Learning Sparse Fixed-Structure Gaussian Bayesian Networks

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Abstract

Gaussian Bayesian networks (a.k.a. linear Gaussian structural equation models) are widely used to model causal interactions among continuous variables. In this work, we study the problem of learning a fixed-structure Gaussian Bayesian network up to a bounded error in total variation distance. We analyze the commonly used node-wise least squares regression \texttt{LeastSquares} and prove that it has the near-optimal sample complexity. We also study a couple of new algorithms for the problem:

- \texttt{BatchAvgLeastSquares} takes the average of several batches of least squares solutions at each node, so that one can interpolate between the batch size and the number of batches. We show that \texttt{BatchAvgLeastSquares} also has near-optimal sample complexity.
- \texttt{CauchyEst} takes the median of solutions to several batches of linear systems at each node. We show that the algorithm specialized to polytrees, \texttt{CauchyEstTree}, has near-optimal sample complexity.

Experimentally\(^1\), we show that for uncontaminated, realizable data, the \texttt{LeastSquares} algorithm performs best, but in the presence of contamination or DAG misspecification, \texttt{CauchyEst/CauchyEstTree} and \texttt{BatchAvgLeastSquares} respectively perform better.

1 Introduction

Linear structural equation models (SEMs) are widely used to model interactions among multiple variables, and they have found applications in diverse areas, including economics, genetics, sociology, psychology and education; see \cite{Mue99, Mul09} for pointers to the extensive literature in this area. Gaussian Bayesian networks are a popularly used form of SEMs where: (i) there are no hidden/unobserved variables, (ii) each variable is a linear combination of its parents plus a Gaussian noise term, and (iii) all noise terms are independent. The structure of a Bayesian network refers to the directed acyclic graph (DAG) that prescribes the parent nodes for each node in the graph.

This work studies the task of learning a Gaussian Bayesian network given its structure. The problem is obviously quite fundamental and has been subject to extensive prior work. The usual formulation of this problem is in terms of parameter estimation, where one wants a consistent estimator that exactly recovers the parameters of the Bayesian network in the limit, as the the number of samples approaches infinity. In contrast, we consider the problem from the viewpoint of distribution learning \cite{KMR+94}. Analogous to Valiant’s famous PAC model for learning Boolean functions \cite{Val84}, the goal here is to learn, with high probability, a distribution \(\hat{P}\) that is close to the ground-truth distribution \(P\), using an efficient algorithm. In this setting, pointwise convergence of the parameters is no longer a requirement; the aim is rather to approximately learn the induced distribution. Indeed, this relaxed objective may be achievable when the former may not be (e.g., for ill-conditioned systems) and can be the more relevant requirement for downstream inference tasks. Diakonikolas \cite{Dia16} surveys the current state-of-the-art in distribution learning from an algorithmic perspective.

\(^1\)Code is available at https://github.com/YohannaWANG/CauchyEst
Consider a Gaussian Bayesian network $\mathcal{P}$ with $n$ variables with parameters in the form of coefficients\footnote{We write $i \leftarrow j$ to emphasize that $X_j$ is the parent of $X_i$ in the Bayesian network.} $a_{i \leftarrow j}$’s and variances $\sigma_i$’s. For each $i \in [n]$, the linear structural equation for variable $X_i$, with parent indices $\pi_i \subseteq [n]$, is as follows:

$$X_i = \eta_i + \sum_{j \in \pi_i} a_{i \leftarrow j} X_j, \quad \eta_i \sim N(0, \sigma_i^2)$$

for some unknown parameters $a_{i \leftarrow j}$’s and $\sigma_i$’s. If a variable $X_i$ has no parents, then $X_i \sim N(0, \sigma_i^2)$ is simply an independent Gaussian. Our goal is to efficiently learn a distribution $Q$ such that

$$d_{TV}(\mathcal{P}, Q) \leq \varepsilon$$

while minimizing the number of samples we draw from $\mathcal{P}$ as a function of $n$, $\varepsilon$ and relevant structure parameters. Here, $d_{TV}$ denotes the total variation or statistical distance between two distributions:

$$d_{TV}(\mathcal{P}, Q) = \frac{1}{2} \int_{\mathbb{R}^n} |\mathcal{P}(x) - Q(x)| dx.$$

One way to approach the problem is to simply view $\mathcal{P}$ as an $n$-dimensional multivariate Gaussian. In this case, it is known that the Gaussian $Q \sim N(0, \hat{\Sigma})$ defined by the empirical covariance matrix $\hat{\Sigma}$, computed with $O(n^2/\varepsilon^2)$ samples from $\mathcal{P}$, is $\varepsilon$-close in TV distance to $\mathcal{P}$ with constant probability [ABDH+20, Appendix C]. This sample complexity is also necessary for learning general $n$-dimensional Gaussians and hence general Gaussian Bayesian networks on $n$ variables.

We focus therefore on the setting where the structure of the network is sparse.

**Assumption 1.1.** Each variable in the Bayesian network has at most $d$ parents. i.e. $|\pi_i| \leq d, \forall i \in [n]$.

Sparsity is a common and very useful assumption for statistical learning problems; see the book [HTW19] for an overview of the role of sparsity in regression. More specifically, in our context, the assumption of bounded in-degree is popular (e.g., see [Das97, BCD20]) and also very natural, as it reflects the belief that in the correct model, each linear structural equation involves a small number of variables\footnote{More generally, one would want to assume a bound on the “complexity” of each equation. In our context, as each equation is linear, the complexity is simply proportional to the in-degree.}.

### 1.1 Our contributions

1. Analysis of MLE LeastSquares and a distributed-friendly generalization BatchAvgLeastSquares

   The standard algorithm for parameter estimation of Gaussian Bayesian networks is to perform node-wise least squares regression. It is easy to see that LeastSquares is the maximum likelihood estimator. However, to the best of our knowledge, there did not exist an explicit sample complexity bound for this estimator. We show that the sample complexity for learning $\mathcal{P}$ to within TV distance $\varepsilon$ using LeastSquares requires only $O(nd/\varepsilon^2)$ samples, which is nearly optimal.

   We also give a generalization dubbed BatchAvgLeastSquares which solves multiple batches of least squares problems (on smaller systems of equations), and then returns their mean. As each batch is independent from the others, they can be solved separately before their solutions are combined. Our analysis will later show that we can essentially interpolate between “batch size” and “number of batches” while maintaining a similar total sample complexity -- LeastSquares is the special case of a single batch. Notably, we do not require any additional assumptions about the coefficients or variance terms in the analyses of LeastSquares and BatchAvgLeastSquares.

2. New algorithms based on Cauchy random variables: CauchyEst and CauchyEstTree

   We develop a new algorithm CauchyEst. At each node, CauchyEst solves several small linear systems of equations and takes the component-wise median of the obtained solution to obtain an estimate of the coefficients for the corresponding structural equation. In the special case of bounded-degree polytree structures, where the underlying undirected Bayesian network is acyclic, we specialize the algorithm to CauchyEstTree for which we give theoretical guarantees. Polytrees are of particular interest because inference on polytree-structured Bayesian networks can be performed efficiently [KP83, Pea86]. On polytrees,
we show that the sample complexity of CauchyEstTree is also $\tilde{O}(nd/\epsilon^2)$. Somewhat surprisingly, our analysis (as the name of the algorithm reflects) involves Cauchy random variables which usually do not arise in the context of regression.

3. Hardness results

In Section 5, we show that our sample complexity upper-bound is nearly optimal in terms of the dependence on the parameters $n$, $d$, and $\epsilon$. In particular, we show that learning the coefficients and noises of a linear structural equation model (on $n$ variables, with in-degree at most $d$) up to an $\epsilon$-error in $d_{TV}$-distance with probability 2/3 requires $\Omega(nd\epsilon^{-2})$ samples in general. We use a packing argument based on Fano's inequality to achieve this result.

4. Extensive experiments on synthetic and real-world networks

We experimentally compare the algorithms studied here as well as other well-known methods for undirected Gaussian graphical model regression, and investigate how the distance between the true and learned distributions changes with the number of samples. We find that the LeastSquares estimator performs the best among all algorithms on uncontaminated datasets. However, CauchyEst, CauchyEstTree and BatchMedLeastSquares outperform LeastSquares and BatchAvgLeastSquares by a large margin when a fraction of the samples are contaminated. In non-realizable/agnostic learning case, BatchAvgLeastSquares, CauchyEst, and CauchyEstTree performs better than the other algorithms.

1.2 Outline of paper

In Section 2, we relate KL divergence with TV distance and explain how to decompose the KL divergence into $n$ terms so that it suffices for us to estimate the parameters for each variable independently. We also give an overview of our two-phased recovery approach and explain how to use recovered coefficients to estimate the variances via VarianceRecovery. For estimating coefficients, Section 3 covers the estimators based on linear least squares (LeastSquares and BatchAvgLeastSquares) while Section 4 presents our new Cauchy-based algorithms (CauchyEst and CauchyEstTree). To complement our algorithmic results, we provide hardness results in Section 5 and experimental evaluation in Section 6.

For a cleaner exposition, we defer some formal proofs to Appendix B.

1.3 Further related work

Bayesian networks, both in discrete and continuous settings, were formally introduced by Pearl [Pea88] in 1988 to model uncertainty in AI systems. For the continuous case, Pearl considered the case when each node is a linear function of its parents added with an independent Gaussian noise [Pea88, Chapter 7]. The parameter learning problem – recovering the distribution of nodes conditioned on its parents from data – is well-studied in practice, and maximum likelihood estimators are known for various simple settings such as when the conditional distribution is Gaussian or the variables are discrete-valued. See for example the implementation of fit in the R package bnlearn [Scu20].

The focus of our paper is to give formal guarantees for the parameter learning in the PAC framework introduced by Valiant [Val84] in 1984. Subsequently, Haussler [Hau18] generalized this framework for studying parameter and density estimation problems of continuous distributions. Dasgupta [Das97] first looked at the problem of parameter learning for fixed structure Bayesian networks in the discrete and continuous settings and gave finite sample complexity bounds for these problems based on the VC-dimensions of the hypothesis classes. In particular, he gave an algorithm for learning the parameters of a Bayes net on $n$ binary variables of bounded in-degree $d_{KL}$ distance using a quadratic in $n$ samples. Subsequently, tight (linear) sample complexity upper and lower bounds were shown for this problem [BGMV20, BGVP20, CDKS20]. To the best of our knowledge, a finite PAC-style bound for fixed-structure Gaussian Bayesian networks was not known previously.

The question of structure learning for Gaussian Bayesian networks has been extensively studied. A number of works [PB14, GH17, CDW19, PK20, Par20, GDA20] have proposed increasingly general conditions for ensuring identifiability of the network structure from observations. Structure learning algorithms that work for high-dimensional Gaussian Bayesian networks have also been proposed by others (e.g., see [AZ15, AGZ19, GZ20]).
2 Preliminaries

In this section, we discuss why we upper bound the total variational distance using KL divergence and give a decomposition of the KL divergence into \( n \) terms, one associated with each variable in the Bayesian network. This decomposition motivates why our algorithms and analysis focus on recovering parameters for a single variable. We also present our general two-phased recovery approach and explain how to estimate variances using recovered coefficients in Section 2.6.

2.1 Notation

A Bayesian network (Bayes net in short) \( \mathcal{P} \) is a joint distribution \( \mathcal{P} \) over \( n \) variables \( X_1, \ldots, X_n \) defined by the underlying directed acyclic graph (DAG) \( G \). The DAG \( G = (V, E) \) encodes the dependence between the variables where \( V = \{X_1, \ldots, X_n\} \) and \( (X_j, X_i) \in E \) if and only if \( X_j \) is a parent of \( X_i \). For any variable \( X_i \), we use the set \( \pi_i \subseteq [n] \) to represent the indices of \( X_i \)’s parents. Under this notation, each variable \( X_i \) of \( \mathcal{P} \) is independent of \( X_i \)’s non-descendants conditioned on \( \pi_i \). Therefore, using Bayes rule in the topological order of \( G \), we have

\[
\mathcal{P}(X_1, \ldots, X_n) = \prod_{i=1}^{n} \Pr(X_i | \pi_i)
\]

Without loss of generality, by renaming variables, we may assume that each variable \( X_i \) only has ancestors with indices smaller than \( i \). We also define \( p_i = |\pi_i| \) as the number of parents of \( X_i \) and \( d_{\text{avg}} = \frac{1}{n} \sum_{i=1}^{n} p_i \) to be average in-degree. Furthermore, a DAG \( G \) is a polytree if the undirected version of \( G \) is acyclic.

We study the realizable setting where our unknown probability distribution \( \mathcal{P} \) is Markov with respect to the given Bayesian network. We denote the true (hidden) parameters associated with \( \mathcal{P} \) by \( \alpha^* = (\alpha_1^*, \ldots, \alpha_n^*) \). Our algorithms recover parameter estimates \( \hat{\alpha} = (\hat{\alpha}_1, \ldots, \hat{\alpha}_n) \) such that the induced probability distribution \( \mathcal{Q} \) is close in total variational distance to \( \mathcal{P} \). For each \( i \in [n] \), \( \alpha_i^* = (A_i, \sigma_i) \) is the set of ground truth parameters associated with variable \( X_i \). \( A_i \) is the coefficients associated to \( \pi_i \), \( \sigma_i^2 \) is the variance of \( \eta_i \), \( \hat{\alpha}_i^* = (\hat{A}_i, \hat{\sigma}_i) \) is our estimate of \( \alpha_i^* \).

In the course of the paper, we will often focus on the perspective a single variable of interest. This allows us to drop a subscript for a cleaner discussion. Let us denote such a variable of interest by \( Y \in V \) and use the index \( y \in [n] \). Without loss of generality, by renaming variables, we may further assume that the parents of \( Y \) are \( X_1, \ldots, X_p \). By Assumption 1.1, we know that \( p \leq d \). We can write \( Y = \eta_y + \sum_{i=1}^{p} \alpha_{y-i} X_i \), where \( \eta_y \sim N(0, \sigma_y^2) \). We use matrix \( M \in \mathbb{R}^{p \times p} \) to denote the covariance matrix defined by the parents of \( Y \), where \( M_{i,j} = \mathbb{E}[X_i X_j] \) and \( M = LL^\top \) is the Cholesky decomposition of \( M \). Under this notation, we see the vector \((X_1, \ldots, X_p) \sim N(0, M)\) is distributed as a multivariate Gaussian. Our goal is then to produce estimates \( \hat{a}_{y-i} \) for each \( a_{y-i} \). For notational convenience, we can group the coefficients into \( A = [a_{y-1}, \ldots, a_{y-p}]^\top \) and \( \hat{A} = [\hat{a}_{y-1}, \ldots, \hat{a}_{y-p}]^\top \). The vector \( \Delta = (\hat{A} - A)^\top \) captures the entry-wise gap between our estimates and the ground truth.

We write \([n]\) to mean \( \{1, 2, \ldots, n\} \) and \( |S| \) to mean the size of a set \( S \). For a matrix \( M \), \( M_{i,j} \) denotes its \((i,j)\)-th entry. We use \(|\cdot|\) to both mean the operator/spectral norm for matrices and \( L_2\)-norm for vectors, which should be clear from context. We hide absolute constant multiplicative factors and multiplicative factors poly-logarithmic in the argument using standard notations: \( \mathcal{O}(\cdot) \), \( \Omega(\cdot) \), and \( \tilde{\mathcal{O}}(\cdot) \).

2.2 Basic facts and results

We begin by stating some standard facts and results.

**Fact 2.1.** Suppose \( X \sim N(0, \sigma^2) \). Then, for any \( t > 0 \), \( \Pr(X > t) \leq \exp \left( -\frac{t^2}{2\sigma^2} \right) \).

**Fact 2.2.** Consider any matrix \( B \in \mathbb{R}^{n \times m} \) with rows \( B_1, \ldots, B_n \in \mathbb{R}^m \). For any \( i \in [m] \) and any vector \( v \in \mathbb{R}^m \) with i.i.d. \( N(0, \sigma^2) \) entries, we have that \( (Bv)_i = B_i v \sim N(0, \sigma^2 \cdot \|B_i\|^2) \).

**Fact 2.3** (Theorem 2.2 in [Gut09]). Let \( X_1, \ldots, X_p \sim N(0, LL^\top) \) be \( p \) i.i.d. \( n \)-dimensional multivariate Gaussians with covariance \( LL^\top \in \mathbb{R}^{n \times n} \) (i.e. \( L \in \mathbb{R}^{n \times p} \)). If \( X \in \mathbb{R}^{p \times n} \) is the matrix formed by stacking \( X_1, \ldots, X_p \) as rows of \( X \), then \( X = GL^\top \) where \( G \in \mathbb{R}^{p \times p} \) is a random matrix with i.i.d. \( N(0, 1) \) entries.\(^4\)

\(^4\)The transformation stated in [Gut09, Theorem 2.2, page 120] is for a single multivariate Gaussian vector, thus we need to take the transpose when we stack them in rows. Note that \( G \) and \( G^\top \) are identically distributed.
Lemma 2.4 (Equation 2.19 in [Wai19]). Let \( Y = \sum_{k=1}^{n} Z_k^2 \), where each \( Z_k \sim N(0,1) \). Then, \( Y \sim \chi_n^2 \) and for any \( 0 < t < 1 \), we have \( \Pr \left( \left| Y/n - 1 \right| \geq t \right) \leq 2 \exp \left( -nt^2/8 \right) \).

Lemma 2.5 (Consequence of Corollary 3.11 in [BVH+16]). Let \( G \in \mathbb{R}^{n \times m} \) be a matrix with i.i.d. \( N(0,1) \) entries where \( n \leq m \). Then, for some universal constant \( C \), \( \Pr \left( \| G \| \geq 2(\sqrt{n} + \sqrt{m}) \right) \leq \sqrt{n} \cdot \exp \left( -C \cdot m \right) \).

Lemma 2.6. Let \( G \in \mathbb{R}^{k \times d} \) be a matrix with i.i.d. \( N(0,1) \) entries. Then, for any constant \( 0 < c_1 < 1/2 \) and \( k \geq d/c_1^2 \),
\[
\Pr \left( \left\| (G^T G)^{-1} \right\|_{op} \leq \frac{1}{(1 - 2c_1)^2 k} \right) \geq 1 - \exp \left( -\frac{k c_1^2}{2} \right)
\]

Proof. See Appendix B.

Lemma 2.7. Let \( G \in \mathbb{R}^{k \times \sigma^2} \) be a matrix with i.i.d. \( N(0,1) \) entries and \( \eta \in \mathbb{R}^k \) be a vector with i.i.d. \( N(0,\sigma^2) \) entries, where \( G \) and \( \eta \) are independent. Then, for any constant \( c_2 > 0 \),
\[
\Pr \left( \left\| G^T \eta \right\|_2 < 2c_2 \sqrt{k} \sigma \right) \geq 1 - 2p \exp \left( -2k \right) - \exp \left( -c_2^2/k \right)
\]

Proof. See Appendix B.

The next result gives the non-asymptotic convergence of medians of Cauchy random variables. We use this result in the analysis of CauchyEst, and it may be of independent interest.

Lemma 2.8. [Non-asymptotic convergence of Cauchy median] Consider a collection of \( m \) i.i.d. Cauchy\((0,1)\) random variables \( X_1, \ldots, X_m \). Given a threshold \( 0 < \tau < 1 \), we have
\[
\Pr \left( \text{median} \{ X_1, \ldots, X_m \} \notin [-\tau, \tau] \right) \leq 2 \exp \left( -m\tau^2/8 \right)
\]

Proof. See Appendix B.

2.3 Distance and divergence between probability distributions

Recall that we are given sample access to an unknown probability distribution \( \mathcal{P} \) over the values of \( (X_1, \ldots, X_n) \in \mathbb{R}^n \) and the corresponding structure of a Bayesian network \( G \) on \( n \) variables. We denote \( \alpha^* \) as the true (hidden) parameters, inducing the probability distribution \( \mathcal{P} \), which we estimate by \( \hat{\alpha} \). In this work, we aim to recover parameters \( \hat{\alpha} \) such that our induced probability distribution \( \mathcal{Q} \) is as close as possible to \( \mathcal{P} \) in total variational distance.

Definition 2.9 (Total variational (TV) distance). Given two probability distributions \( \mathcal{P} \) and \( \mathcal{Q} \) over \( \mathbb{R}^n \), the total variational distance between them is defined as \( d_{TV}(\mathcal{P}, \mathcal{Q}) = \sup_{A \in \mathbb{R}^n} |\mathcal{P}(A) - \mathcal{Q}(A)| = \frac{1}{2} \int_{\mathbb{R}^n} |\mathcal{P} - \mathcal{Q}| \, dx \).

Instead of directly dealing with total variational distance, we will instead bound the Kullback–Leibler (KL) divergence and then appeal to the Pinsker’s inequality [Tsy08, Lemma 2.5, page 88] to upper bound \( d_{TV} \) via \( d_{KL} \). We will later show algorithms that achieve \( d_{KL}(\mathcal{P}, \mathcal{Q}) \leq \varepsilon \).

Definition 2.10 (Kullback–Leibler (KL) divergence). Given two probability distributions \( \mathcal{P} \) and \( \mathcal{Q} \) over \( \mathbb{R}^n \), the KL divergence between them is defined as \( d_{KL}(\mathcal{P}, \mathcal{Q}) = \int_{A \in \mathbb{R}^n} \mathcal{P}(A) \log \left( \frac{\mathcal{P}(A)}{\mathcal{Q}(A)} \right) \, dA \).

Fact 2.11 (Pinsker’s inequality). For distributions \( \mathcal{P} \) and \( \mathcal{Q} \), \( d_{TV}(\mathcal{P}, \mathcal{Q}) \leq \sqrt{d_{KL}(\mathcal{P}, \mathcal{Q})/2} \).

Thus, if \( s(\varepsilon) \) samples are needed to learn a distribution \( \mathcal{Q} \) such that \( d_{KL}(\mathcal{P}, \mathcal{Q}) \leq \varepsilon \), \( s(\varepsilon^2) \) samples are needed to ensure \( d_{TV}(\mathcal{P}, \mathcal{Q}) \leq \varepsilon \).
2.4 Decomposing the KL divergence

For a set of parameters $\alpha = (\alpha_1, \ldots, \alpha_n)$, denote $\alpha_i$ as the subset of parameters that are relevant to the variable $X_i$. Following the approach of [Das97], we decompose $d_{KL}(P, Q)$ into $n$ terms that can be computed by analyzing the quality of recovered parameters for each variable $X_i$.

For notational convenience, we write $x$ to mean $(x_1, \ldots, x_n)$, $\pi_i(x)$ to mean the values given to parents of variable $X_i$ by $x$, and $P(x)$ to mean $P(X_1 = x_1, \ldots, X_n = x_n)$. Let us define

$$d_{CP}(\alpha_i^*, \hat{\alpha}_i) = \int_{x, \pi_i(x)} P(x, \pi_i(x)) \log \left( \frac{P(x_i \mid \pi_i(x))}{Q(x_i \mid \pi_i(x))} \right) dx_i d\pi_i(x)$$

where each $\hat{\alpha}_i$ and $\alpha_i^*$ represent the parameters that relevant to variable $X_i$ from $\hat{\alpha}$ and $\alpha^*$ respectively. By the Bayesian network decomposition of joint probabilities and marginalization, one can show that

$$d_{KL}(P, Q) = \sum_{i=1}^{n} d_{CP}(\alpha_i^*, \hat{\alpha}_i)$$

See Appendix A for the full derivation details.

2.5 Bounding $d_{CP}$ for an arbitrary variable

We now analyze $d_{CP}(\alpha_i^*, \hat{\alpha}_i)$ with respect to the our estimates $\hat{\alpha}_i = (\hat{A}_i, \hat{\sigma}_i)$ and the hidden true parameters $\alpha_i^* = (A_i, \sigma_i)$ for any $i \in [n]$. For derivation details, see Appendix A.

With respect to variable $X_i$, one can derive $d_{CP}(\alpha_i^*, \hat{\alpha}_i) = \ln \left( \frac{\hat{\sigma}_i}{\sigma_i} \right) + \frac{\sigma_i^2 - \hat{\sigma}_i^2}{2\hat{\sigma}_i^2} + \frac{\Delta_i^\top M_i \Delta_i}{2\hat{\sigma}_i^2}$. Thus,

$$d_{KL}(P, Q) = \sum_{i=1}^{n} d_{CP}(\alpha_i^*, \hat{\alpha}_i) = \sum_{i=1}^{n} \ln \left( \frac{\hat{\sigma}_i}{\sigma_i} \right) + \frac{\sigma_i^2 - \hat{\sigma}_i^2}{2\hat{\sigma}_i^2} + \frac{\Delta_i^\top M_i \Delta_i}{2\hat{\sigma}_i^2} \tag{1}$$

where $M_i$ is the covariance matrix associated with variable $X_i$, $\alpha_i^* = (A_i, \sigma_i)$ is the coefficients and variance associated with variable $X_i$, $\alpha_i = (\hat{A}_i, \hat{\sigma}_i)$ are the estimates for $\alpha_i^*$, and $\Delta_i = \hat{A}_i - A_i$.

**Proposition 2.12** (Implication of KL decomposition). Let $\epsilon \leq 0.17$ be a constant. Suppose $\hat{\alpha}_i$ has the following properties for each $i \in [n]$:

$$|\Delta_i^\top M_i \Delta_i| \leq \sigma_i^2 \cdot \frac{\epsilon \cdot p_i}{n \cdot d_{avg}} \tag{Condition 1}$$

$$\left(1 - \sqrt{\frac{\epsilon \cdot p_i}{n \cdot d_{avg}}} \cdot \frac{\sigma_i^2}{\hat{\sigma}_i} \right) \leq \frac{\sigma_i^2}{\hat{\sigma}_i^2} \leq \left(1 + \sqrt{\frac{\epsilon \cdot p_i}{n \cdot d_{avg}}} \cdot \frac{\sigma_i^2}{\hat{\sigma}_i} \right) \tag{Condition 2}$$

Then, $d_{CP}(\alpha_i^*, \hat{\alpha}_i) \leq 3 \cdot \frac{\epsilon \cdot p_i}{n \cdot d_{avg}}$ for all $i \in [n]$. Thus, $d_{KL}(P, Q) = \sum_{i=1}^{n} d_{CP}(\alpha_i^*, \hat{\alpha}_i) \leq 3\epsilon$.

**Proof.** Consider an arbitrary fixed $i \in [n]$. Denote $\gamma = \sigma_i^2 / \hat{\sigma}_i^2$. Observe that $\gamma - 1 - \ln(\gamma) \leq (\gamma - 1)^2$ for $\gamma \geq 0.316 $. Since $p_i \leq n \cdot d_{avg} = \sum_i p_i$, Eq. (Condition 2) implies that $\gamma \geq 1/(1 + \sqrt{\frac{\epsilon \cdot p_i}{n \cdot d_{avg}}}) \geq 1/2$. Then,

$$\ln \left( \frac{\hat{\sigma}_i}{\sigma_i} \right) + \frac{\sigma_i^2 - \hat{\sigma}_i^2}{2\hat{\sigma}_i^2} = \frac{1}{2} \cdot \left( \frac{\sigma_i^2}{\hat{\sigma}_i^2} - 1 - \ln \left( \frac{\sigma_i^2}{\hat{\sigma}_i^2} \right) \right)$$

$$\leq \frac{1}{2} \cdot (\gamma - 1)^2$$

By Condition 2

$$\leq \frac{1}{2} \cdot \left( \frac{1}{1 - \sqrt{\frac{\epsilon \cdot p_i}{n \cdot d_{avg}}}} - 1 \right)^2$$

Since $\left(1 - \sqrt{\frac{\epsilon \cdot p_i}{n \cdot d_{avg}}} \cdot \frac{\sigma_i^2}{\hat{\sigma}_i} \right) \leq \frac{\sigma_i^2}{\hat{\sigma}_i^2}$

$$\leq \frac{2\epsilon \cdot p_i}{n \cdot d_{avg}}$$

Holds when $0 \leq \frac{\epsilon \cdot p_i}{n \cdot d_{avg}} \leq \frac{1}{4}$

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[Das97] analyzes the non-realizable setting where the distribution $P$ may not correspond to the causal structure of the given Bayesian network. As we study the realizable setting, we have a much simpler derivation.

6 For a cleaner argument, we are bounding $d_{KL}(P, Q) \leq 3\epsilon$. This is qualitatively the same as showing $d_{KL}(P, Q) \leq \epsilon$ since one can repeat the entire analysis with $\epsilon' = \epsilon/3$.

7 This inequality is also used in [ABDH+20, Lemma 2.9].
Meanwhile, 
\[ \frac{\Delta_i^\top M_i \Delta_i}{2\hat{\sigma}_i^2} \leq \frac{|\Delta_i^\top M_i \Delta_i|}{2\hat{\sigma}_i^2} \]  
\[ \leq \frac{p \epsilon_{ndav}}{ndav} \cdot \frac{\sigma_i^2}{2\hat{\sigma}_i^2} \quad \text{By Condition 1} \]  
\[ \leq \frac{p \epsilon_{ndav}}{2ndav} \cdot \frac{1}{1 - \sqrt{\frac{ep_{ndav}}{ndav}}} \quad \text{Since} \left( 1 - \sqrt{\frac{ep_{ndav}}{ndav}} \right) \cdot \sigma_i^2 \leq \hat{\sigma}_i^2 \]  
\[ \leq \epsilon_{ndav} \quad \text{Holds when} 0 \leq \frac{ep_{ndav}}{ndav} \leq \frac{1}{4}. \]  

Putting together, we see that \( d_{CP}(\alpha^*_i, \hat{\alpha}_i) \leq \frac{3ep_{ndav}}{ndav}. \)

### 2.6 Two-phased recovery approach

Algorithm 1 states our two-phased recovery approach. We estimate the coefficients of the Bayesian network in the first phase and use them to recover the variances in the second phase.

#### Algorithm 1 Two-phased recovery algorithm

1. **Input**: DAG \( G \) and sample parameters \( m_1 \) and \( m_2 \)
2. Draw \( m = m_1 + m_2 \) independent samples of \((X_1, \ldots, X_n)\).
3. \( \hat{A}_1, \ldots, \hat{A}_n \) \(-\) Run a coefficient recovery algorithm using first \( m_1 \) samples.
4. \( \hat{\sigma}^2_1, \ldots, \hat{\sigma}^2_n \) \(-\) Run \text{VarianceRecovery} using last \( m_2 \) samples and \( \hat{A}_1, \ldots, \hat{A}_n \)
5. **return** \( \hat{A}_1, \ldots, \hat{A}_n, \hat{\sigma}^2_1, \ldots, \hat{\sigma}^2_n \)

Motivated by Proposition 2.12, we will estimate parameters for each variable in an independent fashion\(^8\). We will provide various coefficient recovery algorithms in the subsequent sections. These algorithms will recover coefficients \( \hat{A}_i \) that satisfy Condition 1 for each variable \( X_i \). We evaluate them empirically in Section 6. For variance recovery, we use \text{VarianceRecovery} for each variable \( Y \) by computing the empirical variance\(^9\) of \( Y - X \hat{A} \) such that the recovered variance satisfies Condition 2.

#### Algorithm 2 VarianceRecovery: Variance recovery algorithm given coefficient estimates

1. **Input**: DAG \( G \), coefficient estimates, and \( m_2 \in \mathcal{O} \left( \frac{ndav}{\epsilon_2} \log \left( \frac{n}{3} \right) \right) \) samples
2. **for** variable \( Y \) with \( p \) parents and coefficient estimate \( \hat{A} \) **do** \( (> 0 \text{ if} p = 0, \text{then} \hat{A} = 0) \)
3. Without loss of generality, by renaming variables, let \( X_1, \ldots, X_p \) be the parents of \( Y \).
4. **for** \( s = 1, \ldots, m_2 \) **do**
5. Define \( Y^{(s)} \) as the \( s \)th sample of \( Y \).
6. Define \( X^{(s)} = [X_1^{(s)}, \ldots, X_p^{(s)}] \) as the \( s \)th sample of \( X_1, \ldots, X_p \) placed in a row vector.
7. Define \( Z^{(s)} = (Y^{(s)} - X^{(s)} \hat{A})^2 \).
8. **end for**
9. Estimate \( \hat{\sigma}^{2}_y = \frac{1}{m_2} \sum_{i=1}^{m_2} Z^{(s)} \)
10. **end for**

To analyze \text{VarianceRecovery}, we first prove guarantees for an arbitrary variable and then take union bound over \( n \) variables.

**Lemma 2.13**. Consider Algorithm 2. Fix any arbitrary variable of interest \( Y \) with \( p \) parents, parameters \((A, \sigma_y)\), and associated covariance matrix \( M \). Suppose we have coefficient estimates \( \hat{A} \) such that \( |\Delta^\top \hat{M} \Delta| \leq \sigma_y^2 \cdot \frac{p \epsilon}{ndav} \).

Suppose \( 0 \leq \epsilon \leq 3 - 2\sqrt{2} \leq 0.17 \). With \( k = \frac{32ndav}{ep} \log \left( \frac{n}{3} \right) \) samples, we recover variance estimate \( \hat{\sigma}_y^2 \) such that
\[
\Pr \left( \left( 1 - \sqrt{\frac{ep_{ndav}}{ndav}} \right) \cdot \sigma_y^2 \leq \hat{\sigma}_y^2 \leq \left( 1 + \sqrt{\frac{ep_{ndav}}{ndav}} \right) \cdot \sigma_y^2 \right) \geq 1 - \delta
\]

\(^8\)Given the samples, parameters related to each variable can be estimated in parallel.

\(^9\)Except in our experiments with contaminated data in Section 6 where we use the classical median absolute deviation (MAD) estimator. See Appendix C for a description.
Proof. We first argue that $\tilde{\sigma}_y^2 \sim (\sigma_y^2 + \Delta^\top M \Delta) \cdot \chi_k^2$, then apply standard concentration bounds for $\chi^2$ random variables (see Lemma 2.4).

For any sample $s \in [k]$, we see that $Y^{(s)} - X^{(s)} \tilde{A} = X^{(s)} A + \eta_y^{(s)} - X^{(s)} \tilde{A} = \eta_y^{(s)} - X^{(s)} \Delta$, where $\Delta = \tilde{A} - A \in \mathbb{R}^p$ is an unknown constant vector (because we do not actually know $A$). For fixed $\Delta$, we see that $X^{(s)} \Delta \sim N(0, \Delta^\top M \Delta)$. Since $\eta_y^{(s)} \sim N(0, \sigma_y^2)$ and $X^{(s)}$ are independent, we have that $Y^{(s)} - X^{(s)} \tilde{A} \sim N(0, \sigma_y^2 + \Delta^\top M \Delta)$. So, for any sample $s \in [k]$, $Z^{(s)} = (Y^{(s)} - X^{(s)} \tilde{A})^2 \sim (\sigma_y^2 + \Delta^\top M \Delta) \cdot \chi_1^2$. Therefore, $\tilde{\sigma}_y = \frac{1}{k} \sum_{s=1}^k Z^{(s)} \sim (\sigma_y^2 + \Delta^\top M \Delta)/k \cdot \chi_k^2$. Let us define

$$\gamma = \frac{\tilde{\sigma}_y^2}{\sigma_y^2} \cdot \left( \frac{1}{1 + \frac{\Delta^\top M \Delta}{\sigma_y^2}} \right) \sim \chi_k^2.$$

Since $p \leq nd_{avg}$, if $\varepsilon \leq 3 - 2\sqrt{2}$, then $\frac{\varepsilon p}{nd_{avg}} \leq 3 - 2\sqrt{2} \leq 3 + 2\sqrt{2}$. We first make two observations:

1. For $0 \leq \frac{\varepsilon p}{nd_{avg}} \leq 3 - 2\sqrt{2}$, \(1 + \sqrt{\frac{\varepsilon p}{nd_{avg}}} \cdot \left( \frac{1}{1 + \frac{\Delta^\top M \Delta}{\sigma_y^2}} \right) \geq 1 + \sqrt{\frac{\varepsilon p}{4nd_{avg}}}\).

2. For $0 \leq \frac{\varepsilon p}{nd_{avg}} \leq 3 + 2\sqrt{2}$, \(1 - \sqrt{\frac{\varepsilon p}{nd_{avg}}} \cdot \left( \frac{1}{1 + \frac{\Delta^\top M \Delta}{\sigma_y^2}} \right) \leq 1 - \sqrt{\frac{\varepsilon p}{4nd_{avg}}}\).

Using Lemma 2.4 with the above discussion, we have

$$\Pr \left( \frac{\tilde{\sigma}_y^2}{\sigma_y^2} \geq 1 + \sqrt{\frac{\varepsilon p}{nd_{avg}}} \right) \text{ or } \frac{\tilde{\sigma}_y^2}{\sigma_y^2} \leq 1 - \sqrt{\frac{\varepsilon p}{nd_{avg}}} \right) \leq \Pr \left( \gamma \geq 1 + \sqrt{\frac{\varepsilon p}{nd_{avg}}} \right) \cdot \left( \frac{1}{1 + \frac{\Delta^\top M \Delta}{\sigma_y^2}} \right)$$

$$\leq \Pr \left( |\gamma - 1| \geq \sqrt{\frac{\varepsilon p}{4nd_{avg}}} \right) \leq 2 \exp \left( - \frac{k \varepsilon p}{32 nd_{avg}} \right).$$

The claim follows by setting $k = \frac{32nd_{avg}}{\varepsilon p} \log \left( \frac{2}{\delta} \right).$ \hfill $\square$

**Corollary 2.14** (Guarantees of VarianceRecovery). Consider Algorithm 2. Suppose $0 \leq \varepsilon \leq 3 - 2\sqrt{2} \leq 0.17$ and we have coefficient estimates $A_i$ such that $|\Delta_i^\top M_i \Delta_i| \leq \sigma_i^2 \cdot \frac{\varepsilon p}{nd_{avg}}$ for all $i \in [n]$. With $m_2 \in \mathcal{O}\left( \frac{nd_{avg}}{\varepsilon} \log \left( \frac{2}{\delta} \right) \right)$ samples, we recover variance estimate $\tilde{\sigma}_i$ such that

$$\Pr \left( \forall i \in [n], \left( 1 - \sqrt{\frac{\varepsilon p_i}{nd_{avg}}} \right) \cdot \sigma_i^2 \leq \tilde{\sigma}_i^2 \leq \left( 1 + \sqrt{\frac{\varepsilon p_i}{nd_{avg}}} \right) \cdot \sigma_i^2 \right) \geq 1 - \delta$$

The total running time is $\mathcal{O}\left( \frac{n^2 d_{avg}^2}{\varepsilon} \log \left( \frac{1}{\delta} \right) \right).$

Proof. For each $i \in [n]$, apply Lemma 2.13 with $\delta' = \delta/n$ and $m_2 = \frac{32nd_{avg}}{\varepsilon} \log \left( \frac{2}{\delta} \right) \geq \max_{i \in [n]} \frac{32nd_{avg}}{\varepsilon p_i} \log \left( \frac{2}{\delta} \right)$, then take the union bound over all $n$ variables.

The computational complexity for a variable with $p$ parents is $\mathcal{O}(m_2 \cdot p)$. Since $\sum_{i=1}^n p_i = nd_{avg}$, the total runtime is $\mathcal{O}(m_2 \cdot n \cdot d_{avg}).$ \hfill $\square$

In Section 5, we show that the sample complexity is nearly optimal in terms of the dependence on $n$ and $\varepsilon$. We remark that we use one batch of samples to use for all the nodes; this is possible as we can obtain high-probability bounds on the error events at each node.
3 Coefficient estimators based on linear least squares

In this section, we provide algorithms LeastSquares and BatchAvgLeastSquares for recovering the coefficients in a Bayesian network using linear least squares. As discussed in Section 2.6, we will recover the coefficients for each variable such that Condition 1 is satisfied. To do so, we estimate the coefficients associated with each individual variable using independent samples. At each node, LeastSquares computes an estimate by solving the linear least squares problem with respect to a collection of sample observations. In Section 3.2, we generalize this approach via BatchAvgLeastSquares by allowing any interpolation between “batch size” and “number of batches” -- LeastSquares is a special case of a single batch. Since each solution to batch can be computed independently before their results are combined, BatchAvgLeastSquares facilitates parallelism.

3.1 Vanilla least squares

Consider an arbitrary variable $Y$ with $p$ parents. Using $m_1$ independent samples, we form matrix $X \in \mathbb{R}^{m_1 \times p}$, where the $r$th row consists of sample values $X_1^{(r)}, \ldots, X_p^{(r)}$, and the column vector $B = [Y^{(1)}, \ldots, Y^{(m_1)}]^\top \in \mathbb{R}^{m_1}$. Then, we define $\tilde{A} = (X^\top X)^{-1}X^\top B$ as the solution to the least squares problem $X\tilde{A} = B$. The pseudocode of LeastSquares is given in Algorithm 3 and Theorem 3.1 states its guarantees.

Algorithm 3 LeastSquares: Coefficient recovery algorithm for general Bayesian networks

1: Input: DAG $G$ and $m_1 \in \mathcal{O}\left(\frac{nd_{avg}}{\epsilon} \cdot \ln\left(\frac{2}{\delta}\right)\right)$ samples
2: for variable $Y$ with $p \geq 1$ parents do
3: Without loss of generality, by renaming variables, let $X_1, \ldots, X_p$ be the parents of $Y$.
4: Form matrix $X \in \mathbb{R}^{m_1 \times p}$, where the $r$th row consists of sample values $X_1^{(r)}, \ldots, X_p^{(r)}$
5: Form column vector $B = [Y^{(1)}, \ldots, Y^{(m_1)}]^\top \in \mathbb{R}^{m_1}$
6: Define $\tilde{A} = (X^\top X)^{-1}X^\top B$ as the solution to the least squares problem $X\tilde{A} = B$
7: end for

Theorem 3.1 (Distribution learning using LeastSquares). Let $\epsilon, \delta \in (0, 1)$. Suppose $G$ is a fixed directed acyclic graph on $n$ variables with degree at most $d$. Given $\mathcal{O}\left(\frac{nd_{avg}}{\epsilon \cdot \log\left(\frac{2}{\delta}\right)}\right)$ samples from an unknown Bayesian network $P$ over $G$, if we use LeastSquares for coefficient recovery in Algorithm 1, then with probability at least $1 - \delta$, we recover a Bayesian network $Q$ over $G$ such that $d_{TV}(P, Q) \leq \epsilon$ in $\mathcal{O}\left(\frac{n^2d_{avg}d}{\epsilon^2} \log\left(\frac{1}{\delta}\right)\right)$ time.\(^{10}\)

Our analysis begins by proving guarantees for an arbitrary variable.

Lemma 3.2. Consider Algorithm 3. Fix an arbitrary variable $Y$ with $p$ parents, parameters $(A, \sigma_y)$, and associated covariance matrix $M$. With $k \geq \frac{4c_d^2}{(1-\epsilon^2)c_3} \cdot \frac{nd_{avg}}{\epsilon^2}$ samples, for any constants $0 < c_1 < 1/2$ and $c_2 > 0$, we recover the coefficients $\tilde{A}$ such that

$$\text{Pr}\left(\left|\Delta^\top M\Delta\right| \geq \sigma_y^2 \cdot \frac{pe}{nd_{avg}}\right) \leq \exp\left(-\frac{kc_1^2}{2}\right) + 2p\exp(-2k) + p\exp\left(-\frac{c_2^2}{2}\right)$$

Proof. Since $|\Delta^\top M\Delta| = |\Delta^\top LL^\top \Delta| = \|L^\top \Delta\|^2$, it suffices to bound $\|L^\top \Delta\|$.

Without loss of generality, the parents of $Y$ are $X_1, \ldots, X_p$. Define $X \in \mathbb{R}^{k \times p}$, $B \in \mathbb{R}^k$, and $\tilde{A} \in \mathbb{R}^p$ as in Algorithm 3. Let $\eta = [\eta_y^{(1)}, \ldots, \eta_y^{(d)}] \in \mathbb{R}^k$ be the instantiations of Gaussian $\eta_y$ in the $k$ samples. By the structural equations, we know that $B = XA + \eta$. So,

$$\tilde{A} = (X^\top X)^{-1}X^\top B = (X^\top X)^{-1}X^\top (XA + \eta) = A + (X^\top X)^{-1}X^\top \eta$$

By Fact 2.3, we can express $X = GL^\top$ where matrix $G \in \mathbb{R}^{k \times p}$ is a random matrix with i.i.d. $N(0, 1)$ entries. Since $\Delta = \tilde{A} - A$, we see that $\Delta = (L^\top)^{-1}(G^\top G)^{-1}G^\top \eta$. Rearranging, we have $L^\top \Delta = (G^\top G)^{-1}G^\top \eta$ and so

\(^{10}\)In particular, this gives a $d_{KL}(P, Q) \leq \epsilon$ guarantee for learning centered multivariate Gaussians using $\tilde{O}(n^2\epsilon^{-1})$ samples. See e.g. [ABDH\textsuperscript{+}20] for an analogous $d_{KL}(Q, P) \leq \epsilon$ guarantee.
The total running time is $\|G^\top G\|^{-1}\cdot \|G^\top \eta\|$. Combining Lemma 2.6 and Lemma 2.7, which bound $\|G^\top G\|^{-1}$ and $\|G^\top \eta\|$ respectively, we get

$$
\Pr \left( \|L^\top \Delta\| > \frac{\epsilon_p c_2 \sqrt{p}}{(1 - 2c_1)^2 \sqrt{k}} \right) \leq \exp \left( - \frac{kc_1^2}{2} \right) + 2p \exp \left( -2k \right) + p \exp \left( -\frac{c_2^2}{2} \right)
$$

(2)

for any constants $0 < c_1 < 1/2$ and $c_2 > 0$. The claim follows by setting $k = \frac{4\epsilon_p^2 (1-c_1)^2}{\epsilon_p n_{d_{avg}}}$.

We can now establish Condition 1 of Proposition 2.12 for LeastSquares.

**Lemma 3.3.** Consider Algorithm 3. With $m_1 \in O \left( \frac{n_{d_{avg}}}{\epsilon} \cdot \ln \left( \frac{n}{\delta} \right) \right)$ samples, we recover the coefficients $\hat{A}_1, \ldots, \hat{A}_n$ such that

$$
\Pr \left( \forall i \in [n], |\Delta_i^\top M_i \Delta_i| \geq \sigma_i^2 \cdot \frac{\epsilon_p i}{n_{d_{avg}}} \right) \leq \delta
$$

The total running time is $O \left( \frac{n^2 d_{avg}^2}{\epsilon} \cdot \ln \left( \frac{1}{\delta} \right) \right)$.

**Proof.** By setting $c_1 = 1/4, c_2 = \sqrt{2 \ln (3n/\delta)}$, and $k = \frac{32n_{d_{avg}}}{\epsilon} \ln \left( \frac{3n}{\delta} \right) \geq \frac{4\epsilon_p^2 (1-c_1)^2}{\epsilon_p n_{d_{avg}}}$ in Lemma 3.2, we have

$$
\Pr \left( |\Delta_i^\top M_i \Delta_i| \geq \sigma_i^2 \cdot \frac{p_i \epsilon}{n_{d_{avg}}} \right) \leq \exp \left( - \frac{kc_1^2}{2} \right) + \frac{p \exp \left( -2k \right) + \exp \left( -\frac{c_2^2}{2} \right)}{\delta \ln \left( \frac{1}{\delta} \right)}
$$

for any $i \in [n]$. The claim holds by a union bound over all $n$ variables.

The computational complexity for a variable with $p$ parents is $O(p^2 \cdot m_1)$. Since $\max_{i \in [n]} p_i \leq d$ and $\sum_{i=1}^{n} p_i = n_{d_{avg}}$, the total runtime is $O(m_1 \cdot n \cdot d_{avg} \cdot d)$.

Theorem 3.1 follows from combining the guarantees of LeastSquares and VarianceRecovery (given in Lemma 3.3 and Corollary 2.14 respectively) via Proposition 2.12.

**Proof of Theorem 3.1.** We will show sample and time complexities before giving the proof for the dTV distance.

Let $m_1 \in O \left( \frac{n_{d_{avg}}}{\epsilon} \cdot \ln \left( \frac{n}{\delta} \right) \right)$ and $m_2 \in O \left( \frac{n_{d_{avg}}}{\epsilon} \ln \left( \frac{n}{\delta} \right) \right)$. Then, the total number of samples needed is $m = m_1 + m_2 \in O \left( \frac{n^2 d_{avg}^2}{\epsilon} \ln \left( \frac{1}{\delta} \right) \right)$. LeastSquares runs in $O \left( \frac{n^2 d_{avg}^2}{\epsilon} \ln \left( \frac{1}{\delta} \right) \right)$ time while VarianceRecovery runs in $O \left( \frac{n^2 d_{avg}^2}{\epsilon} \ln \left( \frac{1}{\delta} \right) \right)$ time. Therefore, the overall running time is $O \left( \frac{n^2 d_{avg}^2}{\epsilon} \ln \left( \frac{1}{\delta} \right) \right)$.

By Lemma 3.3, LeastSquares recovers coefficients $\hat{A}_1, \ldots, \hat{A}_n$ such that

$$
\Pr \left( \forall i \in [n], |\Delta_i^\top M_i \Delta_i| \geq \sigma_i^2 \cdot \frac{\epsilon_p i}{n_{d_{avg}}} \right) \leq \delta
$$

By Corollary 2.14 and using the recovered coefficients from LeastSquares, VarianceRecovery recovers variance estimates $\hat{\sigma}_i^2$ such that

$$
\Pr \left( \forall i \in [n], \left( 1 - \sqrt{\frac{\epsilon_p i}{n_{d_{avg}}}} \right) \cdot \sigma_i^2 \leq \hat{\sigma}_i^2 \leq \left( 1 + \sqrt{\frac{\epsilon_p i}{n_{d_{avg}}}} \right) \cdot \sigma_i^2 \right) \geq 1 - \delta
$$

As our estimated parameters satisfy Condition 1 and Condition 2, Proposition 2.12 tells us that $d_{KL}(P, Q) \leq 3\epsilon$. Thus, $d_{TV}(P, Q) \leq \sqrt{d_{KL}(P, Q)/2} \leq \sqrt{3\epsilon/2}$. The claim follows by setting $\epsilon' = \sqrt{3\epsilon/2}$ throughout.

### 3.2 Interpolating between batch size and number of batches

We now discuss a generalization of LeastSquares. In a nutshell, for each variable with $p \geq 1$ parents, BatchAvgLeastSquares solves $b \geq 1$ batches of linear systems made up of $k > p$ samples and then uses the mean of the recovered solutions as an estimate for the coefficients. Note that one can interpolate between different values of $k$ and $b$, as long as $k \geq p$ (so that the batch solutions are correlated to the true parameters). The pseudocode of BatchAvgLeastSquares is provided in Algorithm 4 and the guarantees are given in Theorem 3.1.

In Section 6, we also experimented on a variant of BatchAvgLeastSquares dubbed BatchMedLeastSquares, where $A$ is defined to be the coordinate-wise median of the $A(s)$ vectors. However, in the theoretical analysis below, we only analyze BatchAvgLeastSquares.
Algorithm 4 \textbf{BatchAvgLeastSquares}: Coefficient recovery for general Bayesian networks

1: \textbf{Input:} DAG $G$ and $m_1 = \mathcal{O}\left(\frac{nd_{avg}}{\epsilon^2} (d + \ln \left(\frac{n}{\epsilon^2}\right))\right)$ samples
2: \textbf{for} variable $Y$ with $p \geq 1$ parents \textbf{do}
3: \hspace{1em} Without loss of generality, by renaming variables, let $X_1, \ldots, X_p$ be the parents of $Y$.
4: \hspace{1em} \textbf{for} $s = 1, \ldots, b$ \textbf{do}
5: \hspace{2em} Form matrix $X \in \mathbb{R}^{k \times p}$, where the $r$\textsuperscript{th} row consists of sample values $X_1^{(s,r)}, \ldots, X_p^{(s,r)}$
6: \hspace{2em} Form column vector $B = \left[Y^{(s,1)}, \ldots, Y^{(s,k)}\right]^\top \in \mathbb{R}^k$
7: \hspace{2em} Define $\bar{A}^{(s)} = (X^\top X)^{-1}X^\top B$ as the solution to the least squares problem $X \bar{A}^{(s)} = B$
8: \hspace{1em} \textbf{end for}
9: \hspace{1em} Define $\hat{A} = \frac{1}{b} \sum_{s=1}^b \bar{A}^{(s)}$
10: \textbf{end for}

\textbf{Theorem 3.4} (Distribution learning using \textbf{BatchAvgLeastSquares}). Let $\epsilon, \delta \in (0, 1)$. Suppose $G$ is a fixed directed acyclic graph on $n$ variables with degree at most $d$. Given $\mathcal{O}\left(\frac{nd_{avg}}{\epsilon^2} (d + \ln \left(\frac{n}{\epsilon^2}\right))\right)$ samples from an unknown Bayesian network $\mathcal{P}$ over $G$, if we use \textbf{BatchAvgLeastSquares} for coefficient recovery in Algorithm 1, then with probability at least $1 - \delta$, we recover a Bayesian network $\mathcal{Q}$ over $G$ such that $d_{TV}(\mathcal{P}, \mathcal{Q}) \leq \epsilon$ in $\mathcal{O}\left(\frac{n^2d_{avg}d}{\epsilon^2} (d + \ln \left(\frac{n}{\epsilon^2}\right))\right)$ time.

Our approach for analyzing \textbf{BatchAvgLeastSquares} is the same as our approach for \textbf{LeastSquares}: we prove guarantees for an arbitrary variable and then take union bound over $n$ variables. At a high-level, for each node $Y$, for every fixing of the randomness in generating $X_1, \ldots, X_p$, we show that each $\bar{A}^{(s)}$ is a gaussian. Since the $b$ iterations are independent, $\frac{1}{b} \sum_s \bar{A}^{(s)}$ is also a gaussian. Its variance is itself a random variable but can be bounded with high probability using concentration inequalities.

\textbf{Lemma 3.5}. Consider Algorithm 4. Fix any arbitrary variable of interest $Y$ with $p$ parents, parameters $(A, \sigma_y)$, and associated covariance matrix $M$. With $k > C_k \cdot \left(p + \ln \left(\frac{n}{d}\right)\right)$ and $kb = C_{kb} \cdot \left(\frac{nd_{avg}}{\epsilon^2} (d + \ln \left(\frac{n}{\epsilon^2}\right))\right)$, for some universal constants $C_k$ and $C_{kb}$, we recover coefficients estimates $\hat{A}$ such that

$$
\Pr \left( |A^\top M A| \leq \sigma_y^2 \frac{\epsilon p}{nd_{avg}} \right) \geq 1 - \delta
$$

\textbf{Proof}. Without loss of generality, the parents of $Y$ are $X_1, \ldots, X_p$. For $s \in [n]$, define $X^{(s)} \in \mathbb{R}^{k \times p}$, $B^{(s)} \in \mathbb{R}^k$, and $\bar{A}^{(s)} \in \mathbb{R}^p$ as the quantities involved in the $s$\textsuperscript{th} batch of Algorithm 4. Let $\eta^{(s)} = [\eta^{(s,1)}, \ldots, \eta^{(s,k)}] \in \mathbb{R}^k$ be the instantiations of Gaussian $\eta_y$ in the $k$ samples for the $s$\textsuperscript{th} batch. By the structural equations, we know that $B^{(s)} = X^{(s)}A + \eta^{(s)}$. So,

$$
\bar{A}^{(s)} = ((X^{(s)})^\top X^{(s)})^{-1}(X^{(s)})^\top B
= ((X^{(s)})^\top X^{(s)})^{-1}(X^{(s)})^\top (X^{(s)}A + \eta^{(s)})
= A + ((X^{(s)})^\top X^{(s)})^{-1}(X^{(s)})^\top \eta^{(s)}
$$

By Fact 2.3, we can express $X^{(s)} = G^{(s)}L^\top$ where matrix $G^{(s)} \in \mathbb{R}^{k \times p}$ is a random matrix with i.i.d. $N(0, 1)$ entries. So, we see that

$$
L^\top \Delta = \frac{1}{b} \sum_{s=1}^b ((G^{(s)})^\top G^{(s)})^{-1}(G^{(s)})^\top \eta^{(s)}
$$

For any $i \in [p]$, Fact 2.2 tells us that

$$
(L^\top \Delta)_i = \frac{1}{b} \sum_{s=1}^b \left(((G^{(s)})^\top G^{(s)})^{-1}(G^{(s)})^\top \eta^{(s)}\right)_i \sim N \left(0, \frac{\sigma_y^2}{b^2} \sum_{s=1}^b \left\| ((G^{(s)})^\top G^{(s)})^{-1}(G^{(s)})^\top \eta^{(s)} \right\|_i^2 \right)
$$

We can upper bound each $\left\| ((G^{(s)})^\top G^{(s)})^{-1}(G^{(s)})^\top \eta^{(s)} \right\|_i$ term as follows:

$$
\left\| ((G^{(s)})^\top G^{(s)})^{-1}(G^{(s)})^\top \eta^{(s)} \right\|_i \leq \left\| ((G^{(s)})^\top G^{(s)})^{-1}(G^{(s)})^\top \right\| \cdot \left\| G^{(s)} \right\|_i
$$
When \( k \geq 4p \), Lemma 2.6 tells us that \( \Pr \left( \|G(s)^{\top}\| \geq \frac{4}{k} \right) \leq \exp \left( -\frac{b}{32} \right) \). Meanwhile, Lemma 2.5 tells us that \( \Pr \left( \|G(s)^{\top}\| \geq 2(\sqrt{k} + \sqrt{\beta}) \right) \leq \sqrt{\beta} \cdot \exp \left( -C \cdot k \right) \) for some universal constant \( C \). Let \( \mathcal{E} \) be the event that \( \|((G^{(s)})^{\top}G^{(s)})^{-1}(G^{(s)})^{\top})\| < \frac{8(\sqrt{k} + \sqrt{\beta})}{k} \) for any \( s \in [b] \). Applying union bound with the conclusions from Lemma 2.6 and Lemma 2.5, we have

\[
\Pr (\mathcal{E}) = \Pr \left( \exists s \in [b], \left\| (G^{(s)})^{\top}G^{(s)} - 1(G^{(s)})^{\top} \right\| \geq \frac{8(\sqrt{k} + \sqrt{\beta})}{k} \right)
\leq b \cdot \exp \left( -\frac{k}{32} \right) + b \cdot \sqrt{\beta} \cdot \exp \left( -C \cdot k \right)
\]

Conditioned on event \( \mathcal{E} \), standard Gaussian tail bounds (e.g. see Fact 2.1) give us

\[
\Pr \left( \|L^{\top}\Delta\| \geq \sigma_y \cdot \sqrt{\frac{\varepsilon}{nd_{avg}}} \mid \mathcal{E} \right) \leq \exp \left( -\frac{\sigma_y^2 \cdot nd_{avg}}{2 \cdot \frac{\varepsilon}{nd_{avg}} \sum_{s=1}^{b} \left\| (G^{(s)})^{\top}G^{(s)} - 1(G^{(s)})^{\top} \right\|^2} \right)
\leq \exp \left( -\frac{\varepsilon \cdot b \cdot k}{128 \cdot n \cdot d_{avg} \cdot (\sqrt{k} + \sqrt{\beta})^2} \right)
\leq \exp \left( -\frac{\varepsilon \cdot b \cdot k}{512 \cdot n \cdot d_{avg}} \right)
\]

where the second last inequality is because of event \( \mathcal{E} \) and the last inequality is because \((\sqrt{k} + \sqrt{\beta})^2 \leq (2\sqrt{k})^2 = 4k\), since \( k \geq p \).

Thus, applying a union bound over all \( p \) entries of \( L^{\top}\Delta \) and accounting for \( \Pr (\mathcal{E}) \), we have

\[
\Pr \left( \|L^{\top}\Delta\| \geq \sigma_y \cdot \sqrt{\frac{\varepsilon}{nd_{avg}}} \right)
\leq \Pr \left( \|L^{\top}\Delta\| \geq \sigma_y \cdot \sqrt{\frac{\varepsilon}{nd_{avg}}} \mid \mathcal{E} \right) + \Pr (\mathcal{E})
\leq p \cdot \exp \left( -\frac{\varepsilon \cdot b \cdot k}{512 \cdot n \cdot d_{avg}} \right) + b \cdot \exp \left( -\frac{k}{32} \right) + b \cdot \sqrt{\beta} \cdot \exp \left( -C \cdot k \right)
\]

for some universal constant \( C \).

The claim follows by observing that \( \|\Delta^{\top}M\Delta\| = \|\Delta^{\top}LL^{\top}\Delta\| = \|L^{\top}\Delta\|^2 \) and applying the assumptions on \( k \) and \( b \).

We can now establish Condition 1 of Proposition 2.12 for BatchAvgLeastSquares.

**Lemma 3.6 (Coefficient recovery guarantees of BatchAvgLeastSquares).** Consider Algorithm 4. With \( m_1 \in \mathcal{O} \left( \frac{nd_{avg}}{\varepsilon} \left( d + \ln \left( \frac{n}{\varepsilon g} \right) \right) \right) \) samples, where \( k \in \Omega \left( d + \ln \left( \frac{n}{\varepsilon g} \right) \right) \) and \( b = \frac{m_1}{k} \), we recover coefficient estimates \( \hat{A}_1, \ldots, \hat{A}_n \) such that

\[
\Pr \left( \forall i \in [n], \|\Delta_i^{\top}M_i\Delta_i\| \geq \sigma_i^2 \cdot \frac{\varepsilon p_i}{nd_{avg}} \right) \leq \delta
\]

The total running time is \( \mathcal{O} \left( m_1 \cdot n \cdot d_{avg} \cdot d \right) \).

**Proof.** For each \( i \in [n] \), apply Lemma 3.5 with \( \delta' = \delta/n \), then take the union bound over all \( n \) variables.

The computational complexity for a variable with \( p \) parents is \( \mathcal{O} \left( b \cdot p^2 \cdot k \right) = \mathcal{O} \left( p^2 \cdot m_1 \right) \). Since \( \max_{i \in [n]} p_i \leq d \) and \( \sum_{i=1}^{n} p_i = nd_{avg} \), the total runtime is \( \mathcal{O} \left( m_1 \cdot n \cdot d_{avg} \cdot d \right) \).

**Theorem 3.4** follows from combining the guarantees of BatchAvgLeastSquares and VarianceRecovery (given in Lemma 3.6 and Corollary 2.14 respectively) via Proposition 2.12.

**Proof of Theorem 3.4.** We will show sample and time complexities before giving the proof for the \( d_{TV} \) distance.

Let \( m_1 \in \mathcal{O} \left( \frac{nd_{avg}}{\varepsilon} \left( d + \ln \left( \frac{n}{\varepsilon g} \right) \right) \right) \) and \( m_2 \in \mathcal{O} \left( \frac{nd_{avg}}{\varepsilon} \log \left( \frac{n}{\varepsilon g} \right) \right) \). Then, the total number of samples needed is \( m = m_1 + m_2 \in \mathcal{O} \left( \frac{nd_{avg}}{\varepsilon} \left( d + \ln \left( \frac{n}{\varepsilon g} \right) \right) \right) \). BatchAvgLeastSquares runs in \( \mathcal{O} \left( m_1 nd_{avg}d \right) \) time while VarianceRecovery runs in \( \mathcal{O} \left( \frac{n^2 d_{avg}^2}{\varepsilon} \log \left( \frac{1}{\epsilon} \right) \right) \) time. Therefore, the overall running time is \( \mathcal{O} \left( \frac{n^2 d_{avg}^2 \log \left( \frac{1}{\epsilon} \right)}{\varepsilon} \left( d + \ln \left( \frac{n}{\varepsilon g} \right) \right) \right) \).
By Lemma 3.6, \( \text{BatchAvgLeastSquares} \) recovers coefficients \( \hat{A}_1, \ldots, \hat{A}_n \) such that

\[
\Pr \left( \forall i \in [n], |\Delta^\top_i M_i \Delta_i| \geq \sigma_i^2 \cdot \frac{\varepsilon r_i}{n d_{avg}} \right) \leq \delta
\]

By Corollary 2.14 and using the recovered coefficients from \( \text{BatchAvgLeastSquares} \), \( \text{VarianceRecovery} \) recovers variance estimates \( \tilde{\sigma}_i^2 \) such that

\[
\Pr \left( \forall i \in [n], \left( 1 - \sqrt{\frac{\varepsilon r_i}{n d_{avg}}} \right) \cdot \sigma_i^2 \leq \tilde{\sigma}_i^2 \leq \left( 1 + \sqrt{\frac{\varepsilon r_i}{n d_{avg}}} \right) \cdot \sigma_i^2 \right) \geq 1 - \delta
\]

As our estimated parameters satisfy Condition 1 and Condition 2, Proposition 2.12 tells us that \( d_{\text{KL}}(P, Q) \leq 3\varepsilon \). Thus, \( d_{\text{TV}}(P, Q) \leq \sqrt{d_{\text{KL}}(P, Q)/2} \leq \sqrt{3\varepsilon}/2 \). The claim follows by setting \( \varepsilon' = \sqrt{3\varepsilon}/2 \) throughout.

## 4 Coefficient recovery algorithm based on Cauchy random variables

In this section, we provide novel algorithms \( \text{CauchyEst} \) and \( \text{CauchyEstTree} \) for recovering the coefficients in polytree Bayesian networks. We will show that \( \text{CauchyEstTree} \) has near-optimal sample complexity, and later in Section 6, we will see that both these algorithms outperform \( \text{LeastSquares} \) and \( \text{BatchAvgLeastSquares} \) on randomly generated Bayesian networks. Of technical interest, our analysis involves Cauchy random variables, which are somewhat of a rarity in statistical learning. As in \( \text{LeastSquares} \) and \( \text{BatchAvgLeastSquares} \), \( \text{CauchyEst} \) and \( \text{CauchyEstTree} \) use independent samples to recover the coefficients associated to each individual variable in an independent fashion.

Consider an arbitrary variable \( Y \) with \( p \) parents. The intuition is as follows: if \( \eta_i = 0 \), then one can form a linear system of equations using \( p \) samples to solve for the coefficients \( a_{y \to i} \) exactly for each \( i \in \pi(y) \). Unfortunately, \( \eta_i \) is non-zero in general. Instead of exactly recovering \( A \), we partition the \( m_1 \) independent samples into \( k = [m_1/p] \) batches involving \( p \) samples and form intermediate estimates \( \hat{A}^{(1)}, \ldots, \hat{A}^{(k)} \) by solving a system of linear equation for each batch (see Algorithm 5). Then, we “combine” these intermediate estimates to obtain our estimate \( \hat{A} \).

### Algorithm 5 Batch coefficient recovery algorithm for variable with \( p \) parents

1. **Input:** DAG \( G \), a variable \( Y \) with \( p \) parents, and \( p \) samples
2. Without loss of generality, by renaming variables, let \( X_1, \ldots, X_p \) be the parents of \( Y \).
3. Form matrix \( X \in \mathbb{R}^{p \times p} \) where the \( r \)th row equals \( [X_{1}^{(r)}, \ldots, X_{p}^{(r)}] \), corresponding to \( Y^{(r)} \).
4. Define \( \hat{A} = [\hat{a}_{y \to 1}, \ldots, \hat{a}_{y \to p}]^\top \) as any solution to \( XA = [Y^{(1)}, \ldots, Y^{(p)}] \).
5. **return** \( \hat{A} \)

Consider an arbitrary copy of recovered coefficients \( \hat{A} \). Let \( \Delta = [\Delta_1, \ldots, \Delta_p]^\top = \hat{A} - A \) be a vector measuring the gap between these recovered coefficients and the ground truth, where \( \Delta_i = \hat{a}_{y \to i} - a_{y \to i} \). Lemma 4.1 gives a condition where a vector is term-wise Cauchy. Using this, Lemma 4.2 shows that each entry of the vector \( L^\top \Delta \) is distributed according to \( \sigma_y \cdot \text{Cauchy}(0, 1) \), although the entries may be correlated with each other in general.

**Lemma 4.1.** Consider the matrix equation \( AB = E \) where \( A \in \mathbb{R}^{n \times n} \), \( B \in \mathbb{R}^{n \times 1} \), and \( E \in \mathbb{R}^{n \times 1} \) such that entries of \( A \) and \( E \) are independent Gaussians, elements in each column of \( A \) have the same variance, and all entries in \( E \) have the same variance. That is, \( A_{i,j} \sim N(0, \sigma^2) \) and \( E_i \sim N(0, \sigma^2_{n+1}) \). Then, for all \( i \in [n] \), we have that \( B_i \sim \frac{\sigma_{n+1}}{\sigma_i} \cdot \text{Cauchy}(0, 1) \).

**Proof.** As the event that \( A \) is singular has measure zero, we can write \( B = A^{-1}E \). By Cramer’s rule,

\[
A^{-1} = \frac{1}{\det(A)} \cdot \text{adj}(A) = \frac{1}{\det(A)} \cdot C^\top
\]

where \( \det(A) \) is the determinant of \( A \), \( \text{adj}(A) \) is the adjugate/adjoint matrix of \( A \), and \( C \) is the cofactor matrix of \( A \). Recall that the \( \det(A) \) can defined with respect to elements in \( C \): For any column \( i \in [n] \),

\[
\det(A) = A_{1,i} \cdot C_{1,i} + A_{2,i} \cdot C_{2,i} + \ldots + A_{n,i} \cdot C_{n,i}
\]
So, \( \det(A) \sim N \left( 0, \sigma_i^2 \left( C_{1,i} + \ldots + C_{n,i} \right) \right) \). Thus, for any \( i \in [n] \),
\[
B_i = \left( \frac{1}{\det(A)} \right) \left( \begin{array}{c} C_{1,i} \end{array} \right) \sim N \left( 0, \frac{\sigma_{n+1}^2 \left( C_{1,i} + \ldots + C_{n,i} \right)}{\sigma_i} \right) = \frac{\sigma_{n+1}}{\sigma_i} \cdot \text{Cauchy}(0,1)
\]

\[ \square \]

**Lemma 4.2.** Consider a batch estimate \( \tilde{A} \) from Algorithm 5. Then, \( L^\top \Delta \) is entry-wise distributed as \( \sigma_y \cdot \text{Cauchy}(0,1) \), where \( \Delta = \tilde{A} - A \). Note that the entries of \( L^\top \Delta \) may be correlated in general.

**Proof.** Observe that each row of \( X \) is an independent sample drawn from a multivariate Gaussian \( N(0,M) \). By denoting \( \eta = \left[ \eta_y(1), \ldots, \eta_y(p) \right]^\top \) as the \( p \) samples of \( \eta_y \), we can write \( X \tilde{A} = XA + \eta \) and thus \( X\Delta = \eta \) by rearranging terms. By Fact 2.3, we can express \( X = GL^\top \) where matrix \( G \in \mathbb{R}^{p \times p} \) is a random matrix with i.i.d. \( N(0,1) \) entries. By substituting \( X = GL^\top \) into \( X\Delta = \eta \), we have \( L^\top \Delta = G^{-1}\eta \).

By applying Lemma 4.1 with the following parameters: \( A = G, B = L^\top \Delta, E = \eta \), we conclude that each entry of \( L^\top \Delta \) is distributed as \( \sigma_y \cdot \text{Cauchy}(0,1) \). However, note that these entries are generally correlated.

\[ \square \]

If we have direct access to the matrix \( L \), then one can do the following (see Algorithm 6): for each coordinate \( i \in [p] \), take medians\(^\text{12} \) of \( \left( L^\top \left[ \tilde{a}_{y_1-1}, \ldots, \tilde{a}_{y_p-1} \right] \right)_i \) to form \( \text{MED}_i \) and then estimate \( \left[ \tilde{a}_{y_1-1}, \ldots, \tilde{a}_{y_p-1} \right] = (L^\top)^{-1} \text{MED}_1 \ldots, \text{MED}_p \). By the convergence of Cauchy random variables to their median, one can show that each \( \tilde{a}_{y_1-1} \) converges to the true coefficient \( a_{y_1} \) as before. Unfortunately, we do not have \( L \) and can only hope to estimate it with some matrix \( \tilde{L} \) using the empirical covariance matrix \( \tilde{M} \).

**Algorithm 6 CauchyEst: Coefficient recovery algorithm for general Bayesian networks**

1: **Input:** DAG \( G \) and \( m \) samples
2: **for** variable \( Y \) with \( p \geq 1 \) parents **do** \( \triangleright \) By Assumption 1.1, \( p \leq d \)
3: \hspace{0.5cm} Without loss of generality, by renaming variables, let \( X_1, \ldots, X_p \) be the parents of \( Y \).
4: \hspace{0.5cm} Let \( \tilde{M} \) be the empirical covariance matrix with respect to \( X_1, \ldots, X_p \).
5: \hspace{0.5cm} Compute the Cholesky decomposition \( \tilde{M} = \tilde{L} \tilde{L}^\top \) of \( \tilde{M} \).
6: \hspace{0.5cm} **for** \( s = 1, \ldots, [m/p] \) **do**
7: \hspace{1cm} Using \( p \) samples and Algorithm 5, compute a batch estimate \( \tilde{A}(s) \).
8: \hspace{0.5cm} **end for**
9: \hspace{0.5cm} For each \( i \in [n] \), define \( \text{MED}_i = \text{median} \{ (\tilde{L}^\top \tilde{A}(1))_i, \ldots, (\tilde{L}^\top \tilde{A}(m/p))_i \} \).
10: \hspace{0.5cm} **return** \( \tilde{A} = \left[ \tilde{a}_{y_1-1}, \ldots, \tilde{a}_{y_p-1} \right]^\top = (\tilde{L}^\top)^{-1} \text{MED}_1 \ldots, \text{MED}_p \).
11: **end for**

### 4.1 Special case of polytree Bayesian networks

If the Bayesian network is a polytree, then \( L \) is diagonal. In this case, we specialize \text{CauchyEst} to \text{CauchyEstTree} and are able to give theoretical guarantees. We begin with simple corollary which tells us that the \( i^{th} \) entry of \( \Delta \) is distributed according to \( \sigma_y / \sigma_i \cdot \text{Cauchy}(0,1) \).

**Corollary 4.3.** Consider a batch estimate \( \tilde{A} \) from Algorithm 5. If the Bayesian network is a polytree, then \( \Delta_i = (\tilde{A} - A)_i \sim \frac{\sigma_y}{\sigma_i} \cdot \text{Cauchy}(0,1) \).

**Proof.** Observe that each row of \( X \) is an independent sample drawn from a multivariate Gaussian \( N(0,M) \). By denoting \( \eta = \left[ \eta_y(1), \ldots, \eta_y(p) \right]^\top \) as the \( p \) samples of \( \eta_y \), we can write \( X \tilde{A} = XA + \eta \) and thus \( X\Delta = \eta \) by rearranging terms. Since the parents of any variable in a polytree are not correlated, each element in the \( i^{th} \) column of \( X \) is a \( N(0, \sigma_i^2) \) Gaussian random variable.

By applying Lemma 4.1 with the following parameters: \( A = X, B = \Delta E = \eta \), we conclude that \( \Delta_i = (\tilde{A} - A)_i \sim \frac{\sigma_y}{\sigma_i} \cdot \text{Cauchy}(0,1) \).

\[ \square \]

\(^{11}\)Note that event that \( G \) is singular has measure 0.

\(^{12}\)The typical strategy of averaging independent estimates does not work here as the variance of a Cauchy variable is unbounded.
For each \(i \in \pi(y)\), we combine the \(k\) independently copies of \(\tilde{a}_{y \to i}\), \(\dot{\ldots} \tilde{a}_{y \to i}^{(k)}\) using the median. For arbitrary sample \(s \in [k]\) and parent index \(i \in \pi(y)\), observe that \(\Delta_i^{(s)} = \tilde{a}_{y \to i}^{(s)} - a_{y \to i}\). Since \(a_{y \to i}\) is just an unknown constant,
\[
\hat{a}_{y \to i} = \text{median}_{s \in [k]} \left\{ \tilde{a}_{y \to i}^{(s)} \right\} = \text{median}_{s \in [k]} \left\{ \Delta_i^{(s)} \right\} + a_{y \to i}
\]
Since each \(\Delta_i^{(s)}\) term is i.i.d. distributed as \(\sigma_y \cdot \text{Cauchy}(0,1)\), the term median_{s \in [k]} \left\{ \Delta_i^{(s)} \right\} converges to 0 with sufficiently large \(k\), and thus \(\hat{a}_{y \to i}\) converges to the true coefficient \(a_{y \to i}\).

The goal of this section is to prove Theorem 4.4 given CauchyEstTree, whose pseudocode we provide in Algorithm 7.

**Algorithm 7 CauchyEstTree**: Coefficient recovery algorithm for polytree Bayesian networks

1. **Input**: A polytree \(G\) and \(m_1 \in \mathcal{O} \left( \frac{nd_{avg}d}{\varepsilon^2} \log \left( \frac{n}{\delta} \right) \right)\) samples
2. **for** variable \(Y\) with \(p \geq 1\) parents **do**
   - By Assumption 1.1, \(p \leq d\)
   - Without loss of generality, by renaming variables, let \(X_1, \ldots, X_p\) be the parents of \(Y\).
3. **for** \(s = 1, \ldots, \lfloor m_1/p \rfloor\) **do**
   - Using \(p\) samples and Algorithm 5, compute a batch estimate \(\tilde{A}^{(s)}\).
4. **end for**
5. **return** \(\hat{A} = [\hat{a}_{y \to 1}, \dot{\ldots} \hat{a}_{y \to p}]^\top\)
6. **end for**

**Theorem 4.4** (Distribution learning using CauchyEstTree). Let \(\varepsilon, \delta \in (0,1)\). Suppose \(G\) is a fixed directed acyclic graph on \(n\) variables with degree at most \(d\). Given \(\mathcal{O} \left( \frac{nd_{avg}d}{\varepsilon} \log \left( \frac{n}{\delta} \right) \right)\) samples from an unknown Bayesian network \(\mathcal{P}\) over \(G\), if we use CauchyEstTree for coefficient estimation in Algorithm 1, then with probability at least \(1 - \delta\), we recover a Bayesian network \(\mathcal{Q}\) over \(G\) such that \(d_{TV}(\mathcal{P}, \mathcal{Q}) \leq \varepsilon\) in \(\mathcal{O} \left( \frac{n^2d_{avg}d^{-1}}{\varepsilon} \log \left( \frac{n}{\delta} \right) \right)\) time.

Note that for polytrees, \(d_{avg}\) is just a constant. As before, we will first prove guarantees for an arbitrary variable and then take union bound over \(n\) variables.

**Lemma 4.5.** Consider Algorithm 7. Fix an arbitrary variable of interest \(Y\) with \(p\) parents, parameters \((A, \sigma_y)\), and associated covariance matrix \(M\). With \(k = \frac{8nd_{avg}}{\varepsilon} \log \left( \frac{n}{\delta} \right)\) samples, we recover coefficient estimates \(\hat{A}\) such that
\[
\Pr \left( \left| \Delta^\top M \Delta \right| \leq \sigma_y^2 \cdot \frac{\varepsilon p}{nd_{avg}} \right) \geq 1 - \delta
\]

**Proof.** Since \(M = LL^\top\), it suffices to bound \(\|L^\top \Delta\|\). Lemma 4.2 tells us that each entry of the vector \(L^\top \Delta\) is the median of \(k\) copies of Cauchy \((0,1)\) random variables multiplied by \(\sigma_y\). Setting \(k = \frac{8nd_{avg}}{\varepsilon} \log \left( \frac{n}{\delta} \right)\) and \(0 < \tau = \sqrt{\varepsilon/(nd_{avg})} < 1\) in Lemma 2.8, we see that
\[
\Pr \left( \text{median of \(k\) i.i.d. Cauchy\((0,1)\) random variables} \notin \left[ -\sqrt{\frac{\varepsilon}{nd_{avg}}} \cdot \sqrt{\frac{\varepsilon}{nd_{avg}}} \right] \right) \leq \delta
\]
That is, each entry of \(L^\top \Delta\) has absolute value at most \(\sigma_y \cdot \sqrt{\frac{\varepsilon}{nd_{avg}}}\). By summing across all \(p\) entries of \(L^\top \Delta\), we see that
\[
\left| \Delta^\top M \Delta \right| = \left| \Delta^\top L L^\top \Delta \right| = \|L^\top \Delta\|^2 \leq p \cdot \sigma_y^2 \cdot \frac{\varepsilon}{nd_{avg}} = \sigma_y^2 \cdot \frac{\varepsilon p}{nd_{avg}}
\]

We can now establish Condition 1 of Proposition 2.12 for CauchyEstTree.

**Lemma 4.6.** Consider Algorithm 7. Suppose the Bayesian network is a polytree. With \(m_1 \in \mathcal{O} \left( \frac{nd_{avg}d}{\varepsilon} \log \left( \frac{n}{\delta} \right) \right)\) samples, we recover coefficient estimates \(\hat{A}_1, \dot{\ldots} \hat{A}_n\) such that
\[
\Pr \left( \forall i \in [n], \Delta_i^\top M_i \Delta_i \geq \sigma_i^2 \cdot \frac{\varepsilon p_i}{nd_{avg}} \right) \leq \delta
\]
The total running time is $\mathcal{O}\left(\frac{n^2d_{avg}^2d^{-1}}{\varepsilon} \log \left(\frac{n}{\delta}\right)\right)$ where $\omega$ is the matrix multiplication exponent.

Proof. For each $i \in [n]$, apply Lemma 4.5 with $\delta' = \delta/n$ and $m_1 = \frac{8nd_{avg}}{\varepsilon} \log \left(\frac{2n}{\delta}\right)$, then take the union bound over all $n$ variables.

The runtime of Algorithm 5 is the time to find the inverse of a $p \times p$ matrix, which is $\mathcal{O}(p^\omega)$ for some $2 < \omega < 3$. Therefore, the computational complexity for a variable with $p$ parents is $\mathcal{O}(p^{\omega-1} \cdot m_1)$. Since $\max_{i \in [n]} p_i \leq d$ and $\sum_{i=1}^n p_i = nd_{avg}$, the total runtime is $\mathcal{O}(m_1 \cdot n \cdot d_{avg} \cdot d^{\omega-2})$.

We are now ready to prove Theorem 4.4.

Theorem 4.4 follows from combining the guarantees of CauchyEstTree and VarianceRecovery (given in Lemma 4.6 and Corollary 2.14 respectively) via Proposition 2.12.

Proof of Theorem 4.4. We will show sample and time complexities before giving the proof for the $d_{TV}$ distance.

Let $m_1 \in \mathcal{O}\left(\frac{nd_{avg}}{\varepsilon} \log \left(\frac{\Delta_i}{\delta}\right)\right)$ and $m_2 \in \mathcal{O}\left(\frac{d_{avg}}{\varepsilon} \log \left(\frac{n}{\delta}\right)\right)$. Then, the total number of samples needed is $m = m_1 + m_2 \in \mathcal{O}\left(\frac{nd_{avg}}{\varepsilon} \log \left(\frac{\Delta_i}{\delta}\right)\right)$. CauchyEstTree runs in $\mathcal{O}\left(\frac{n^2d_{avg}^2d^{-1}}{\varepsilon} \log \left(\frac{n}{\delta}\right)\right)$ time while VarianceRecovery runs in $\mathcal{O}\left(\frac{n^2d_{avg}^2d^{-1}}{\varepsilon} \log \left(\frac{n}{\delta}\right)\right)$ time, where $\omega$ is the matrix multiplication exponent. Therefore, the overall running time is $\mathcal{O}\left(\frac{n^2d_{avg}^2d^{-1}}{\varepsilon} \log \left(\frac{n}{\delta}\right)\right)$.

By Lemma 4.6, CauchyEstTree recovers coefficients $\hat{A}_1, \ldots, \hat{A}_n$ such that

$$\Pr\left(\forall i \in [n], |\hat{A}_i^\top \Sigma_i A_i| \geq \sigma_i^2 \cdot \frac{\varepsilon p_i}{nd_{avg}}\right) \leq \delta$$

By Corollary 2.14 and using the recovered coefficients from CauchyEstTree, VarianceRecovery recovers variance estimates $\hat{\sigma}_i^2$ such that

$$\Pr\left(\forall i \in [n], \left(1 - \sqrt{\frac{\varepsilon p_i}{nd_{avg}}}ight) \cdot \sigma_i^2 \leq \hat{\sigma}_i^2 \leq \left(1 + \sqrt{\frac{\varepsilon p_i}{nd_{avg}}}ight) \cdot \sigma_i^2\right) \geq 1 - \delta$$

As our estimated parameters satisfy Condition 1 and Condition 2, Proposition 2.12 tells us that $d_{KL}(P, Q) \leq 3\varepsilon$. Thus, $d_{TV}(P, Q) \leq \sqrt{d_{KL}(P, Q)/2} \leq \sqrt{3\varepsilon/2}$. The claim follows by setting $\varepsilon' = \sqrt{3\varepsilon/2}$ throughout.

5 Hardness for learning Gaussian Bayesian networks

In this section, we present our hardness results. We first show a tight lower-bound for the simpler case of learning Gaussian product distributions in total variation distance (Theorem 5.2). Next, we show a tight lower-bound for learning Gaussian Bayes nets with respect to total variation distance. (Theorem 5.3). In both cases, our hardness applies to the problems of learning the covariance matrix of a centered multivariate Gaussian, which is equivalent to recovering the coefficients and noises of the underlying linear structural equation.

We will need the following fact about the variation distance between multivariate Gaussians and a Frobenius norm $\|\cdot\|_F$ between the covariance matrices.

Fact 5.1 ([DMR18]). There exists two universal constants $\frac{1}{100} \leq c_1 \leq c_2 \leq \frac{3}{2}$, such that for any two covariance matrices $\Sigma_1$ and $\Sigma_2$,

$$c_1 \leq d_{TV}(N(0, \Sigma_1), N(0, \Sigma_2)) \|\Sigma_1^{1/2} \Sigma_2 - I\|_F \leq c_2.$$ 

Theorem 5.2. Given samples from a $n$-fold Gaussian product distribution $P$, learning a $\tilde{P}$ such that in $d_{TV}(P, \tilde{P}) = \mathcal{O}(\varepsilon)$ with success probability $2/3$ needs $\Omega(\sqrt{n\varepsilon^{-2}})$ samples in general.

Proof. Let $C \subseteq \{0, 1\}^n$ be a set with the following properties: 1) $|C| = 2^{\Theta(n)}$ and 2) every $i \neq j \in C$ have a Hamming distance $\Theta(n)$. Existence of such a set is well-known. We create a class of Gaussian product distributions $\mathcal{P}_C$ based on $C$ as follows. For each $s \in C$, we define a distribution $P_s \in \mathcal{P}_C$ such that if the $i$-th bit of $s$ is 0, we use the distribution $N(0, 1)$ for the $i$-th component of $P_s$; else if the $i$-th bit is 1, we use the distribution $N(0, 1 + \frac{\varepsilon}{\sqrt{n}})$. Then for any $P_s \neq P_t$, $d_{KL}(P_s, P_t) = \mathcal{O}(\varepsilon^2)$. Fano’s inequality tells us that guessing a random distribution from $\mathcal{P}_C$ correctly with $2/3$ probability needs $\Omega(n\varepsilon^{-2})$ samples.
Then, \( \text{such that learning a Gaussian Bayes net} \)
\( \text{For any} \ P \ \text{such that} \ \text{Theorem 5.3.} \)
\( \text{probability. We need the following fact about the} \)
\( N \)
\( P \)
\( define \)
\( m \)
\( pair of vertices differing in at least \( \text{largest-sized subset with any pair of distributions in the subset differing in at least} \)
\( X \)
\( \ell \)
\( \text{corresponding to the bit-pattern of} \)
\( C \)
\( \text{Hamming distance} \)
\( \text{nd} \epsilon \)
\( P \)
\( of \)
\( c \)
\( \text{choice of} \)
\( \text{for learning a random distribution} \)
\( d \)
\( \text{and guess the random distribution correctly. Hence, the lower-bound follows.} \)
\( \text{Now, we present the lower-bound for learning general Bayes nets.} \)

**Theorem 5.3.** For any \( 0 < \epsilon < 1 \) and \( n, d \) such that \( d \leq n/2 \), there exists a DAG \( G \) over \([n]\) of in-degree \( d \) such that learning a Gaussian Bayes net \( \hat{P} \) on \( G \) such that \( d_{\text{TV}}(P, \hat{P}) \leq \epsilon \) with success probability \( 2/3 \) needs \( \Omega(n d e^{-2}) \) samples in general.

Let \( C \subseteq \{0, 1\}^d \) be a set with the following properties: 1) \( |C| = 2^{\Theta(d)} \) and 2) every \( i \neq j \in C \) have a Hamming distance \( \Theta(d) \). Existence of such a set is well-known. We define a class of distributions \( \mathcal{P}_C \) based on \( C \) and the graph \( G \) shown in Fig. 1 as follows. Each vertex of each distribution in \( \mathcal{P}_C \) has a \( N(0, 1) \) noise, and hence no learning is required for the noises. Each coefficient \( a_{i \rightarrow j} \) takes one of two values \( \left\{ \frac{1}{\sqrt{d(n-d)}}, \frac{1+\epsilon}{\sqrt{d(n-d)}} \right\} \) corresponding to bits \( \{0, 1\} \) respectively. For each \( s \in C \), we define \( A_s \) to be the vector of coefficients corresponding to the bit-pattern of \( s \) as above. We have \( 2^{\Theta(d)} \) possible bit-patterns, which we use to define each conditional probability \( (X_i | X_1, X_2, \ldots, X_d) \). Then, we have a class \( \mathcal{Q}_P \) of \( |C|^{(n-d)} \) distributions for the overall Bayes net. We prune some of the distributions to get the desired subclass \( \mathcal{P}_C \subseteq \mathcal{Q}_P \), such that \( \mathcal{P}_C \) is the largest-sized subset with any pair of distributions in the subset differing in at least \( (n-d)/2 \) bit-patterns (out of \( (n-d)/2 \)) many for the \( (X_i | X_1, X_2, \ldots, X_d) \)’s.

**Claim 5.4.** \( |\mathcal{P}_C| \geq 2^{\Theta(d(n-d))} \).

**Proof.** Let \( \ell = |C| = 2^{\Theta(d)} \) and \( m = n-d \). Then, there are \( N = \ell^m \) possible coefficient-vectors/distributions in \( \mathcal{Q}_C \). We create an undirected graph \( G \) consisting of a vertex for each coefficient, and edges between any pair of vertices differing in at least \( m/2 \) bit-patterns. Note that \( G \) is \( r \)-regular for \( r = \left( \frac{m}{0.5m} \right)(\ell-1)^{0.5m} + \cdots + \left( \frac{m}{0.5m+1} \right)(\ell-1)^{0.5m+1} + \cdots + (\ell-1)^m \). Turan’s theorem says that there is a clique of size \( \alpha = (1 - \frac{r}{\ell})^{-1} \). We define \( \mathcal{P}_C \) to be the vertices of this clique.

To show that \( \alpha \) is as large as desired, it suffices to show \( N - r \leq N/2^{\Theta(dm)} \). The result follows by noting \( N - r = 1 + \binom{m}{1}(\ell-1) + \cdots + \binom{m}{m}(\ell-1)^m + \cdots + \binom{m}{0.5m}(\ell-1)^{0.5m} \leq m \cdot (4(\ell-1))^{0.5m} \).

We also get for any two distributions \( P_a, P_b \) in this model with the coefficients \( a, b \) respectively, \( d_{\text{KL}}(P_a, P_b) = \frac{1}{2} ||a - b||_2^2 \) from (1). Hence, any pair of \( \mathcal{P}_C \) has \( d_{\text{KL}} = \Theta(\epsilon^2) \). Then, Fano’s inequality tells us that given a random distribution \( P \in \mathcal{P}_C \), it needs at least \( \Omega(d(n-d)\epsilon^{-2}) \) samples to guess the correct one with \( 2/3 \) probability. We need the following fact about the \( d_{\text{TV}} \)-distance among the members of \( \mathcal{P}_C \).

**Claim 5.5.** Let \( P_a, P_b \in \mathcal{P}_C \) be two distinct distributions (i.e. \( P_a \neq P_b \)) with coefficient-vectors \( a, b \) respectively. Then, \( d_{\text{TV}}(P_a, P_b) \in \Theta(\epsilon) \).
Proof. By Pinsker’s inequality, we have $d_{\text{TV}}(P_a, P_b) \leq \Omega(\epsilon)$. Here we show $d_{\text{TV}}(P_a, P_b) \in O(\epsilon)$. Let $n-d=m$. By construction, $a$ and $b$ differ in $m' \geq m/2$ conditional probabilities. Let $a' \subseteq a, b' \subseteq b$ be the coefficient-vectors on the coordinates where they differ. Let $P_{a'}, \Sigma_{a'}$ and $P_{b'}, \Sigma_{b'}$ be the corresponding marginal distributions on $(m'+d)$ variables, and their covariance matrices. In the following, we show $||\Sigma_{a'}^{-1}\Sigma_{b'} - I||_F = O(\epsilon)$. This proves the claim from Fact 5.1.

Let $M_a = \begin{bmatrix} 0_{m' \times m'} & 0_{m' \times d} \\ A_{d \times m'} & 0_{d \times d} \end{bmatrix}$ be the adjacency matrix for $P_a$, where the sources appear last in the rows and columns and in the matrix $A$, each $A_{ij} \in \{\frac{1}{\sqrt{md}}, \frac{1+\epsilon}{\sqrt{md}}\}$ denote the coefficient from source $i$ to sink $j$. Similarly, we define $M_b$ using a coefficient matrix $B_{d \times m'}$. Let $\{A_i : 1 \leq i \leq m'\}$ and $\{B_i : 1 \leq i \leq m'\}$ denote the columns of $A$ and $B$. Then for every $i$, $A_i$ and $B_i$ differ in at least $\Theta(d)$ coordinates by construction.

By definition $\Sigma_{b'} = \begin{bmatrix} B & 0_d \\ 0_d & I_{d \times d} \end{bmatrix}$ and $\Sigma_{a'}^{-1} = \begin{bmatrix} I_{m' \times m'} & -A^T \\ -A & -I \end{bmatrix}$, where $\bullet$ corresponds to certain matrices not relevant to our discussion. Let $J = \Sigma_{a'}^{-1}\Sigma_{b'} = \begin{bmatrix} \bullet & X_{m' \times d} \\ \bullet & \bullet \end{bmatrix}$. It can be checked that $X_{ij} = (B_i(j) - A_i(j))$ for every $1 \leq i \leq m'$ and $m' + 1 \leq j \leq m' + d$. Now for every $i$, each of the $\Theta(d)$ places that $A_i$ and $B_i$ differ, $X_{ij} \in \frac{\epsilon}{\sqrt{md}}$. Hence, their total contribution in $||J-I||_F^2 = \Omega(\epsilon^2)$. 

Proof of Theorem 5.3. Consider any algorithm which learns a random distribution $P = N(0, \Sigma)$ from $P_C$ in $d_{\text{TV}}$ distance $c_1\epsilon$, for a small enough constant $c_1$. Let the learnt distribution be $\hat{P} = N(0, \hat{\Sigma})$. Then, from Fact 5.1, and triangle inequality of $d_{\text{TV}}$, only the unique distribution $P$ with $\Sigma' = \Sigma$ would satisfy $||\hat{\Sigma}^{-1}\Sigma' - I||_F \leq c_1\epsilon$ for every covariance matrix $\Sigma'$ from $P_C$, for an appropriate choice of $c_4$. This would reveal the random distribution, hence the lower-bound follows.

6 Experiments

General Setup For our experiments, we explored both polytree networks (generated using random Prüfer sequences) and $G(n, p)$ Erdős-Rényi graphs with bounded expected degrees (i.e. $p = d/n$ for some bounded degree parameter $d$) using the Python package networkx [HSSC08]. Our non-zero edge weights are uniformly drawn from the range $(-2, 1] \cup [1, 2)$. Once the graph is generated, the linear i.i.d. data $X \in \mathbb{R}^{m \times n}$ (with $n$ variables and sample size $m \in \{1000, 2000, \ldots, 5000\}$) is generated by sampling the model $X = B^T X + \eta$, where $\eta \sim N(0, I_{n \times n})$ and $B$ is a strictly upper triangular matrix. We report KL divergence between the ground truth and our learned distribution using Eq. (1), averaged over 20 random repetitions. All experiments were conducted on an Intel Core i7-9750H 2.60GHz CPU.

Algorithms The algorithms used in our experiments are as follows: Graphical Lasso [FHT08], MLE (empirical) estimator, CLIME [CLL11], LeastSquares, BatchAvgLeastSquares, BatchMedLeastSquares, CauchyEstTree, and CauchyEst. Specifically, we use BatchAvg_LS+x and BatchMed_LS+x to represent the BatchAvgLeastSquares and BatchMedLeastSquares algorithms respectively with a batch size of $p + x$ at each node, where $p$ is the number of parents of that node.

Synthetic data Fig. 2 compares the KL divergence between the ground truth and our learned distribution over 100 variables between the eight estimators mentioned above. The first three estimators are for undirected graph structure learning. For this reason, we are not using Eq. (1) but the common equation in [Duc07, page 13] for calculating the KL divergence between multivariate Gaussian distributions. Fig. 2(a) and Fig. 2(b) shows the results on ER graphs while Fig. 2(c) shows the results for random tree graphs. The performances of MLE and CLIME are very close to each other, thus are overlapped in Fig. 2(a). In figure Fig. 2(b), we take a closer look at the results from Fig. 2(a) for LeastSquares, BatchMedLeastSquares, BatchAvgLeastSquares, CauchyEstTree, and CauchyEst estimators for a clear comparison. In our experiments, we find that the latter five outperform the GLASSO, CLIME and MLE (empirical) estimators. With a degree 5 ER graph, CauchyEst performs better than CauchyEstTree, while LeastSquares performs best. In our experiments for
(a) Eight algorithms evaluated on ER graph with $d = 5$

(b) A closer look at some of the algorithms in the plot of Fig. 2(a)

(c) A closer look at some of the algorithms evaluated on random tree graphs

Figure 2: Experiment on well-conditioned uncontaminated data

our random tree graphs with in-degree 1 (see Fig. 2(c), we find that the performances between CauchyEstTree and CauchyEst are very close to each other and their plots overlap.

In our experiments, CauchyEst outperforms CauchyEstTree when the $G(n,p)$ graph is generated with a higher degree parameter $d$ (e.g. $d > 5$) and the resultant graph is unlikely to yield a polytree structure.

Real-world datasets We also evaluated our algorithms on four real Gaussian Bayesian networks from R package bnlearn [Scu09]. The ECOLI170 graph provided by [SS05] contains 46 nodes and 70 edges. The MAGIC-NIAB graph from [SHBM14] contains 44 nodes and 66 edges. The MAGIC-IRRI graph contains 64 nodes and 102 edges, and the ARTH150 [ORS07] graph contains 107 nodes and 150 edges. Experimental results in Fig. 3 show that the error for LeastSquares is smaller than CauchyEst and CauchyEstTree for all the above datasets.

Contaminated synthetic data The contaminated synthetic data is generated in the following way: we randomly choose 5% samples with 5 nodes to be contaminated from the well-conditioned data over $n = 100$ node graphs. The well-conditioned data has a $N(0, 1)$ noise for every variable, while the small proportion of the contaminated data has either $N(1000, 1)$ or Cauchy(1000, 1). In our experiments in Fig. 4 and Fig. 5, CauchyEst, CauchyEstTree, and BatchMedLeastSquares outperform BatchAvgLeastSquares and LeastSquares by a large margin. With more than 1000 samples, BatchMedLeastSquares with a batch size of $p + 20$ performs similar to CauchyEst and CauchyEstTree, but performs worse with less samples. When comparing the performance between LeastSquares and BatchAvgLeastSquares over either a random tree or a ER graph, the experiment in Fig. 4(a) based on a random tree graph shows that LeastSquares performs better than BatchAvgLeastSquares when sample size is smaller than 2000, while BatchAvgLeastSquares performs relatively better with more samples. Experiment results in Fig. 5(a) based on ER degree 5 graphs is slightly different from Fig. 4(a). In Fig. 5(a), BatchAvgLeastSquares performs better than LeastSquares by a large margin. Besides, we can also observe that the performances of CauchyEst, CauchyEstTree, and BatchMedLeastSquares are better than the above two estimators and are consistent over different types of graphs. For all five algorithms, we use the median absolute deviation for robust variance recovery [Hub04] in the contaminated case only (see Algorithm 8
This is because both LeastSquares and BatchAvgLeastSquares use the sample covariance (of the entire dataset or its batches) in the coefficient estimators for the unknown distribution. The presence of a small proportion of outliers in the data can have a large distorting influence on the sample covariance, making them sensitive to atypical observations in the data. On the contrary, our CauchyEstTree and BatchMedLeastSquares estimators are developed using the sample median and hence are resistant to outliers in the data.

Contaminated real-world datasets To test the robustness of the real data in the contaminated condition, we manually contaminate 5% samples of 5 nodes from observational data in ECOLI70 and ARTH150. The results are reported in Fig. 6 and Fig. 7. In our experiments, CauchyEst and CauchyEstTree outperforms BatchAvgLeastSquares and LeastSquares by a large margin, and therefore are stable in both contaminated and well-conditioned case. Besides, note that different from the well-conditioned case, here CauchyEstTree performs slightly better than CauchyEst. This is because the Cholesky decomposition used in CauchyEst estimator takes contaminated-data into account.
Figure 5: Experiment results on contaminated data (ER graph with Cauchy noise)

Figure 6: Ecoli70 under contaminated condition

Figure 7: Arth150 under contaminated condition
Ill-conditioned synthetic data  The ill-conditioned data is generated in the following way: we classify the node sets $V$ into either well-conditioned or ill-conditioned nodes. The well-conditioned nodes have a $N(0, 1)$ noise, while ill-conditioned nodes have a $N(0, 10^{-20})$ noise. In our experiments, we choose 3 ill-conditioned nodes over 100 nodes. Synthetic data is sampled from either a random tree or an Erdős Rényi (ER) model with an expected number of neighbors $d = 5$. Experiments over ill-conditioned Gaussian Bayesian networks through 20 random repetitions are presented in Fig. 8. For the ill-conditioned settings, we sometimes run into numerical issues when computing the Cholesky decomposition of the empirical covariance matrix $\hat{M}$ in our CauchyEst estimator. Thus, we only show the comparison results between LeastSquares, BatchAvgLeastSquares, BatchMedLeastSquares, and CauchyEstTree. Here also, the error for LeastSquares decreases faster than the other three estimators. The performance of BatchMedLeastSquares is worse than BatchAvgLeastSquares but slightly better than CauchyEstTree estimator.

Agnostic Learning  Our theoretical results treat the case that the data is realized by a distribution consistent with the given DAG. In this section, we explore learning of non-realizable inputs, so that there is a non-zero KL divergence between the input distribution $P$ and any distribution consistent with the given DAG.

We conduct agnostic learning experiments by fitting a random sub-graph of the ground truth graph. To do this, we first generate a 100-node ground truth graph $G$, either a random tree with 4 random edges removed or a random ER graph with 9 random edges removed. Our algorithm will try to fit the data from the original Bayes net on $G$ on the edited graph $G^*$. Fig. 9 reports the KL divergence learned over our five estimators. We find that BatchAvgLeastSquares estimator performs slightly better than all other estimators in both cases.

Effect of changing batch size  Next, we experiment the trade off between the batch-size (eg. batch size = $[5, 20, 100]$) and the KL-divergence of our BatchAvgLeastSquares and BatchMedLeastSquares estimators in detail. As shown in Fig. 10 and Fig. 11, when batch size increases, the results are closer.

\footnote{We use batch size up to 100 to ensure there are enough batch size from simulation data, so that either mean and median can converge.}
Figure 10: Effect of changing batch size over Batch Average

(a) ER graph, $d = 2$

(b) ER graph, $d = 5$

Figure 11: Effect of changing batch size over Batch Median (ER)

(a) ER graph, $d = 2$

(b) ER graph, $d = 5$
to the \texttt{LeastSquares} estimator. In other words, \texttt{LeastSquares} can be seen as a special case of either \texttt{BatchAvgLeastSquares} or \texttt{BatchMedLeastSquares} with one batch only. Thus, when batch size increases, the performances of \texttt{BatchAvgLeastSquares} and \texttt{BatchMedLeastSquares} are closer to the \texttt{LeastSquares} estimator. On the contrary, the \texttt{CauchyEstTree} estimator can be seen as the estimator with a batch size of $p$. Therefore, with smaller batch size (e.g. batch size $= p + 5$), \texttt{BatchAvgLeastSquares} and \texttt{BatchMedLeastSquares} performs closer to the \texttt{CauchyEstTree} estimator.

\textbf{Runtime comparison} We now give the amount of time spent by each algorithm to process a degree-5 ER graph on 100 nodes with 500 samples. \texttt{LeastSquares} algorithm takes 0.0096 seconds, \texttt{BatchAvgLeastSquares} with a batch size of $p + 20$ takes 0.0415 seconds, \texttt{BatchMedLeastSquares} with a batch size of $p + 20$ takes 0.0290 seconds, \texttt{CauchyEstTree} takes 0.6063 seconds, and \texttt{CauchyEst} takes 0.6307 seconds. The timings given above are representative of the relative running times of these algorithms across different graph sizes.

\textbf{Takeaways} In summary, the \texttt{LeastSquares} estimator performs the best among all algorithms on uncontaminated datasets (both real and synthetic) generated from Gaussian Bayesian networks. This holds even when the data is ill-conditioned. However, if a fraction of the samples are contaminated, \texttt{CauchyEst}, \texttt{CauchyEstTree} and \texttt{BatchMedLeastSquares} outperform \texttt{LeastSquares} and \texttt{BatchAvgLeastSquares} by a large margin under different noise and graph types. If the data is not generated according to the input graph (i.e., the non-realizable/agnostic learning setting), then \texttt{BatchAvgLeastSquares}, \texttt{CauchyEst}, and \texttt{CauchyEstTree} have a better tradeoff between the error and sample complexity than the other algorithms, although we do not have a formal explanation.

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A  Details on decomposition of KL divergence

In this section, we provide the full derivation of Eq. (1).
For notational convenience, we write $x$ to mean $(x_1, \ldots, x_n)$, $\pi_i(x)$ to mean the values given to parents of variable $X_i$ by $x$, and $P(x)$ to mean $P(X_1 = x_1, \ldots, X_n = x_n)$. Observe that

\[
d_{\text{KL}}(P, Q) = \int_x P(x) \log \left( \frac{P(x)}{Q(x)} \right) dx
\]

\[
= \int_x P(x) \log \left( \prod_{i=1}^n P(x_i | \pi_i(x)) \right) dx
\]

\[
= \sum_{i=1}^n \int_{x_i, \pi_i(x)} P(x_i | \pi_i(x)) \log \left( \frac{P(x_i | \pi_i(x))}{Q(x_i | \pi_i(x))} \right) dx_i d\pi_i(x)
\]

where $(*)$ is due to the Bayesian network decomposition of joint probabilities. Let us define

\[
d_{\text{CP}}(\alpha_i^*, \tilde{\alpha}_i) = \int_{x_i, \pi_i(x)} P(x_i, \pi_i(x)) \log \left( \frac{P(x_i | \pi_i(x))}{Q(x_i | \pi_i(x))} \right) dx_i d\pi_i(x)
\]

where each $\tilde{\alpha}_i$ and $\alpha_i^*$ represent the parameters that relevant to variable $X_i$ from $\tilde{\alpha}$ and $\alpha^*$ respectively. Under this notation, we can write $d_{\text{KL}}(P, Q) = \sum_{i=1}^n d_{\text{CP}}(\alpha_i^*, \tilde{\alpha}_i)$.

Fix a variable of interest $Y$ with parents $X_1, \ldots, X_p$, each with coefficient $c_i$, and variance $\sigma^2$. That is, $Y = \eta_y + \sum_{i=1}^p c_i X_i$ for some $\eta_y \sim N(0, \sigma^2)$ that is independent of $X_1, \ldots, X_p$. By denoting $X = x$ (i.e. $X_1 = x_1, \ldots, X_p = x_p$) and $c = (c_1, \ldots, c_p)$, we can write the conditional distribution density of $Y$ as

\[
Pr(y | x, c, \sigma) = \frac{1}{\sigma \sqrt{2\pi}} \exp \left( -\frac{1}{2\sigma^2} \cdot \left( y - \sum_{i=1}^p c_i X_i \right)^2 \right)
\]

We now analyze $d_{\text{CP}}(\alpha_y^*, \tilde{\alpha}_y)$ with respect to the our estimates $\tilde{\alpha}_y = (\tilde{A}, \tilde{\sigma}_y)$ and the hidden true parameters $\alpha_y^* = (A, \sigma_y)$, where $\tilde{A} = (\tilde{a}_{y-1}, \ldots, \tilde{a}_{y-p})$ and $A = (a_{y-1}, \ldots, a_{y-p})$.

With respect to variable $Y$, we see that

\[
d_{\text{CP}}(\alpha_y^*, \tilde{\alpha}_y)
\]

\[
= \int_{x,y} P(x, y) \ln \left( \frac{1}{\sigma \sqrt{2\pi}} \exp \left( -\frac{1}{2\sigma^2} \cdot (y - \sum_{i=1}^p a_{y-i} X_i)^2 \right) \right) dy dx
\]

\[
= \ln \left( \frac{\tilde{\sigma}_y}{\sigma_y} \right) - \frac{1}{2\sigma_y^2} \cdot E_{x,y} \left( y - \sum_{i=1}^p a_{y-i} X_i \right)^2 + \frac{1}{2\sigma_y^2} \cdot E_{x,y} \left( y - \sum_{i=1}^p \tilde{a}_{y-i} X_i \right)^2
\]

\[
= \ln \left( \frac{\tilde{\sigma}_y}{\sigma_y} \right) - \frac{1}{2\sigma_y^2} \cdot E_{x,y} \left( y - A^T X \right)^2 + \frac{1}{2\sigma_y^2} \cdot E_{x,y} \left( y - \tilde{A}^T X \right)^2
\]

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By defining $\Delta = \hat{A} - A$, we can see that for any instantiation of $y, X_1, \ldots, X_p$, 

$$
\left( y - \hat{A}^\top X \right)^2 = \left( y - (\Delta + A)^\top X \right)^2
$$

By definition of $\Delta$

$$
= \left( (y - A^\top X) - \Delta^\top X \right)^2
$$

$$
= \left( (y - A^\top X)^2 - 2(y - A^\top X)(\Delta^\top X) + (\Delta^\top X)^2 \right)
$$

$$
= \left( (y - A^\top X)^2 - 2(yA^\top X - A^\top X\Delta^\top X) + (\Delta^\top X)^2 \right)
$$

$$
= \left( (y - A^\top X)^2 - 2(yX^\top \Delta - A^\top XX^\top \Delta) + \Delta^\top XX^\top \Delta \right)
$$

Since $\Delta^\top X$ is just a number

Denote the covariance matrix with respect to $X_1, \ldots, X_p$ as $M \in \mathbb{R}^{p \times p}$, where $M_{i,j} = \mathbb{E}[X_iX_j]$. Then, we can further simplify $d_{\text{CP}}(\alpha^*_y, \tilde{\alpha}_y)$ as follows:

$$
d_{\text{CP}}(\alpha^*_y, \tilde{\alpha}_y) = \ln \left( \frac{\sigma_y}{\tilde{\sigma}_y} \right) - \frac{1}{2\sigma_y^2} \cdot \mathbb{E}_{x,y} \left( y - A^\top X \right)^2 + \frac{1}{2\tilde{\sigma}_y^2} \cdot \mathbb{E}_{x,y} \left( y - \tilde{A}^\top X \right)^2 \quad \text{From above}
$$

$$
= \ln \left( \frac{\sigma_y}{\tilde{\sigma}_y} \right) - \frac{1}{2\sigma_y^2} \cdot \mathbb{E}_{x,y} \left( y - A^\top X \right)^2
$$

$$
+ \frac{1}{2\tilde{\sigma}_y^2} \cdot \mathbb{E}_{x,y} \left[ (y - A^\top X)^2 - 2(yA^\top X - A^\top XX^\top \Delta) + \Delta^\top XX^\top \Delta \right] \quad \text{From above}
$$

$$
= \ln \left( \frac{\sigma_y}{\tilde{\sigma}_y} \right) - \frac{1}{2\sigma_y^2} \cdot \mathbb{E}_{x,y} \eta_y^2 + \frac{1}{2\tilde{\sigma}_y^2} \cdot \mathbb{E}_{x,y} \left[ \eta_y^2 - 2(\eta_yX^\top \Delta) + \Delta^\top XX^\top \Delta \right] \quad (\dagger)
$$

$$
= \ln \left( \frac{\sigma_y}{\tilde{\sigma}_y} \right) - \frac{1}{2\sigma_y^2} \cdot \mathbb{E}_{x,y} \eta_y^2 + \frac{1}{2\tilde{\sigma}_y^2} \cdot \left( \sigma_y^2 - 2\sigma_y^2 + \Delta^\top XX^\top \Delta \right) \quad (\ast)
$$

$$
= \ln \left( \frac{\sigma_y}{\tilde{\sigma}_y} \right) - \frac{1}{2} + \frac{\sigma_y^2 - \Delta^\top XX^\top \Delta}{2\sigma_y^2} + \frac{\Delta^\top M \Delta}{2\sigma_y^2}
$$

where $(\dagger)$ is because $y = \eta_y + A^\top X$ while $(\ast)$ is because $\eta_y \sim N(0, \sigma_y^2)$, $\mathbb{E}_{x,y} (\eta_yX^\top \Delta) = \mathbb{E}_{x,y} \eta_y \cdot \mathbb{E}_{x,y} X^\top \Delta = 0$, and $\mathbb{E}_{x,y} \Delta^\top XX^\top \Delta = \Delta^\top (\mathbb{E}_{x,y} XX^\top) \Delta = \Delta^\top M \Delta$.

In conclusion, we have

$$
d_{\text{KL}}(P, Q) = \sum_{i=1}^n d_{\text{CP}}(\alpha^*_i, \tilde{\alpha}_i) = \sum_{i=1}^n \ln \left( \frac{\alpha^*_i}{\tilde{\alpha}_i} \right) + \frac{\sigma_i^2 - \tilde{\sigma}_i^2}{2\tilde{\sigma}_i^2} + \frac{\Delta_i^\top M_i \Delta_i}{2\tilde{\sigma}_i^2} \quad (3)
$$

where $M_i$ is the covariance matrix associated with variable $X_i$, $\alpha^*_i = (A_i, \sigma_i)$ is the coefficients and variance associated with variable $X_i$, $\alpha_i = (\hat{A}_i, \tilde{\sigma}_i)$ are the estimates for $\alpha^*_i$, and $\Delta_i = \hat{A}_i - A_i$.

## B Deferring proofs

This section provides the formal proofs that were deferred in favor for readability. For convenience, we will restate the statements before proving them.

The next two lemmata, Lemma 2.6 and Lemma 2.7 are used in the proof of Lemma 3.2, which is in turn used in the proof of Theorem 3.1. We also use Lemma 2.6 in the proof of Lemma 3.5. The proof of Lemma 2.6 uses the standard result of Lemma B.1.

**Lemma B.1** ([RV09]: Theorem 6.1 and Equation 6.10 in [Wai19]). Let $\ell \geq d$ and $G \in \mathbb{R}^{\ell \times d}$ be a matrix with i.i.d. $N(0, 1)$ entries. Denote $\sigma_{\min}(G)$ as the smallest singular value of $G$. Then, for any $0 < \ell < 1$, we have

$$
\Pr \left( \sigma_{\min}(G) \geq \sqrt{\ell} (1 - t) - \sqrt{d} \right) \leq \exp \left( -\ell t^2/2 \right).
$$
Lemma 2.6. Let $G \in \mathbb{R}^{k \times d}$ be a matrix with i.i.d. $N(0, 1)$ entries. Then, for any constant $0 < c_1 < 1/2$ and $k \geq d/c_1^2$,

$$\Pr \left( \|(G^T G)^{-1}\|_{op} \leq \frac{1}{1 - 2c_1^2 k} \right) \geq 1 - \exp \left( -\frac{k c_1^2}{2} \right)$$

Proof of Lemma 2.6. Observe that $G^T G$ is symmetric, thus $(G^T G)^{-1}$ is also symmetric and the eigenvalues of $G^T G$ equal the singular values of $G^T G$. Also, note that event that $G^T G$ is singular has measure 0.\(^{16}\)

By definition of operation norm, $\|(G^T G)^{-1}\|$ equals the square root of maximum eigenvalue of

$$((G^T G)^{-1})^\top ((G^T G)^{-1}) = ((G^T G)^{-1})^2,$$

where the equality is because $(G^T G)^{-1}$ is symmetric. Since $G^T G$ is invertible, we have $\|(G^T G)^{-1}\| = 1/\|G^T G\|$, which is equal to the inverse of minimum eigenvalue $\lambda_{\min}(G^T G)$ of $G^T G$, which is in turn equal to the square of minimum singular value $\sigma_{\min}(G)$ of $G$.

Therefore, the following holds with probability at least $1 - \exp (-kc_1^2/2)$:

$$\|{(G^T G)^{-1}}\| = \frac{1}{\|G^T G\|} = \frac{1}{\lambda_{\min}(G^T G)} = \frac{1}{\sigma_{\min}^2(G)} \leq \frac{1}{\sqrt{k(1 - c_1)} - \sqrt{d}} \leq \frac{1}{(1 - 2c_1)^2 k}$$

where the second last inequality is due to Lemma B.1 and the last inequality holds when $k \geq d/c_1^2$. \(\square\)

Lemma 2.7. Let $G \in \mathbb{R}^{k \times p}$ be a matrix with i.i.d. $N(0, 1)$ entries and $\eta \in \mathbb{R}^k$ be a vector with i.i.d. $N(0, \sigma^2)$ entries, where $G$ and $\eta$ are independent. Then, for any constant $c_2 > 0$,

$$\Pr \left( \|G^T \eta\|_2 < 2\sigma c_2 \sqrt{kp} \right) \geq 1 - 2p \exp (-2k) - p \exp \left( -\frac{c_2^2}{2} \right)$$

Proof of Lemma 2.7. Let us denote $g_r \in \mathbb{R}^k$ as the $r$th row of $G$. Then, we see that $\|G^T \eta\|_2^2 = \sum_{r=1}^p (g_r, \eta)^2$. For any row $r$, we see that $(g_r, \eta) = \|\eta\|_2 \cdot (g_r, \eta/\|\eta\|_2)$. We will bound values of $\|\eta\|_2$ and $|(g_r, \eta/\|\eta\|_2)|$ separately.

It is well-known (e.g. see [JNG+19, Lemma 2]) that the norm of a Gaussian vector concentrates around its mean. So, $\Pr \left( \|\eta\|_2 \leq 2\sigma \sqrt{k} \right) \leq 2 \exp (-2k)$. Since $g_r \sim N(0, I_k)$ and $\eta$ are independent, we see that $(g_r, \eta/\|\eta\|_2) \sim N(0, 1)$. By standard Gaussian bounds, we have that $\Pr \left( \|g_r, \eta/\|\eta\|_2\| \geq c_2 \right) \leq \exp \left( -c_2^2/2 \right)$.

By applying a union bound over these two events, we see that $\|g_r, \eta/\|\eta\|_2\| \leq 2\sigma c_2 \sqrt{k}$ for any row with probability $2 \exp (-2k) + \exp (-c_2^2/2)$. The claim follows from applying a union bound over all $p$ rows. \(\square\)

Lemma 2.8. [Non-asymptotic convergence of Cauchy median] Consider a collection of $m$ i.i.d. Cauchy$(0, 1)$ random variables $X_1, \ldots, X_m$. Given a threshold $0 < \tau < 1$, we have

$$\Pr \left( \text{median} \{X_1, \ldots, X_m\} \notin [-\tau, \tau] \right) \leq 2 \exp \left( -\frac{m\tau^2}{8} \right)$$

Proof of Lemma 2.8. Let $S_{>\tau} = \sum_{i=1}^m 1_{X_i > \tau}$ be the number of values that are larger than $\tau$, where $\mathbb{E}[1_{X_i > \tau}] = \Pr(X \geq \tau)$. Similarly, let $S_{<\tau}$ be the number of values that are smaller than $-\tau$. If $S_{>\tau} < m/2$ and $S_{<\tau} < m/2$, then we see that median $\{X_1, \ldots, X_m\} \in [-\tau, \tau]$.

For a random variable $X \sim \text{Cauchy}(0, 1)$, we know that $\Pr(X \leq x) = 1/2 + \arctan(x)/\pi$. For $0 < \tau < 1$, we see that $\Pr(X \geq \tau) = 1/2 - \arctan(\tau)/\pi \leq 1/2 - \tau/4$. By additive Chernoff bounds, we see that

$$\Pr \left( S_{>\tau} \geq \frac{m}{2} \right) \leq \exp \left( -\frac{2m^2\tau^2}{16m} \right) = \exp \left( -\frac{m\tau^2}{8} \right)$$

Similarly, we have $\Pr \left( S_{<\tau} \geq m/2 \right) \leq \exp \left( -m\tau^2/8 \right)$. The claim follows from a union bound over the events $S_{>\tau} \geq m/2$ and $S_{<\tau} \geq m/2$. \(\square\)

\(^{16}\)Consider fixing all but one arbitrary entry of $G$. The event of this independent $N(0, 1)$ entry making $\det(G^T G) = 0$ has measure 0.
C Median absolute deviation

In this section, we give a pseudo-code of the well-known Median Absolute Deviation (MAD) estimator (see [Hub04] for example) which we use for the component-wise variance recovery in the contaminated setting. The scale factor, $1/\Phi^{-1}(3/4) \approx 1.4826$ below, is needed to make the estimator unbiased.

Algorithm 8 MAD: Variance recovery in the contaminated setting

1: **Input**: Contaminated samples $\{x_1, x_2, \ldots, x_m\}$ from a univariate Gaussian
2: $\mu \leftarrow$ median $\{x_1, x_2, \ldots, x_m\}$.
3: $\tilde{\sigma} \leftarrow 1.4826 \cdot \text{median}\{|x_1 - \tilde{\mu}|, |x_2 - \tilde{\mu}|, \ldots, |x_m - \tilde{\mu}|\}$.
4: **return** $\tilde{\sigma}$