For each network we set the number of samples \( m = e^{C \log n} \), and ran Algorithm 1 once. For the true edge set \( E \) and recovered edge set \( \hat{E} \), we define the edge precision as \(|\hat{E} \cap E|/|\hat{E}|\), and the edge recall as \(|\hat{E} \cap E|/|E|\). The F1 score was computed from the previously defined precision and recall. As we can observe in Table 3 both networks achieved an edge precision of 1.0, which indicates that all the edges that our algorithm learned are indeed part of the true network. Finally, both networks also achieved an edge recall of 1.0, which indicates that all edges (including the transitive edges) were correctly recovered.

Table 3: Results on real-world continuous networks. For each network, we show the number of nodes, \( n \), the number of edges, \(|E|\), the number of transitive edges, \(|RE|\), the constant \( C \), the maximum domain size, \( r \), the edge precision, \(|\hat{E} \cap E|/|\hat{E}|\), the edge recall, \(|\hat{E} \cap E|/|E|\), and the F1 score.

| Network     | \( n \) | \(|E|\) | \(|RE|\) | \( C \) | Edge precision | Edge recall | F1 score |
|-------------|---------|--------|---------|-------|----------------|-------------|---------|
| Magic-Irri  | 64      | 102    | 25      | 11    | 1.00           | 1.00        | 1.00    |
| Magic-Niab  | 44      | 66     | 12      | 7     | 1.00           | 1.00        | 1.00    |

E.4 DAG recovery on real-world genetics data

In this section we show experimental results on real-world interventional data. We selected 15 genes from the interventional data in “Transcriptional regulatory code of a eukaryotic genome” [9]. A few observations from the learned BN are: the gene YBL054W reaches 9 genes directly and indirectly; the gene YLR278C is reached by 13 genes directly and indirectly; finally, YER130C is an isolated gene.

![Figure 7: DAG structure recovered from interventional data in [9].](image)