
Learning 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 structure of 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. Finally, we experimentally validate the correctness of our algorithm in synthetic and real-world networks.

1. Introduction

Bayesian networks (BNs) are a powerful representation of joint probability distributions. BNs are also used to describe causal relationships among variables (Koller & Friedman 2009). The structure of a *causal* BN 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 BN 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.¹ 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 (Hauser & Bühlmann 2012, He & Geng 2008, Murphy 2001). This data is produced after performing

¹Two 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 (Verma & Pearl 1991). (A v-structure consists of converging directed edges into the same node, such as $X \rightarrow Y \leftarrow Z$).

an ideal experiment (intervention) (Pearl 2000), in which one or several random variables are forced to take some specific values, irrespective of their causal parents.

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). Höffgen (1993) provides a score-maximizing algorithm that is likelihood consistent, but that needs super-exponential time. Spirtes et al. (2000), Cheng et al. (2002) 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). Chickering & Meek (2002) show that greedy hill-climbing is structure consistent in the infinite sample limit, with unbounded time. Zuk et al. (2006) show structure consistency of a single network and do not provide uniform consistency for all candidate networks (the authors discuss the issue of not using the union bound in their manuscript).

From the *active learning* literature, most of the works first find a Markov equivalence class from purely *observational* data and then direct the edges by using as few *interventions* as possible. Murphy (2001), Tong & Koller (2001) propose an exponential-time Bayesian approach relying on structural priors and MCMC. Hauser & Bühlmann (2012), He & Geng (2008), Shanmugam et al. (2015) present methods to find an optimal set of interventions in polynomial time for a restrictive class of chordal DAGs. Unfortunately, finding the initial Markov equivalence class remains NP-hard (Chickering 1996). Eaton & Murphy (2007) propose an exponential-time dynamic programming algorithm for learning DAG structures exactly. Triantafillou & Tsamardinos (2015) propose a constrain-based method to combine heterogeneous (observational and interventional) datasets but relies on solving instances of the (NP-hard) *boolean satisfiability problem*, as well as on the strong assumption that intervened nodes can only affect their children. The work of Eberhardt et al. (2005) analyzed the number of interventions sufficient and in the worst-case necessary to determine the structure of any DAG, although no algorithm or sample complexity analysis was provided. Literature on learning *structural equation models* from observational data, include the work on continuous (Peters et al. 2014) and discrete (Peters et al. 2010) additive noise models. Correctness was shown for the continuous case (Peters et al. 2014) but only in the infinite-sample limit.

Compared to the above literature, to the best of our knowledge, we are the first to propose a polynomial-time algorithm with logarithmic sample complexity for correctly learning the exact DAG structure of a causal BN, from purely interventional data. Our interest on interventional data stems from our goal of discovering the true causal relationships, and not just a compact representation of the joint distribution. We perform one intervention for each node, which agrees with the numbers of interventions sufficient and in the worst-case necessary to identify any DAG, as shown in Eberhardt et al. (2005).

Our contributions are as follows. We propose a polynomial time algorithm for learning BNs with provable guarantees of DAG structure recovery by using interventional path queries. For n nodes, the time complexity of our algorithm is dominated by fast matrix multiplication, $\mathcal{O}(n^{2.3729})$ (LeGall 2014). We analyze the sample complexity required for answering every path query. We show that for a BN of discrete random variables with maximum domain size r , the sample complexity is $\mathcal{O}(\log(nr))$; whereas for BNs of sub-Gaussian random variables, the sample complexity is $\mathcal{O}(\sigma_{ub}^2 \log n)$ where σ_{ub}^2 is an upper bound of the variable variances (marginally as well as after interventions.) Finally, we validate our theoretical results in synthetic and real-world

datasets.

Our manuscript is organized as follows. In Section 2, we provide some important notations and definitions, and a list of our main technical assumptions. In Section 3, we present our polynomial time algorithm for learning the exact structure of a BN, and discuss the sample complexity of the interventional data required per path query. Finally, in Section 4, we validate our theoretical results on synthetic and real-world structures. Concluding remarks are provided in Section 5.

2. Preliminaries

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

Let $G = (V, E)$ be *directed acyclic graph* (DAG) with vertex set $V = \{1, \dots, n\}$ 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 path of length k from node i to node j is a sequence of nodes $(i, v_1, v_2, \dots, v_{k-1}, j)$ such that $\{(i, v_1), (v_1, v_2), \dots, (v_{k-2}, v_{k-1}), (v_{k-1}, j)\}$ is a subset of the edge set E .

Let $\mathbf{X} = \{X_1, \dots, X_n\}$ 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 \mathbf{X} is a pair $\mathcal{B} = (G, \mathcal{P}_G)$ that represents a distribution over the joint space of \mathbf{X} . Here, G is a DAG, whose nodes correspond to the random variables in \mathbf{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) $P(X_i | \mathbf{X}_{\pi_G(i)})$. We use $\mathbf{X}_{\pi_G(i)}$ 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 \mathbf{X} , i.e., $P(X_1, \dots, X_n) = \prod_{i=1}^n P(X_i | \mathbf{X}_{\pi_G(i)})$.

Viewed as a probabilistic model, a BN can answer any “conditioning” query of the form $P(\mathbf{Z} | \mathbf{E} = \mathbf{e})$ where \mathbf{Z} and \mathbf{E} are sets of variables and \mathbf{e} is an assignment of values to \mathbf{E} . Nonetheless, a BN can also be viewed as a *causal model* (Pearl 2000). Under this perspective, the BN 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 (Spirtes et al. 2000, Pearl 2000) 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. We follow the standard notation (Pearl 2000) 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 $P(X_1, \dots, X_{i-1}, X_{i+1}, \dots, X_n | do(X_i = x_i)) = \mathbb{1}[X_i = x_i] \prod_{j \neq i} P(X_j | \mathbf{X}_{\pi_G(j)})$.

We refer as discrete BNs to BNs in which all random variables X_i have finite domain $\text{Dom}[X_i]$. 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 $\mathbf{p}(Y) \in [0, 1]^{|\text{Dom}[Y]|}$ indexed by the elements of $\text{Dom}[Y]$, i.e., $p_j(Y) = P(Y = j), \forall j \in \text{Dom}[Y]$. We refer to networks with variables that have continuous domains as continuous BNs.

The class of BNs that our methods can learn are DAGs without *redundant edges*. Next, we formally define redundant edges.

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

We then refer as non-redundant DAGs (NRDAGs) to DAGs that do not have redundant edges. Likewise, we refer as non-redundant Bayesian networks (NRBN) to BNs whose graph structure are NRDAGs. The algorithm for removing redundant edges from a DAG is called *transitive reduction* and it was introduced by Aho, Garey & Ullman (1972). 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 $Q_G : V \times V \rightarrow \{0, 1\}$ such that $Q_G(i, j) = 1$ if there exists a path in G from i to j , and $Q_G(i, j) = 0$ otherwise.

We will use $Q(i, j)$ to denote $Q_G(i, j)$ since for our problem, the DAG G is fixed (but unknown). Furthermore, some DAGs are also non-identifiable by using path queries. For instance, consider the two graphs shown in Figure 1. In both cases, we have that $Q(1, 2) = Q(1, 3) = Q(3, 2) = 1$. Thus, by using path queries, it is impossible to discern whether the edge $(1, 2)$ exists or not. Hence our motivation to analyze NRBNs.



Figure 1: 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. In fact, since we answer path queries by using a finite number of samples, then it is a rather hopeless attempt to answer them almost surely. Therefore, we make use of noisy queries as defined below.

Definition 3 (Noisy path query). Let $G = (V, E)$ be a DAG, and let Q_G be a path query. A noisy path query is a function $\tilde{Q}_G : V \times V \rightarrow \{0, 1\}$ such that $\tilde{Q}_G(i, j) = Q_G(i, j)$ with high probability if $i \in \pi_G(j)$ or if there is no path from i to j .

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 path between both variables. We do not require correctness when there is a path of length greater than 1 between both variables. Additionally, note that the uncertainty of the exact recovery of a BN relies on answering multiple noisy path queries.

2.1. Assumptions

Before diving into our technical contributions. We state our main assumptions for clarity.

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

Assumption 2 (Causal Markov). The data is generated from an underlying NRBN (G, \mathcal{P}_G) over \mathbf{X} .

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

Assumption 1 has been widely used in the active learning literature (Murphy 2001, Tong & Koller 2001, He & Geng 2008, Hauser & Bühlmann 2012, Shanmugam et al. 2015). By assuming that a causal graph is *causally Markov*, 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, we ensure that the population has exactly these and no additional independencies (Spirtes et al. 2000, Tong & Koller 2001, Shanmugam et al. 2015, He & Geng 2008, Triantafillou & Tsamardinos 2015). In the literature, other stronger assumptions include a locality condition, denoting that the intervention of each manipulated variable should not directly affect any variable other than its children (Triantafillou & Tsamardinos 2015). In this paper, we *do not* assume locality.

3. Algorithms and sample complexity

In this section we present our results and provide a formal analysis on the sample complexity of queries, as well as, the characterization of the class of NRBNs that our methods can learn.

3.1. Algorithm for learning NRBNs

We now present a simple algorithm for learning the structure of NRBNs exactly. Algorithm 1 performs $\mathcal{O}(n^2)$ path queries for all possible node pairs, and then calls the *transitive reduction* algorithm. As proved by Aho, Garey & Ullman (1972), 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 LeGall (2014), which has $\mathcal{O}(n^{2.3729})$ time complexity. As a result, the time complexity of Algorithm 1 is dominated by the computation of the transitive reduction. 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 done in Eberhardt et al. (2005).

Algorithm 1 Learning a NRBN from interventions

Input: Vertex set V

Output: Edge set \hat{E}

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1:  $\hat{E} \leftarrow \emptyset$ 
2: for  $i = 1 \dots n$  do
3:   for  $j = 1 \dots n$  do
4:     if  $i \neq j$  and  $\tilde{Q}(i, j) = 1$  then
5:        $\hat{E} \leftarrow \hat{E} \cup \{(i, j)\}$ 
6:     end if
7:   end for
8: end for
9:  $\hat{E} \leftarrow \text{TransitiveReduction}(\hat{E})$ 
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While Algorithm 1 may seem a rather trivial algorithm, we briefly present some negative results which show that $\Omega(n^2)$ path queries are necessary for reconstructing a general DAG. (Please see Appendix A for detailed proofs.)

Theorem 1. *In order to reconstruct a sparse disconnected directed acyclic graph of n nodes, any deterministic algorithm requires at least $\Omega(n^2)$ time.*

Theorem 2. *In order to reconstruct a sparse connected directed acyclic graph of n nodes, any deterministic algorithm requires at least $\Omega(n^2)$ time.*

Assuming that we have correct answers for all path queries, Algorithm 1 will indeed recover any NR DAG exactly. However, this is not necessary. We can recover the true structure of a NR DAG if we have correct answers for queries $Q_G(i, j)$ when $i \in \pi_G(j)$, and when there is no path from i to j , and arbitrary answers when there is a path from i to j . This is because the *transitive reduction* step will remove any path of length greater than 1 between true parent and children (with respect to the true NR DAG). It is the previous observation that motivated our characterization of noisy queries given in Definition 3. In what follows, we focus on analyzing noisy queries in the context of causal BNs and interventions. We also analyze the conditions under which we can recover the true structure of a NRBN with high probability.

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

Lemma 1. *Let $\mathcal{B} = (G, \mathcal{P}_G)$ be a Bayesian network with $X_i, X_j \in \mathbf{X}$ being any two random variables in the network. If there is no path from i to j in G , then X_i and X_j are independent random variables after performing an intervention on X_i , i.e., $P(X_j | do(X_i = x_i)) = P(X_j)$.*

As described later in our results, Lemma 1 is a key property that will help us to determine the answer for a path query. Next, we show an important lemma.

Lemma 2. *Let X_i and X_j be two random variables, such that $i \in \pi_G(j)$. Then, the following propositions hold:*

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

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 BNs. Alternatively, we can use the expected value of X_j , since $E[X_j] \neq E[X_j | do(X_i = x_i)]$ implies that $P(X_j) \neq P(X_j | do(X_i = x_i))$ (Claim 1).

3.2. Noisy path query algorithm

Next, we propose a polynomial time algorithm for answering a particular path query. Algorithm 2 presents our algorithm for answering a noisy path query $\tilde{Q}(i, j)$ motivated by Theorems 3 and 4. For discrete NRBNs, we first create a list \mathcal{L} of size $d = |Dom[X_i]|$, containing the empirical PMFs of X_j after intervening X_i with all the possible values from its domain $Dom[X_i]$. Next, if the ℓ_∞ -norm of the difference of any pair of PMFs in \mathcal{L} is greater than a constant γ , then we answer the query with 1, and 0 otherwise. For continuous NRBNs, 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.

3.3. Discrete Random Variables

To answer a path query in a discrete NRBN, our algorithm compares two empirical probability mass functions (PMFs), therefore, we need a good estimation of these PMFs. In this paper we use conditional probability tables (CPTs) as the representation of the CPDs. The following lemma shows the sample complexity required to estimate several PMFs simultaneously by using maximum likelihood estimation.

Algorithm 2 Query algorithm

(a) <i>Discrete variables</i>	(b) <i>Continuous variables</i>
Input: Nodes i and j , number of samples m , and constant γ Output: $\tilde{Q}(i, j)$ 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 $x_j^{(1)}, \dots, x_j^{(m)}$ of X_j 4: $\hat{p}_k = \sum_{l=1}^m \mathbb{1}[x_j^{(l)} = k] \quad \forall k \in \text{Dom}[X_j]$ 5: Add $\hat{\mathbf{p}}$ to the list \mathcal{L} 6: end for 7: $\tilde{Q}(i, j) \leftarrow \mathbb{1}[(\exists \hat{\mathbf{p}}, \hat{\mathbf{q}} \in \mathcal{L}) \ \hat{\mathbf{p}} - \hat{\mathbf{q}}\ _\infty > \gamma]$	Input: Nodes i and j , number of samples m , and constant z Output: $\tilde{Q}(i, j)$ 1: Intervene X_i by setting its value to z , and obtain m samples $x_j^{(1)}, \dots, x_j^{(m)}$ of X_j 2: $\hat{\mu} \leftarrow \frac{1}{m} \sum_{k=1}^m x_j^{(k)}$ 3: $\tilde{Q}(i, j) \leftarrow \mathbb{1}[\hat{\mu} > 1/2]$

Lemma 3. Let Y_1, \dots, 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 $y_i^{(1)}, \dots, y_i^{(m)}$ be m independent samples of Y_i . The maximum likelihood estimator, $\hat{\mathbf{p}}(Y_i)$, is obtained as follows:

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

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

$$P \left(\|\hat{\mathbf{p}}(Y_1) - \mathbf{p}(Y_1)\|_\infty \leq t \wedge \dots \wedge \|\hat{\mathbf{p}}(Y_L) - \mathbf{p}(Y_L)\|_\infty \leq t \right) \geq 1 - \delta$$

Lemma 3 states that simultaneously for all L PMFs, the maximum likelihood estimator $\hat{\mathbf{p}}(Y_i)$ is at most t -away of $\mathbf{p}(Y_i)$ in ℓ_∞ -norm with probability at least $1 - \delta$. Next, we present a theorem that formally characterizes the class of discrete NRBNS that our algorithm can learn, and provides the sample complexity for each noisy path query.

Theorem 3. Let $\mathcal{B} = (G, \mathcal{P}_G)$ be a discrete NRBNS, such that each variable X_j has a finite domain $\text{Dom}[X_j]$, with $|\text{Dom}[X_j]| \leq r$. Furthermore, let

$$\gamma = \min_{\substack{j \in V \\ i \in \pi_G(j)}} \min_{\substack{x_i, x'_i \in \text{Dom}[X_i] \\ \mathbf{p}(X_j | \text{do}(X_i = x_i)) \neq \mathbf{p}(X_j | \text{do}(X_i = x'_i))}} \left\| \mathbf{p}(X_j | \text{do}(X_i = x_i)) - \mathbf{p}(X_j | \text{do}(X_i = x'_i)) \right\|_\infty.$$

If $\gamma > 0$, then for a fixed probability of error $\delta \in (0, 1)$, we can learn the exact structure of the NRBNS by using Algorithm 1 and $\mathcal{O}(\frac{r}{\gamma^2} (\ln n + \ln \frac{r}{\delta}))$ interventional samples per path query in Algorithm 2 (a).

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

3.4. Continuous Random Variables

For continuous NRBNs, our algorithm compares two empirical expected values for answering a path query. This is related to Claim 1 in Lemma 2, since $E[X_j] \neq E[X_j | do(X_i = x_i)]$ implies $P(X_j) \neq P(X_j | X_i = x_i)$. Next, we present a theorem that formally characterizes the class of continuous NRBNs that our algorithm can learn, and provides the sample complexity for each noisy path query for *sub-Gaussian* distributions. The class of sub-Gaussian variates 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 the sample complexity using sub-Gaussian variables have been studied in the past for other models, such as Markov random fields (Ravikumar et al. 2011).

Theorem 4. *Let $\mathcal{B} = (G, \mathcal{P}_G)$ be a continuous NRBN such that each variable X_j is a sub-Gaussian random variable with full support on \mathbb{R} , with mean $\mu_j = 0$ and variance σ_j^2 . Let $\mu_{j|do(X_i=z)}$ and $\sigma_{j|do(X_i=z)}^2$ denote the expected value and variance of X_j after intervening X_i with a value z . Furthermore, let*

$$\mu(\mathcal{B}, z) = \min_{\substack{j \in V \\ i \in \pi_G(j)}} |\mu_{j|do(X_i=z)}|, \quad \sigma^2(\mathcal{B}, z) = \max \left(\max_{\substack{j \in V \\ i \in \pi_G(j)}} \sigma_{j|do(X_i=z)}^2, \max_{j \in V} \sigma_j^2 \right).$$

If there exist an upper bound σ_{ub}^2 and a finite value z such that $\sigma^2(\mathcal{B}, z) \leq \sigma_{ub}^2$ and $\mu(\mathcal{B}, z) \geq 1$, then for a fixed probability of error $\delta \in (0, 1)$, we can learn the exact structure of the NRBN by using Algorithm 1 and $\mathcal{O}(\sigma_{ub}^2 \log \frac{n}{\delta})$ interventional samples per path query in Algorithm 2 (b).

It is worth noting that there is nothing special about the conditions $\mu_j = 0, \forall j \in V$, and $\mu(\mathcal{B}, z) \geq 1$, other than it offers clarity in the derivations. One could for instance set an upper bound for the magnitude of μ_j , and have $\mu(\mathcal{B}, z)$ be greater than some other constant besides 1. This will clearly affect the sample complexity results since it will depend in such bounds, nevertheless, the proof follows a similar approach. 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.

We now present a specific model, as a corollary, that fulfills the conditions presented in Theorem 4. Next, we define the additive sub-Gaussian noise model (ASGN).

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

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

with N_i being an independent sub-Gaussian “noise” variable with full support on \mathbb{R} , with zero mean and variance σ_i^2 for all $i \in V$, and $W_{i,j} \neq 0$ if and only if $(i, j) \in E$.

Corollary 4.1 (Additive sub-Gaussian noise model). *Let $\mathcal{B} = (G, \mathcal{P}(\mathbf{W}, \mathcal{S}))$ be a ASGN network as in Definition 4, such that $\sigma_j^2 \leq \sigma_{max}^2, \forall j \in V$. Also, let $w_{min} = \min_{(i,j) \in E} |W_{i,j}|$. If $z = 1/w_{min}$, and $\sigma_{ub}^2 = \sigma_{max}^2 \|(\mathbf{I} - \mathbf{W})^{-1}\|_{2,\infty}^2$, then for a fixed probability of error $\delta \in (0, 1)$, we can learn the exact structure of the NRBN by using Algorithm 1 and $\mathcal{O}(\sigma_{ub}^2 \log \frac{n}{\delta})$ interventional samples per path query in Algorithm 2 (b).*

In practice, the values of w_{min} and σ_{ub}^2 are unknown. Fortunately, knowing a lower bound of w_{min} and an upper bound of σ_{ub}^2 suffices for structure recovery.

4. Experiments

In this section, we validate our theoretical results on synthetic and real-world data. In the first set of experiments, our objective is to characterize the number of samples per query needed by our algorithm for learning the NR DAG structure of a NRB N exactly. Our experimental setup is as follows. We sample a random DAG structure G over n nodes and calculate its transitive reduction, i.e., G is a NR DAG. We then generate a NRB N as follows: for a discrete NRB N, the domain of a variable X_i is $Dom[X_i] = \{1, \dots, d\}$, where d is the size of the domain, which is selected uniformly at random from $\{2, \dots, 5\}$, i.e., $r = 5$ in terms of Theorem 3. Then, each row of a CPT is generated uniformly at random. Finally, We ensure that the generated NRB N fulfills $\gamma \geq 0.01$. For a continuous NRB N, 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., $\sigma_{max}^2 = 5$, in terms of Corollary 4.1. 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 \mathbf{W} fulfills $\|(\mathbf{I} - \mathbf{W})^{-1}\|_{2,\infty}^2 \leq 20$. After generating a NRB N, 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 NR DAG structure \hat{G} matched the true NR DAG structure G exactly, across 40 randomly sampled NRB Ns. 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 NRB Ns, and $e^C \log n$ for continuous NRB Ns, where C was the control parameter, chosen to be in $[0, 16]$. Figure 2 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 3 and 4.

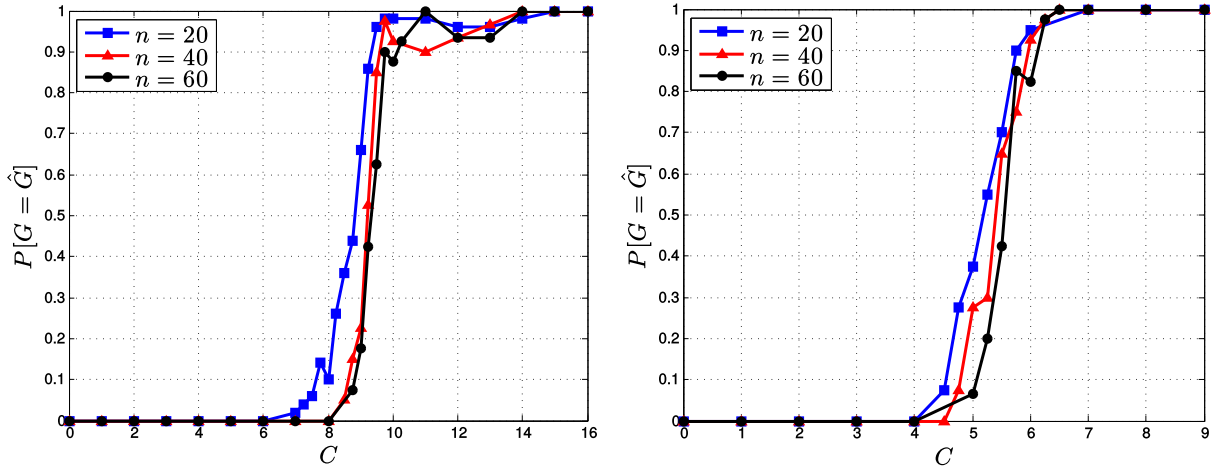


Figure 2: (Left) Probability of correct structure recovery of a discrete NRB N vs. number of samples per query, where the latter is set to $e^C \log nr$, with all NRB Ns having $r = 5$ and $\gamma \geq 0.01$. (Right) Similarly, for continuous NRB Ns, the number of samples per query were set to $e^C \log n$, with all NRB Ns having $\|(\mathbf{I} - \mathbf{W})^{-1}\|_{2,\infty}^2 \leq 20$. 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 3 and 4.

Finally, we test our algorithm on real-world networks that may contain redundant edges, thus violating our assumption. We use some widely known datasets publicly available at <http://compbio.cs.huji.ac.il/Repository/networks.html>. For each network we set the

number of samples $m = e^{12} \log nr$, 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, almost all of the networks achieved edge precision of 1.0, which indicates that the edges that our algorithm learned are indeed part of the true DAG. The Hailfinder network did not achieve an edge precision of 1.0 due to one edge being incorrect. Finally, the edge recall in Carpo is 1.0 because the network does not have any redundant edge, while Child, Hailfinder, and Win95pts have redundant edges. In these datasets, the loss in edge recall is fully explained by the inability of our method to recover redundant edges.

Table 1: Results on real-world datasets. For each network, we show the number of nodes (n) and edges ($|E|$), number of redundant edges, maximum domain size (r), edge precision, edge recall and F1 score.

Network	n	$ E $	Number of redundant edges	r	Edge precision	Edge recall	F1 score
Carpo	60	74	0	4	1.000	1.000	1.000
Child	20	25	1	6	1.000	0.960	0.979
Hailfinder	56	66	4	11	0.984	0.939	0.961
Win95pts	76	112	8	2	1.000	0.928	0.963

5. Concluding remarks

There are several ways of extending this work. For instance, it would be interesting to relax the assumption of perfect interventions, as in the work of Eaton & Murphy (2007) which also deals with imperfect and uncertain interventions. For continuous BNs, 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 (Liu et al. 2012) could be beneficial.

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Appendix A Detailed Proofs

We now present the proofs of Lemmas, Theorems and Corollaries respectively.

Proof of Lemma 1. The proof follows a d-separation argument. Let $\bar{\mathcal{B}}$ be the network after we perform an intervention on X_i with value x_i , i.e., $\bar{\mathcal{B}}$ has the edge set $E \setminus \{(p_i, i) \mid p_i \in \pi_G(i)\}$. Let $anc_G(i)$ and $anc_G(j)$ be the ancestor set of i and j respectively. Now, if there is no path from i to j in \mathcal{B} then there is no path in $\bar{\mathcal{B}}$ either, therefore, $i \notin anc_G(j)$. Also, $anc_G(i) = \emptyset$ 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 $\bar{\mathcal{B}}$. Since $anc_G(i) = \emptyset$, 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., $P(X_j) = P(X_j|X_i)$ in $\bar{\mathcal{B}}$. Finally, since $P(X_j|\mathbf{X}_{\pi_G(j)})$ 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 \mathcal{B} remains unchanged in $\bar{\mathcal{B}}$, i.e., $P(X_j|do(X_i = x_i)) = P(X_j)$. ■

Proof of Lemma 2. Both claims follow a proof by contradiction. For Claim 1, if for all $x_i \in Dom[X_i]$ we have that $P(X_j) = P(X_j|do(X_i = x_i))$ 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 $x_i, x'_i \in Dom[X_i]$ we have that $P(X_j|do(X_i = x_i)) = P(X_j|do(X_i = x'_i))$ 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 $i \in \pi_G(j)$. ■

Proof of Lemma 3. We use the Dvoretzky-Kiefer-Wolfowitz inequality (Massart 1990, Dvoretzky, Kiefer & Wolfowitz 1956):

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

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

$$\begin{aligned} |\hat{p}_j(Y_i) - p_j(Y_i)| &= \left| (\hat{F}_j(Y_i) - \hat{F}_{j-1}(Y_i)) - (F_j(Y_i) - F_{j-1}(Y_i)) \right| \\ &\leq \left| \hat{F}_j(Y_i) - F_j(Y_i) \right| + \left| \hat{F}_{j-1}(Y_i) - F_{j-1}(Y_i) \right| \end{aligned}$$

therefore, for a specific i , we have

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

Then by the union bound, we have:

$$P\left(\|\hat{\mathbf{p}}(Y_1) - \mathbf{p}(Y_1)\|_\infty > t \vee \dots \vee \|\hat{\mathbf{p}}(Y_L) - \mathbf{p}(Y_L)\|_\infty > t\right) \leq 2Le^{-mt^2/2}, \quad t > 0.$$

Let $\delta = 2Le^{-mt^2/2}$, then for $m \geq \frac{2L}{t^2} \ln \frac{2L}{\delta}$, we have:

$$P\left(\|\hat{\mathbf{p}}(Y_1) - \mathbf{p}(Y_1)\|_\infty \leq t \wedge \dots \wedge \|\hat{\mathbf{p}}(Y_L) - \mathbf{p}(Y_L)\|_\infty \leq t\right) \geq 1 - \delta, \quad \delta \in (0, 1), \quad t > 0.$$

Which concludes our proof. ■

Proof of Theorem 1. 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. ■

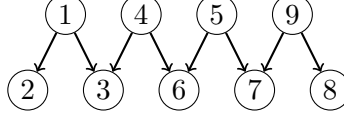


Figure 3: A “v-structured two-layered” directed acyclic graph.

Proof of Theorem 2. 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 3. 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.) ■

Proof of Theorem 3. We analyze a path query $\tilde{Q}(i, j)$ 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 path from i to j . To detect the latter, we opt to use Claim 2 from Lemma 2.

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

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

That is, with probability at least $1 - \delta$, simultaneously for all i, j, k , the estimators $\hat{\mathbf{p}}_{ij}^{(k)}$ are at most $\tau/4$ -away from the true distributions $\mathbf{p}_{ij}^{(k)}$ in ℓ_{∞} norm, provided that $m \geq \frac{32}{\tau^2} \left(2 \ln n + \ln \frac{2r}{\delta}\right)$ 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 $\mathbf{p}_{ij}^{(u)}, \mathbf{p}_{ij}^{(v)}$ where $x_u, x_v \in \text{Dom}[X_i]$, either $\mathbf{p}_{ij}^{(u)} = \mathbf{p}_{ij}^{(v)}$ or $\|\mathbf{p}_{ij}^{(u)} - \mathbf{p}_{ij}^{(v)}\|_{\infty} > \tau$ (recall the definition of γ and τ). Next, for a specific i, j , we show how to test if two distributions $\mathbf{p}_{ij}^{(u)}, \mathbf{p}_{ij}^{(v)}$ are equal or not. Let us assume $\mathbf{p}_{ij}^{(u)} = \mathbf{p}_{ij}^{(v)}$, then

we have

$$\begin{aligned}\left\|\hat{\mathbf{p}}_{ij}^{(u)} - \hat{\mathbf{p}}_{ij}^{(v)}\right\|_{\infty} &= \left\|\hat{\mathbf{p}}_{ij}^{(u)} - \mathbf{p}_{ij}^{(u)} - \left(\hat{\mathbf{p}}_{ij}^{(v)} - \mathbf{p}_{ij}^{(v)}\right)\right\|_{\infty} \\ &\leq \left\|\hat{\mathbf{p}}_{ij}^{(u)} - \mathbf{p}_{ij}^{(u)}\right\|_{\infty} + \left\|\hat{\mathbf{p}}_{ij}^{(v)} - \mathbf{p}_{ij}^{(v)}\right\|_{\infty} \\ &\leq \tau/2.\end{aligned}$$

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

$$\begin{aligned}\left\|\mathbf{p}_{ij}^{(u)} - \mathbf{p}_{ij}^{(v)}\right\|_{\infty} &= \left\|\mathbf{p}_{ij}^{(u)} - \hat{\mathbf{p}}_{ij}^{(u)} - \left(\mathbf{p}_{ij}^{(v)} - \hat{\mathbf{p}}_{ij}^{(v)}\right) + \hat{\mathbf{p}}_{ij}^{(u)} - \hat{\mathbf{p}}_{ij}^{(v)}\right\|_{\infty} \\ &\leq \left\|\hat{\mathbf{p}}_{ij}^{(u)} - \mathbf{p}_{ij}^{(u)}\right\|_{\infty} + \left\|\hat{\mathbf{p}}_{ij}^{(v)} - \mathbf{p}_{ij}^{(v)}\right\|_{\infty} + \left\|\hat{\mathbf{p}}_{ij}^{(u)} - \hat{\mathbf{p}}_{ij}^{(v)}\right\|_{\infty} \\ &\leq \tau.\end{aligned}$$

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

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

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

$$P\left((\forall j = 1, \dots, n \wedge (i \in \pi_G(j) \vee j \notin \text{desc}_G(i))) \tilde{Q}(i, j) = Q_G(i, j)\right) \geq 1 - \delta,$$

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

Proof of Theorem 4. 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 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 NRBN that there exist a finite value z and upper bound σ_{ub}^2 , such that $\mu(\mathcal{B}, z) \geq 1$ and $\sigma^2(\mathcal{B}, z) \leq \sigma_{ub}^2$. Let $x_j^{(1)}, \dots, x_j^{(m)}$ be m i.i.d. samples 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, $\hat{\mu}_{j|\text{do}(X_i=z)}$ has expected value $|\mathbb{E}[\hat{\mu}_{j|\text{do}(X_i=z)}]| = |\mu_{j|\text{do}(X_i=x_i)}| \geq 1$, and variance $\hat{\sigma}_{j|\text{do}(X_i=z)}^2 = \sigma_{j|\text{do}(X_i=z)}^2/m \leq \sigma_{ub}^2/m$. Then, by using Hoeffding's inequality we have

$$\begin{aligned}P\left(\left|\hat{\mu}_{j|\text{do}(X_i=z)} - \mu_{j|\text{do}(X_i=z)}\right| \geq t\right) &\leq 2e^{-t^2/(2\hat{\sigma}_{j|\text{do}(X_i=z)}^2)} \\ &\leq 2e^{-mt^2/(2\sigma_{ub}^2)}.\end{aligned}\tag{4.1}$$

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

As we can observe from both cases described above, the true mean $\mu_{j|do(X_i=z)}$ when $i \in \pi_G(j)$ is at least separated by 1 from the true mean when there is no path. Therefore, to estimate the mean, a suitable value for t in inequality (4.1) is $t \leq 1/2$. The latter allows us to state that if $|\hat{\mu}_{j|do(X_i=z)}| > 1/2$ then $\tilde{Q}(i, j) = 1$, and $\tilde{Q}(i, j) = 0$ otherwise. Replacing $t = 1/2$ and restating inequality 4.1, 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

$$P\left(Q_G(i, j) \neq \tilde{Q}(i, j)\right) \leq 2e^{-m/(8\sigma_{ub}^2)}.$$

The latter inequality is for a single query. Using the union bound we have

$$P\left((\exists j = 1, \dots, n \wedge (i \in \pi_G(j) \vee j \notin desc_G(i))) \tilde{Q}(i, j) \neq Q_G(i, j)\right) \leq 2n^2 e^{-m/(8\sigma_{ub}^2)}.$$

Now, let $\delta = 2n^2 e^{-m/(8\sigma_{ub}^2)}$, if $m \geq 8\sigma_{ub}^2 \log \frac{2n^2}{\delta}$ then

$$P\left((\forall j = 1, \dots, n \wedge (i \in \pi_G(j) \vee j \notin desc_G(i))) \tilde{Q}(i, j) = Q_G(i, j)\right) \geq 1 - \delta.$$

That is, with probability of at least $1 - \delta$, the path query $\tilde{Q}(i, j)$ (in Algorithm 2) 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 path from i to j . Note also that the probability at least $1 - \delta$ is guaranteed after we remove the redundant edges in the network. Therefore, we obtain $m \geq 8\sigma_{ub}^2(2 \log n + \log \frac{2}{\delta})$, i.e., $m \in \mathcal{O}(\sigma_{ub}^2 \log \frac{n}{\delta})$. ■

Proof of Corollary 4.1. Let us first analyze the expected value μ_j of each variable X_j in the network before performing any intervention. From the definition of the model we have that the expected value of X_j is $\mu_j = \sum_{p \in \pi_G(j)} W_{pj} \mu_p$, and from the topological ordering of the NRBN we can observe that the variables without parents have zero mean since these are only affected by a sub-Gaussian noise with zero mean. Therefore, following this ordering we have that the mean of every variable X_j is $\mu_j = 0$.

Next, we analyze if $z = 1/w_{min}$, and $\sigma_{ub}^2 = \sigma_{max}^2 \|(\mathbf{I} - \mathbf{W})^{-1}\|_{2,\infty}^2$ fulfill the conditions given in Theorem 4. First, let $i \in \pi_G(j)$, i.e., $(i, j) \in E$. Then by contradiction there cannot be another path from i to j , else the network would not be a NRBN. This means that when we intervene X_i with value z , it will only affect X_j through (i, j) . Therefore, $|\mu_{j|do(X_i=z)}| = |w_{ij}| \times |z| = |w_{ij}|/w_{min}$. Since $w_{min} \leq |w_{ij}|$ for any i and j , we have that $\mu(\mathcal{B}, z) \geq 1$. Let $v_{j|do(X_i=z)}$ be the variance of X_j after intervening X_i , then we have that

$$v_{j|do(X_i=z)}^2 = \left(\sum_{p \in \pi_G(j) \setminus i} |W_{pj}| v_p \right)^2 + \sigma_j^2 \leq v_j^2,$$

as a result, $\sigma^2(\mathcal{B}, z) = \max_{j \in V} v_j^2$. Then, it remains to find an upper bound σ_{ub}^2 for $\max_{j \in V} v_j^2$ so that we satisfy the condition $\sigma^2(\mathcal{B}, z) \leq \sigma_{ub}^2$. Without loss of generality we assume that the variables in the NRBN are topologically ordered. This implies that \mathbf{W} is an upper triangular matrix with diagonal zero. Also, notice that $W_{ij}^k \in \mathbf{W}^k$ is the sum of the products of weights in a path, across all different paths of length k from i to j , this means that we can express the variance of X_j as follows,

$$v_j^2 = \sum_{i \in V} \sigma_i^2 \left(\sum_{k=1}^{\infty} W_{ij}^k \right)^2 + \sigma_j^2.$$

The term $\sum_{k=1}^{\infty} W_{ij}^k$ can be interpreted as the total *effect* of X_i over X_j . Moreover, $\sum_{k=0}^{\infty} W_{ij}^k$ is the i, j entry of the series $\sum_{k=0}^{\infty} \mathbf{W}^k$, which has a close form equal to $(\mathbf{I} - \mathbf{W})^{-1}$ since \mathbf{W} has all its eigenvalues equal to 0. Now, we think of the worst possible scenario to upper bound v_j^2 , that is, setting all noise variances equal to σ_{max}^2 , and finding the maximum value for $\sum_{i \in V} (\sum_{k=1}^{\infty} W_{ij}^k)^2$ among all different j 's which is given by $\|(\mathbf{I} - \mathbf{W})^{-1}\|_{2,\infty}^2$, i.e., $\sigma_{ub}^2 = \sigma_{max}^2 \|(\mathbf{I} - \mathbf{W})^{-1}\|_{2,\infty}^2$.

Second, let be the case that there is no 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 $\sigma_{ub}^2 = \sigma_{max}^2 \|(\mathbf{I} - \mathbf{W})^{-1}\|_{2,\infty}^2$, we fulfill the conditions given in Theorem 4, therefore, we can learn the structure of this class of networks by using Algorithm 1 and $\mathcal{O}(\sigma_{ub}^2 \log \frac{n}{\delta})$ interventional samples per path query in Algorithm 2 (b). ■