Linear Polytree Structural Equation Models: Structural Learning and Inverse Correlation Estimation

Xingmei Lou¹, Yu Hu², and Xiaodong Li¹

¹Department of Statistics, University of California, Davis ²Department of Mathematics and Division of Life Science, Hong Kong University of Science and Technology

Abstract

We are interested in the problem of learning the directed acyclic graph (DAG) when data are generated from a linear structural equation model (SEM) and the causal structure can be characterized by a polytree. Specially, under both Gaussian and sub-Gaussian models, we study the sample size conditions for the well-known Chow-Liu algorithm to exactly recover the equivalence class of the polytree, which is uniquely represented by a CPDAG. We also study the error rate for the estimation of the inverse correlation matrix under such models. Our theoretical findings are illustrated by comprehensive numerical simulations, and experiments on benchmark data also demonstrate the robustness of the method when the ground truth graphical structure can only be approximated by a polytree.

Keywords. polytree, linear structural equation models, equivalence class, CPDAG, Chow-Liu algorithm, minimum spanning trees

1 Introduction

Over the past three decades, the problem of learning directed graphical models from data has received enormous amount of attention since they provide a compact and flexible way to represent the joint distribution of the data, especially when the associated graph is a directed acyclic graph (DAG). A directed graph is called a DAG if it does not contain directed cycles. DAG models are popular in practice with applications in biology, genetics, machine learning and causal inference (Sachs et al., 2005; Zhang et al., 2013; Koller and Friedman, 2009; Spirtes et al., 2000). There exists an extensive literature on learning the graph structure from data under the assumption that the graph is a DAG. For a summary, see the survey of Drton and Maathuis (2017); Heinze-Deml et al. (2018). Existing approaches generally fall into two categories, constrain-based methods (Spirtes et al., 2000; Pearl, 2009) and score-based methods (Chickering, 2002). Constraint-based methods utilize conditional independence test to determine whether there exists an edge between two nodes and then orient the edges in the graph, such that the resulting graph is compatible with the conditional independencies seen in the data. Score-based methods formulate the structure learning task as optimizing a score function based on the unknown graph and the data.

A polytree is a DAG which does not contain any cycles even if the directions of all edges are ignored. It has been popularly used in practice due to tractability in both structure learning and

inference. To the best of our knowledge, structure learning of polytree models was originally studied in Rebane and Pearl (1987), in which the skeleton of the polytree was estimated by applying the Chow-Liu algorithm (Chow and Liu, 1968) to pairwise mutual information quantities, a method that has been widely used in the literature of Markov random field to fit undirected tree models. Polytree graphical model has received a significant amount of research interests both empirically and theoretically ever since, see, e.g., Huete and de Campos (1993); Dasgupta (1999); Ouerd et al. (2004). Skeleton recovery via Chow-Liu algorithm has also been used as an initial step for fitting general DAGs; see, e.g., Cheng et al. (2002).

This paper aims to study the finite sample properties of the method proposed in Rebane and Pearl (1987) for the recovery of polytree structures. In particular, we would like to understand the sample complexity requirements for consistent recovery of the underlying polytree structure, and we intend to restrict our study to the case of linear structure equation models (SEM). Furthermore, we will also establish an upper error bound for the estimation of the inverse correlation matrix under the same models.

An important line of research that inspires our study is regarding the structure learning for tree-structured undirected graphical models, including both discrete cases (Heinemann and Globerson, 2014; Bresler et al., 2020; Netrapalli et al., 2010; Anandkumar et al., 2012b,a) and Gaussian cases (Tan et al., 2010; Tavassolipour et al., 2018; Nikolakakis et al., 2019; Katiyar et al., 2019). In particular, the sample complexity of undirected tree structure learning via Chow-Liu algorithm has been well-studied for both Ising and Gaussian models (Bresler et al., 2020; Tavassolipour et al., 2018; Nikolakakis et al., 2019), and the analysis relies crucially on the so-called "correlation decay" property over the ground truth undirected tree, and the correlation decay can be explicitly quantified by the pairwise population correlations corresponding to the edges of the underlying true tree. Based on this result and some perturbation results of pairwise sample correlations to their population counterparts, the required sample complexity for tree recovery with the Chow-Liu algorithm can be straightforwardly conducted.

In order to apply the above technical framework to study the sample complexity requirement for polytree learning, a natural question is whether we have similar correlation decay phenomenon for the polytree models. In fact, this is suggested in the seminal paper Rebane and Pearl (1987). To be concrete, under some nondegeneracy assumptions, it has been shown in Rebane and Pearl (1987) that there holds the "mutual information decay" over the skeleton of the underlying polytree. Roughly speaking, the mutual information decay is a direct implication of the well known "Data Processing Inequality" in information theory (Cover, 1999). Restricted to the very special case of Gaussian linear SEM, the mutual information decay is indeed equivalent to the property of population correlation decay.

However, to obtain some meaningful sample complexity result, we need to quantify such correlation decay explicitly as what has been done in the study of Chow-Liu algorithm for undirected tree models (Bresler et al., 2020; Tavassolipour et al., 2018; Nikolakakis et al., 2019). The mutual information decay given in Rebane and Pearl (1987) holds for general polytree models, but one can expect to further quantify such decay under more restrictive models. In fact, if we restrict the polytree model to linear SEM, by applying the well-known Wright's formula (Wright, 1960; Nowzohour et al., 2017; Foygel et al., 2012), the population correlation decay property can be quantified by the pairwise correlations corresponding to the tree edges. Note that such quantification of correlation decay holds even for non-Gaussian linear polytree SEM. This is interesting since in general mutual information decay does not directly imply population correlation decay for non-Gaussian models.

With such quantification of correlation decay over the underlying polytree skeleton, we can apply the ideas from undirected tree structure learning to establish the sample complexity requirement for polytree learning via the Chow-Liu algorithm.

The paper is organized as follows: In Section 2, we will review the concept of linear polytree SEM, the concepts of Markov equivalence and CPDAG, and the polytree learning method introduced in Rebane and Pearl (1987); In Section 3, we will first explain the phenomenon of correlation decay under linear polytree models, and then establish sample complexity requirement results for both Gaussian and sub-Gaussian cases. In addition, for the estimation of the inverse correlation matrices, an upper bound that depends on the model parameters, including the number of variables, the sample size, the maximum in-degree, and the maximum and minimum absolute correlations over the tree-skeleton, is established under the entry-wise ℓ_1 norm. We will illustrate our theoretical findings with numerical evidences in Section 4. A brief summary of our work and some potential future research will be provided in Section 5.

2 Linear Polytree Models and Learning

2.1 Linear Polytree Models

Let G = (V, E) be a directed graph with vertex set $V = \{1, 2, ..., p\}$ and edge set E. We use $i \to j \in E$ to denote that there is a directed edge from node i to node j in G. If there are no directed cycles in G, we call it a directed acyclic graph (DAG). The parent set of node j in G is denoted as $Pa(j) := \{i \in V : i \to j \in E\}$. Let $\mathbf{X} = [X_1, ..., X_p]^{\mathsf{T}}$ be a random vector where each random variable X_j corresponds to a node $j \in V$. The edge set E encodes the direct causal relationships among the variables. The random vector \mathbf{X} is said to be Markov on a DAG G if its joint density function (or mass function) $p(\mathbf{x})$ can be factorized according to G as follow.

$$p(\mathbf{x}) = \prod_{j=1}^{p} p(x_j | x_{Pa(j)}), \tag{2.1}$$

where $p(x_j|x_{Pa(j)})$ is the conditional density/probability of X_j given its parents $X_{Pa(j)} := \{X_i : i \in Pa(j)\}.$

For any DAG, if we ignore the directions of all its directed edges, the resulting undirected graph is referred to as the *skeleton* of the DAG. A polytree is a DAG whose skeleton does not possess any undirected cycles. Polytree-structured graphical models are multivariate probability distributions that are Markov on a polytree T = (V, E), which have turned out to be an important and tractable class of directed graphical models, largely because they permit fast exact inference.

One interesting fact we would like to emphasize is that tree-structured undirected graphical models (Markov random fields) can be viewed as special cases of polytree DAGs. Suppose $\mathcal{T} = (V, \mathcal{E})$ is an undirected tree. An undirected tree model is a joint distribution on X with joint pdf/pmf

$$p(\boldsymbol{x}) = \prod_{i=1}^{p} p_i(x_i) \prod_{(i,j) \in \mathcal{E}} \frac{p_{ij}(x_i, x_j)}{p_i(x_i) p_j(x_j)}.$$

Notice that if we choose any node in a tree as the root, then we can transform the undirected tree into a unique *rooted tree*, i.e., a directed tree in which each non-root node has a unique parent node.

Without loss of generality, let's choose node 1 as the root, and let T = (V, E) be the resulting rooted tree, which implies that \mathcal{E} is the skeleton of E. Then we can rewrite the joint pdf/pmf as

$$p(\mathbf{x}) = p_1(x_1) \prod_{i=2}^{p} p_i(x_i) \frac{p_{iPa(i)}(x_i, x_{Pa(i)})}{p_i(x_i) p_{Pa(i)}(x_{Pa(i)})}$$

$$= p_1(x_1) \prod_{i=2}^{p} \frac{p_{iPa(i)}(x_i, x_{Pa(i)})}{p_{Pa(i)}(x_{Pa(i)})}$$

$$= \prod_{j=1}^{p} p(x_j | x_{Pa(j)}),$$

which is the DAG model with the rooted tree T = (V, E).

Throughout this work, we restrict our discussion to an important subclass of DAGs: linear structure equation models (SEM), in which the dependence of each X_j on its parents is linear with an additive noise. The parameterization of the linear SEM with directed graph G = (V, E) would be

$$X_j = \sum_{i=1}^p \beta_{ij} X_i + \epsilon_j = \sum_{i \in Pa(j)} \beta_{ij} X_i + \epsilon_j, \quad j = 1, \dots, p.$$

where $\beta_{ij} \neq 0$ if and only if $i \to j \in E$, and all ϵ_j are independent with mean zero, usually with different variances. Here we don't specify the distributional requirements on the independent noises, but in our theoretical analysis we will discuss two important cases: Gaussian noises and sub-Gaussian noises. Let $\mathbf{B} = ((\beta_{ij})) \in \mathbb{R}^{p \times p}$ and $\mathbf{\epsilon} = [\epsilon_1, \dots, \epsilon_p]^{\top}$. Then the SEM can be represented as

$$X = B^{\top}X + \epsilon. \tag{2.2}$$

Denote $Cov(X) = \Sigma = ((\sigma_{ij}))$ and $Cov(\epsilon) = \Omega = Diag((\omega_{jj}))$. Notice that Ω is diagonal since all additional noises are assumed to be mutually independent.

Under the linear SEM (2.2), a natural question is how to represent the covariance structure of X by B and Ω . Notice that we first have $(I - B)^{\top}X = \epsilon$. The assumption that G is a DAG implies that B is permutationally similar to an upper triangular matrix. This implies that all eigenvalues of I - B are 1's and I - B is thereby invertible. Therefore, we can represent the vector of node variables by that of noise in that

$$X = (I - B)^{-\top} \epsilon, \tag{2.3}$$

which implies that X is mean-zero. This further characterizes the relationship between the covariance structure of X and that of the additional noises ϵ :

$$\Sigma = (I - B)^{-\top} \Omega (I - B)^{-1}. \tag{2.4}$$

If the DAG is a polytree T = (V, E), we refer to this linear SEM as a linear polytree model. If we further assume that the noises ϵ_i 's are Gaussian, then the linear polytree model is referred to as a Gaussian linear polytree model. Recall that we have explained that undirected tree model can be viewed as a special case of polytree model by transforming the undirected tree into a rooted tree. In the Gaussian regime, any tree-structure Gaussian undirected graphical model is equivalent to a Gaussian linear polytree by the same transformation. We don't give a detailed derivation here.

2.2 Markov equivalence and CPDAG

Let's briefly review the concept of Markov equivalence of DAGs. In fact, there are several equivalent definitions for this concept. The most intuitive definition is perhaps the following: if any joint distribution p(x) that can be factorized according to G_1 as in Eq. (2.1), can also be factorized according to G_2 , and vice versa, then we say G_1 and G_2 are Markov equivalent. Another intuitive definition is from the concept of conditional independence. In fact, each DAG G entails a list of statements of conditional independence, which are satisfied by any joint distribution factorized to G. Then two DAGs are equivalent if they entail the same list of conditional independencies.

It is interesting that the concept of Markov equivalence can be characterized under the regime of zero-mean Gaussian linear structural equation models. Notice that each zero-mean multivariate normal distribution is uniquely determined by its population covariance matrix. Therefore, the class of zero-mean multivariate normal distributions factorized to a DAG G can be characterized by the set of covariance matrices

$$\Sigma(G) := \{ (I - B)^{-\top} \Omega (I - B)^{-1} : \forall (B, \Omega) \text{ s.t. } \Omega \in \text{diag}^+, \text{supp}(B) \subseteq \text{supp}(B_G) \}$$

where diag⁺ is the set of diagonal matrices with positive diagonal entries, \mathbf{B}_G is the binary adjacency matrix of G, and supp $(\mathbf{B}) := \{(i, j) : B_{ij} \neq 0\}$. It has recently been shown in Ghassami et al. (2020) (Proposition 1) that two DAGs G_1 and G_2 are Markov equivalent if and only if $\Sigma(G_1) = \Sigma(G_2)$.

In the present paper, the recovery of equivalence class of DAGs hinges on the following famous and neat result given in Verma and Pearl (1991): Two DAGs are Markov equivalent if and only if they have the same skeleton and sets of v-structures, where a v-structure is a node triplet $i \to k \leftarrow j$ where i and j are nonadjacent.

The above result implies directly that for a DAG G, any DAG G' equivalent to G will have the same skeleton, and if $i \to k \leftarrow j$ is a v-structure in G, it must be a v-structure in G'. Then this raises the question that how to determine all of the directed edges that remain the same in all DAGs equivalent to G. This leads to the concept of completed partially DAG (CPDAG): a graph K with both directed and undirected edges representing the Markov equivalence class of a DAG G if: (1) K and G have the same skeleton; (2) K contains a directed edge $i \to j$ if and only if any DAG G' that is Markov equivalent to G contains the same directed edge $i \to j$.

By the definition of CPDAG, we know that we can only hope to identify the CPDAG of a DAG G given a joint distribution that is Markov on G. An interesting result in Meek (1995) guarantees that the CPDAG of G can be efficiently recovered as long as we can determine the skeleton and all the v-structures. More concretely, after determining the skeleton and all v-structures of G, its CPDAG can be recovered by iteratively conducting four orientation propagation rules that have been introduced in Verma and Pearl (1992). In the case of polytrees, it turns out that only the first rule is needed, while the other three rules don't apply. We will elaborate on the first rule in Section 2.3.

It would be interesting to have some intuitions on what the CPDAG of a polytree looks like. To this end, we introduce the following result:

Theorem 2.1. The undirected subgraph containing undirected edges of the CPDAG of a polytree forms a forest. All equivalent DAGs can be obtained by orienting each undirected tree of the forest into a rooted tree, that is, by selecting any node as the root and setting all edges going away from it.

Proof. Each connected component of the undirected edges is a subgraph of the polytree G's skeleton, thus is a tree. If a node of the tree also has directed edges, they must be outgoing according to

Line 6 of Algorithm 2 (Rule 1 in Meek (1995)). This means that when we convert each undirected tree into a rooted tree, it does not create any additional v-structures in the resulting DAG G'. So the original CPDAG is also the CPDAG of G', i.e., G' is equivalent to G. On the other hand, if G' is an equivalent DAG, for each undirected tree T in the CPDAG, let i be a source node of T according to G'. Then T in G' must be a rooted tree with i being the root to avoid having v-structures within T (and hence contradicting with G' shares the same CPDAG). This shows that all equivalent class members can be obtained by orienting undirected trees into rooted trees and completes the proof.

2.3 Polytree learning

A major purpose of this paper is to study the problem of polytree learning, i.e., the recovery of the CPDAG of the polytree T = (V, E) under the linear SEM (2.2) from a finite sample of observations. To be concrete, suppose that we have observed i.i.d. samples $\boldsymbol{X}^{(1)}, \ldots, \boldsymbol{X}^{(n)}$ generated according to the linear SEM (2.2), where the parameter matrix \boldsymbol{B} is compatible to a polytree T = (V, E). We aim to consistently recover the CPDAG of the underlying polytree T, denoted as CPDAG(T), from the data matrix $\boldsymbol{X}^{(1:n)} = [\boldsymbol{X}^{(1)}, \ldots, \boldsymbol{X}^{(n)}]^{\top} \in \mathbb{R}^{n \times p}$.

The procedure of polytree learning we are considering in this paper has been in principle introduced in Rebane and Pearl (1987), and similar methods have also been discussed in some follow-up works, e.g., Ouerd et al. (2004). The key idea is to first recover the skeleton of the polytree by applying the Chow-Liu algorithm (Chow and Liu, 1968) to the pairwise sample correlations of the data matrix, which had been used in undirected tree structured graphical models. After the skeleton is recovered, the set of all v-structures can be correctly identified via a simple thresholding approach to pairwise sample correlations. Finally, the CPDAG can be found by applying Rule 1 introduced in Verma and Pearl (1992), as guaranteed in Meek (1995).

2.3.1 Chow-Liu algorithm for finding the skeleton

To the best of our knowledge, it was first proposed in Rebane and Pearl (1987) to recover the skeleton of a polytree by applying the Chow-Liu algorithm introduced in Chow and Liu (1968) for undirected tree graphical models. Notice that given we are interested in linear polytree models without modeling the joint distribution parametrically, we directly apply the Chow-Liu algorithm to the sample correlations, while the standard Chow-Liu algorithm is usually applied to estimates of pairwise mutual information quantities. The Chow-Liu tree associated to pairwise correlations, which is the estimated skeleton of the underlying polytree, is defined as below.

Definition 1 (Chow-Liu tree associated to pairwise sample correlations). Consider the linear polytree model (2.2) associated to a polytree T = (V, E), whose skeleton is denoted as T = (V, E). Let \mathbb{T}_p denote the set of undirected trees over p nodes. Given n i.i.d. samples $\mathbf{X}^{(1:n)} = [\mathbf{X}^{(1)}, \dots, \mathbf{X}^{(n)}]^{\top} \in \mathbb{R}^{n \times p}$, we obtain the sample correlation $\hat{\rho}_{ij}$ between X_i and X_j for all $1 \le i < j \le p$. The Chow-Liu tree associated to the pairwise sample correlations is defined as the maximum-weight spanning tree over the p nodes where the weights are absolute values of sample correlations:

$$\mathcal{T}^{CL} = \underset{\mathcal{T}=(V,\mathcal{E})\in\mathbb{T}_p}{\operatorname{arg max}} \sum_{i-j\in\mathcal{E}} |\hat{\rho}_{ij}|. \tag{2.5}$$

For tree-structured undirected graphical models, it has been established in Chow and Liu (1968)

that the maximum likelihood estimation of the underlying tree structure is the Chow-Liu tree associated to the empirical mutual information quantities (which are used to find the maximum-weight spanning tree). Under the assumption of multivariate normality, the Chow-Liu tree associated to empirical mutual information quantities is the same as the one associated with pairwise sample correlations. The rationale of applying Chow-Liu algorithm to polytree learning has been carefully explained in Rebane and Pearl (1987), to which interested readers are referred. The step of skeleton recovery can be summarized in Algorithm 1.

Algorithm 1 Chow-Liu algorithm

Input: n i.i.d. samples $X^{(1:n)}$ Output: Estimated skeleton \widehat{T} .

- 1: Compute the pairwise sample correlations $\hat{\rho}_{ij}$ for all $1 \leq i < j \leq p$;
- 2: Construct a maximum-weight spanning tree using $|\hat{\rho}_{ij}|$ as the edge weights, i.e., $\hat{\mathcal{T}} = \mathcal{T}^{CL}$ defined in (2.5).

It is noteworthy that Algorithm 1 can be implemented efficiently by applying the Kruskal's algorithm [Kruskal (1956)] to pairwise sample correlations $|\hat{\rho}_{ij}|$ for the construction of maximum-weight spanning tree. The computational complexity is for Kruskal's algorithm is known to be $O(p^2 \log p)$, which is generally no larger than that for computing the sample correlations, which is $O(p^2 n)$.

2.3.2 Extending the skeleton to the equivalence class

In the second part of the procedure of polytree learning, we aim to extend the estimated skeleton $\hat{T} = T^{CL}$ to an estimated CPDAG of the underlying polytree T. Intuitively speaking, this amounts to figuring out all the edges whose orientations can be determined.

The first step of this part is to identify all the v-structures. Notice that in the linear polytree model (2.2), we assume that $\beta_{ij} \neq 0$ if and only if $i \to j \in E$, which implies the non-degeneracy of the polytree. It has also been observed in Rebane and Pearl (1987) that, for any pair of nonadjacent nodes i and j with common neighbor k, they form a v-structure $i \to k \leftarrow j$ if and only X_i and X_j are mutually independent. Interestingly, the criterion of mutual independence can be replaced with zero correlation under the linear polytree model, even if the noises are non-Gaussian. The details will be deferred to Section 3. Then, we can determine the existence of a v-structure $i \to k \leftarrow j$ when the sample correlation $|\hat{\rho}_{ij}| < \rho_{cirt}$. The discussion on the practical choice of ρ_{cirt} is deferred to Section 4. Theoretical discussions on the threshold will be discussed in Section 3.

After recovering all the v-structures, as aforementioned, it is guaranteed in Meek (1995) that the CPDAG of the polytree can be recovered by iteratively applying the four rules originally introduced in Verma and Pearl (1992). However, given our discussion is restricted to the polytree models, Rules 2, 3, and 4 in Verma and Pearl (1992) and Meek (1995) do not apply. We only need to apply Rule 1 repeatedly. This rule can be stated as follows: Orient any undirected edge j - k into $j \to k$ whenever there is a directed edge $i \to j$ from a third node i.

These two steps in the second part of polytree structure learning are summarized as Algorithm 2.

Algorithm 2 Extending the skeleton to a CPDAG

Input: Estimated skeleton \hat{S} , sample correlations $\hat{\rho}_{ij}$'s, critical value for correlation ρ_{crit} Output: Estimated CPDAG \hat{C}

1: for Each pair of nonadjacent variables i, j with common neighbor k do

- 2: if $|\hat{\rho}_{ij}| < \rho_{crit}$ then
- 3: replace i-k-j in \hat{S} by $i \to k \leftarrow j$
- 4: end if
- 5: end for
- 6: In the resulting graph, orient as many undirected edges as possible by repeatedly applying the rule: orient an undirected edge j-k into $j\to k$ whenever there is a directed edge $i\to j$ for some i.

3 Main Results

3.1 Wright's formula and correlation decay on polytrees

In principle, the equality (2.4) suggests that we can represent the entries of Σ by (β_{ij}) and (ω_{ii}) . In fact, this can be conveniently achieved by using the Wright's path tracing formula [Wright (1960)]. We first introduce some necessary definitions in order to obtain such expression. A trek from node i to node j in a directed graph G = (V, E) is a sequence of non-colliding consecutive edges beginning at i and ending in j. In other words, a trek τ from node i to node j is of the form

$$i = v_l^L \leftarrow v_{l-1}^L \leftarrow \cdots \leftarrow v_1^L \leftarrow v_0 \rightarrow v_1^R \rightarrow \cdots \rightarrow v_{r-1}^R \rightarrow v_r^R = j.$$

We define the left-hand side of τ as $Left(\tau) = v_l^L \leftarrow \cdots \leftarrow v_0$, the right-hand side of τ as $Right(\tau) = v_0 \rightarrow \cdots \rightarrow v_r^R$ (note l or r can be 0) and the head of τ as $H_{\tau} = v_0$. A trek τ is said to be a $simple\ trek$ if $Left(\tau)$ and $Right(\tau)$ do not have common edges.

Denoting the sets of simple treks

$$S^{ij} = \{ \tau : \tau \text{ is a simple trek from } i \text{ to } j \text{ in } G \},$$

the following rules (Wright, 1960; Nowzohour et al., 2017; Foygel et al., 2012) express the off-diagonal entries of the covariance matrix Σ as a summation over treks.

$$\sigma_{ij} = \sum_{\tau \in \mathcal{S}^{ij}} \sigma_{H_{\tau}H_{\tau}} \prod_{s \to t \in \tau} \beta_{st} \qquad (i \neq j).$$

Our approach to learning the structure of a polytree, which has been introduced in Section 2.3, depends solely on the marginal correlation coefficients, and is thereby invariant to scaling. Therefore, without loss of generality, we can assume that X_j 's have unit variance for all $j \in V$, i.e. Σ is the correlation matrix. It is obvious that the standardized version of a linear SEM is still a linear SEM. In fact, let D be the diagonal matrix with the j-th diagonal being the standard deviation of X_j . Then the standardized random variables are $D^{-1}X$, which satisfies

$$\boldsymbol{D}^{-1}\boldsymbol{X} = (\boldsymbol{D}\boldsymbol{B}\boldsymbol{D}^{-1})^{\top}\boldsymbol{D}^{-1}\boldsymbol{X} + \boldsymbol{D}^{-1}\boldsymbol{\epsilon}. \tag{3.1}$$

In other words, the standardized random variables admit a linear SEM with the coefficient matrix $\tilde{B} = DBD^{-1}$ and the diagonal noise variance matrix $\tilde{\Omega} = D^{-1}\Omega D^{-1} = D^{-2}\Omega$. One should notice that \tilde{B} and B follow from the same DAG.

Now let us simplify the above trek rules under the linear polytree models with standardized variables. Notice that in a polytree model, any two nodes i and j are connected by a unique simple trek if and only if i and j have common ancestors¹, otherwise, there is no simple trek connecting them. As a direct consequence of the trek rules introduced before, we have the following result.

Lemma 3.1. Consider the linear polytree model (2.2) with the associated polytree T = (V, E) over p nodes, i.e., $\beta_{ij} \neq 0$ if and only if $i \rightarrow j \in E$. Also assume that X_j has unit variance for all $j \in V$. Then, given $\{\beta_{ij}\}_{1 \leq i,j \leq p}$, we have the following results regarding the entries of Σ and Ω :

(1) The off-diagonal entries of Σ are given by

$$\sigma_{ij} = \begin{cases} \prod_{s \to t \in \tau_{ij}} \beta_{st} & \text{if } i \text{ and } j \text{ have common ancestors;} \\ 0 & \text{otherwise,} \end{cases}$$
(3.2)

where τ_{ij} is the simple trek connecting node i and node j when i and j have common ancestors.

(2) The diagonal entries of Ω are given by

$$\omega_{jj} = 1 - \sum_{i \in Pa(j)} \beta_{ij}^2, \quad j = 1, \dots, p.$$
 (3.3)

Remark 1. Here Eq. (3.3) can be derived by the following simple argument: Since T is a polytree, all variables in Pa(j) are independent and are also independent with ϵ_j . Evaluating the variance on both sides of $X_j = \sum_{i \in Pa(j)} \beta_{ij} X_i + \epsilon_j$ leads to the desired identity.

Notice that if $i \to j \in E$ (or $j \to i \in E$), we know that i and j have common ancestors, and the simple trek connecting them is the directed edge. Then Lemma 3.1 implies that $\sigma_{ij} = \operatorname{corr}(X_i, X_j) = \beta_{ij}$ (or β_{ji}). Let's use the traditional notations to denote the pairwise correlations as $\rho_{ij} := \operatorname{corr}(X_i, X_j)$, and under the assumption of unit variances we actually have $\rho_{ij} = \sigma_{ij} = \beta_{ij}$ (or β_{ji}). Then Lemma 3.1 implies the following corollary.

Corollary 3.2. Consider the linear polytree model (2.2) with the associated polytree T = (V, E) over p nodes. The pairwise population correlation coefficients satisfy that

$$\rho_{ij} = \begin{cases} \prod_{s \to t \in \tau_{ij}} \rho_{st} & \text{if } i \text{ and } j \text{ have common ancestors} \\ 0 & \text{otherwise.} \end{cases}$$
(3.4)

Remark 2. We need to emphasize that in this corollary we don't need to assume that the variables X_1, \ldots, X_p have unit variances. One can simply use (3.1) to standardize the linear polytree and then obtain (3.4), which still holds for the original linear SEM since correlation coefficients are invariant under standardization.

¹We denote by $An(j) := \{i : \exists \text{ directed path from } i \text{ to } j \text{ in } G\} \cup \{j\} \text{ the set of ancestors of node } j, \text{ so } An(j) \text{ includes } j.$

Recall that in Section 2.1, we have explained that any undirected tree-structured Gaussian graphical model can be transformed into a linear polytree SEM by selecting any node as a root. Under this transformation, any two nodes are connected by a simple trek since there are no colliding edges. Then Eq. (3.4) becomes

$$\rho_{ij} = \prod_{s \to t \in \tau_{ij}} \rho_{st}, \quad \forall i \neq j.$$

This is exactly the correlation decay relationship used in the literature to study the sample complexity for undirected tree structure learning, see, e.g. Nikolakakis et al. (2019); Tavassolipour et al. (2018); Bresler et al. (2020). We aim to apply the similar techniques to analyze the sample complexity requirement for linear polytree learning.

For the convenience of quantifying the correlation decay rates, we make the following assumptions:

Assumption 1. There exist positive ρ_{\min} and ρ_{\max} such that

$$0 < \rho_{\min} \le |\rho_{ij}| \le \rho_{\max} < 1, \quad \forall i \to j \in E.$$

Under Assumption 1, we see that a polytree-structured model satisfies correlation decay as a direct consequence of Eq. (3.4), i.e., the correlation between any two nonadjacent variables X_i and X_j is strictly smaller than the correlation between any two consecutive variables on the simple path between X_i and X_j in terms of absolute value.

It is noteworthy that we do not assume that ρ_{\min} and ρ_{\max} are independent of n or p. In fact, ρ_{\min} is generally vanishing when p is large. More specifically, the second part of Lemma 3.1 gives rise to the following relationship between the noise variance and the correlation coefficients with parents for each node: $\sum_{i \in Pa(j)} \rho_{ij}^2 < 1$, which further implies the following corollary.

Corollary 3.3. Let d_* represent the highest in-degree for a polytree. Then,

$$\rho_{\min} < \frac{1}{\sqrt{d_*}}.$$

In contrast, it is reasonable to assume ρ_{\min} to be a positive constant independent of p under the undirected tree-structured Gaussian graphical model, since after transforming it to a rooted tree as in Section 2.1, the highest in-degree satisfies $d_* = 1$.

3.2 Gaussian case

We now introduce our major results on the recovery of polytree structures, with focus on the sample complexity analysis. The discussion in this subsection will be restricted to the Gaussian case, and this assumption is relaxed to sub-Gaussian in the next subsection.

Throughout this subsection, the discussion is based on the linear polytree SEM (2.2) with the associated polytree T = (V, E), for which Corollary 3.2 holds. We also assume that Assumption 1 holds. The additional assumption on Gaussianity can be simply imposed on the noise variables as follows.

Assumption 2. Under the linear polytree SEM (2.2), we assume that $\epsilon_1, \ldots, \epsilon_p$ are independent Gaussian random variables, i.e., $\epsilon_j \sim \mathcal{N}(0, \omega_{jj})$ for $j = 1, \ldots, p$.

In linear SEM, we always assume that the noise variables are independent. Then by $X = (I - B)^{-\top} \epsilon$, we know that X is also multivariate Gaussian. This fact will help quantify the discrepancy between population and sample pairwise correlations:

Lemma 3.4 (Kalisch and Bühlman (2007), Lemma 1). Consider the linear polytree SEM (2.2) with Assumptions 1 and 2 satisfied. For any $0 < \gamma \le 2$, there holds

$$\sup_{i \neq j} \mathbb{P}(|\hat{\rho}_{ij} - \rho_{ij}| \ge \gamma) \le C_1(n-2) \exp\left((n-4)\log\left(\frac{4-\gamma^2}{4+\gamma^2}\right)\right),\,$$

where $C_1 = \frac{(1-\rho_{\min}^2)^{3/2}(3-\rho_{\max})}{(1-\rho_{\max})^{7/2}}$. This further implies that

$$\mathbb{P}\left(\bigcap_{1\leq i< j\leq p} \{|\hat{\rho}_{ij} - \rho_{ij}| < \gamma\}\right) \geq 1 - C_1\binom{p}{2}(n-2)\exp\left((n-4)\log\left(\frac{4-\gamma^2}{4+\gamma^2}\right)\right).$$

3.2.1 Skeleton Recovery

With Corollary 3.2 and Lemma 3.4, we are ready to prove the sample complexity requirement for the tree-skeleton recovery. The proof is standard in the literature of undirected tree structure learning, e.g., Nikolakakis et al. (2019); Tavassolipour et al. (2018); Bresler et al. (2020), but we will give a self-contained proof in this paper. The crux for the proof is the following result regarding the exact recovery of tree skeleton by Chow-Liu algorithm provided the sample correlation decay over the tree.

Lemma 3.5 (e.g. Bresler et al. (2020), Lemma 6.1 and Lemma 8.8). Let \mathcal{T} be the skeleton of true polytree T = (V, E) and $\widehat{\mathcal{T}}$ be the estimated tree through Chow-Liu algorithm (2.5). If an edge $(w, \tilde{w}) \in \mathcal{T}$ and $(w, \tilde{w}) \notin \widehat{\mathcal{T}}$, i.e. this edge is incorrectly missed, then there exists an edge $(v, \tilde{v}) \in \widehat{\mathcal{T}}$ and $(v, \tilde{v}) \notin \mathcal{T}$ such that $(w, \tilde{w}) \in \operatorname{path}_{\mathcal{T}}(v, \tilde{v})$ and $(v, \tilde{v}) \in \operatorname{path}_{\widehat{\mathcal{T}}}(w, \tilde{w})$. On such an error event, we have $|\hat{\rho}_{v\tilde{v}}| \geq |\hat{\rho}_{w\tilde{w}}|$.

Theorem 3.6. Consider the linear polytree SEM (2.2) with Assumptions 1 and 2 satisfied. Let $\widehat{\mathcal{T}}(\mathbf{X}^{(1:n)})$ denote the estimated skeleton from the Chow-Liu algorithm (2.5) and \mathcal{T} denote the true skeleton from the polytree T. For any $\delta \in (0,1)$, we have

$$\mathbb{P}(\widehat{\mathcal{T}}(\boldsymbol{X}^{(1:n)}) \neq \mathcal{T}) < \delta$$

provided

$$\frac{n-4}{\frac{2}{\gamma^2} + \frac{1}{2}} - \log n > \log \frac{3p^2}{2\delta(1-\rho_{\text{max}})^{7/2}}$$
(3.5)

where $\gamma = \rho_{\min}(1 - \rho_{\max})/2$.

Remark 3. The above condition implies some dependence of the sample size on the maximum in-degree d_* . In fact, together with Corollary 3.3, the sample size condition is essentially $n \geq O(d_* \log(p/\sqrt{\delta}))$ if we further assume that ρ_{\max} is controlled well beyond 1.

Proof. With $\gamma = \rho_{\min}(1 - \rho_{\max})/2$, consider the event

$$E = \bigcap_{1 \le i < j \le p} \{ |\hat{\rho}_{ij} - \rho_{ij}| < \gamma \}.$$

By Lemma 3.4, we have

$$\mathbb{P}(E) \ge 1 - C_1 \binom{p}{2} (n-2) \exp\left((n-4) \log\left(\frac{4-\gamma^2}{4+\gamma^2}\right)\right),$$

where $C_1 = \frac{(1-\rho_{\min}^2)^{3/2}(3-\rho_{\max})}{(1-\rho_{\max})^{7/2}}$.

Consider any undirected edge $(w, \tilde{w}) \in \mathcal{T}$ and any nonadjacent pair (v, \tilde{v}) such that $(w, \tilde{w}) \in path_{\mathcal{T}}(v, \tilde{v})$. According to Corollary 3.2, there are two possible cases. If $path_{S_T}(v, \tilde{v})$ corresponds to a simple trek in the polytree T, then $\rho_{v\tilde{v}}$ consists of the product among several correlation coefficients containing $\rho_{w\tilde{w}}$. Hence $|\rho_{v\tilde{v}}| \leq |\rho_{w\tilde{w}}|\rho_{\max}$ by Assumption 1. On the contrary, if $path_{\mathcal{T}}(v, \tilde{v})$ is not a simple trek in T, then we have $\rho_{v\tilde{v}} = 0$. Overall, we can obtain an upper bound for $|\rho_{v\tilde{v}}| - |\rho_{w\tilde{w}}|$.

$$|\rho_{v\tilde{v}}| - |\rho_{w\tilde{w}}| \le |\rho_{w\tilde{w}}|(\rho_{\max} - 1) \le \rho_{\min}(\rho_{\max} - 1). \tag{3.6}$$

Under the event E, the triangular inequality gives that

$$|\hat{\rho}_{v\tilde{v}}| - |\hat{\rho}_{w\tilde{w}}| = |\hat{\rho}_{v\tilde{v}}| - |\rho_{v\tilde{v}}| + |\rho_{v\tilde{v}}| - |\rho_{w\tilde{w}}| - (|\hat{\rho}_{w\tilde{w}}| - |\rho_{w\tilde{w}}|)$$

$$\leq |\hat{\rho}_{v\tilde{v}} - \rho_{v\tilde{v}}| + |\hat{\rho}_{w\tilde{w}} - \rho_{w\tilde{w}}| + |\rho_{v\tilde{v}}| - |\rho_{w\tilde{w}}|$$

$$< 2\gamma + \rho_{\min}(\rho_{\max} - 1) = 0.$$
(3.7)

Notice that this holds uniformly for any undirected edge $(w, \tilde{w}) \in \mathcal{T}$ and any nonadjacent pair (v, \tilde{v}) such that $(w, \tilde{w}) \in path_{\mathcal{T}}(v, \tilde{v})$.

Under the event $\widehat{\mathcal{T}}(X^{(1:n)}) \neq \mathcal{T}$, by Lemma 3.5, we know there is an edge $(w, \tilde{w}) \in \mathcal{T}$ and a nonadjacent pair (v, \tilde{v}) , such that $(w, \tilde{w}) \in path_{\mathcal{T}}(v, \tilde{v})$ while $|\hat{\rho}_{v\tilde{v}}| \geq |\hat{\rho}_{w\tilde{w}}|$. Then we have

$$E \subset {\widehat{\mathcal{T}}(\boldsymbol{X}^{(1:n)}) = \mathcal{T}}.$$

It suffices to study the tail probability of E, which satisfies

$$C_1(n-2)\exp\left((n-4)\log\left(\frac{4-\gamma^2}{4+\gamma^2}\right)\right)\binom{p}{2} \le C_1\exp\left((n-4)\log\left(\frac{4-\gamma^2}{4+\gamma^2}\right)\right)\frac{np^2}{2}.$$

Then we have $\mathbb{P}(E) < \delta$ by requiring the sample size to satisfy

$$n > \log \left(\frac{(1 - \rho_{\min}^2)^{3/2} (3 - \rho_{\max}) n p^2}{2(1 - \rho_{\max})^{7/2} \delta} \right) / \log \left(\frac{4 + \gamma^2}{4 - \gamma^2} \right) + 4.$$

This condition can be implied by the sample complexity condition (3.5) by the equality $\log(1+x) \ge \frac{x}{1+x}$ for any positive x.

3.2.2 Implication in Tree-structured Undirected Gaussian Graphical Models

As we discussed in Section 2.1, tree-structured undirected Gaussian graphical models can be viewed as special cases of Gaussian linear polytree SEM, where the polytree is actually a rooted tree, so it is permissible to assume that $\rho_{\min} = \Omega(1)$ and $1 - \rho_{\max} = \Omega(1)$. In this case, Theorem 3.6 gives a sample complexity result for structural learning of undirected tree-structured Gaussian graphical model. In fact, for undirected Gaussian tree models, structural learning by directly applying the Chow-Liu algorithm to sample correlations has been studied in a recent work (Nikolakakis et al., 2019), and their result is compatible to ours. In fact, our result is a bit better than theirs, since the sufficient number of samples therein is $n = O(\log^4(p/\delta))$, while ours is $n = O(\log(p/\sqrt{\delta}))$.

3.2.3 CPDAG Recovery

As described in Section 2.3.2, after obtaining the estimated skeleton, the next step is to identify all v-structures by comparing ρ_{ij} for all node triplets i-k-j in the skeleton with a threshold ρ_{crit} . Then the orientation propagation rule described in Algorithm 2 can be applied iteratively to orient as many undirected edges as possible. If both the skeleton and v-structures are correctly identified, the orientation rule will be able to recover the true CPDAG, i.e. equivalence class [Meek (1995)].

Theorem 3.7. Consider the Gaussian linear polytree SEM (2.2) with Assumptions 1 and 2 satisfied. Denote by $\hat{C}(\mathbf{X}^{(1:n)})$ the estimated CPDAG from the entire algorithm in Sections 2.3.1 and 2.3.2 with the threshold ρ_{crit} , and by C_T the true CPDAG from the polytree T. Denote $\gamma' = \min\left\{\frac{\rho_{\min}}{3}, \frac{1-\rho_{\max}}{2}\right\}\rho_{\min}$. For any $\delta \in (0,1)$, on an event with probability at least $1-\delta$, we have

$$|\hat{\rho}_{ij} - \rho_{ij}| < \gamma' \quad \forall i < j,$$

and

$$\mathbb{P}(\hat{C}(\boldsymbol{X}^{(1:n)}) \neq C_T) < \delta,$$

provided

C1
$$\gamma' < \rho_{crit} < \rho_{\min}^2 - \gamma';$$

$$C2 \frac{n-4}{\frac{2}{\gamma'^2} + \frac{1}{2}} - \log n > \log \frac{3p^2}{2\delta(1-\rho_{\max})^{7/2}}.$$

Remark 4. It is essential to observe the difference of the sample size conditions in Theorems 3.6 and 3.7, since γ' is usually much smaller than γ . Analogous to Theorem 3.6, together with Corollary 3.3, the above sample size condition is essentially $n \geq O(d_*^2 \log(p/\sqrt{\delta}))$ if we further assume that ρ_{\max} is well controlled beyond 1. In contrast, the sample size condition for skeleton recovery is essentially $n \geq O(d_* \log(p/\sqrt{\delta}))$.

Proof. With $\gamma' = \min\left\{\frac{\rho_{\min}}{3}, \frac{1-\rho_{\max}}{2}\right\} \rho_{\min}$, consider the event

$$E' = \bigcap_{1 \le i < j \le p} \{ |\hat{\rho}_{ij} - \rho_{ij}| < \gamma' \}.$$

By Lemma 3.4, we have

$$\mathbb{P}(E') \ge 1 - C_1 \binom{p}{2} (n-2) \exp\left((n-4) \log\left(\frac{4-\gamma'^2}{4+\gamma'^2}\right)\right),$$

where $C_1 = \frac{(1-\rho_{\min}^2)^{3/2}(3-\rho_{\max})}{(1-\rho_{\max})^{7/2}}$. Similar to the argument in Theorem 3.6, under this event the the Chow–Liu algorithm recovers the true skeleton of the polytree exactly, i.e.,

$$E' \subset {\widehat{\mathcal{T}}(\boldsymbol{X}^{(1:n)}) = \mathcal{T}}.$$

It suffices to show that by choosing ρ_{crit} that satisfies C1 in Algorithm 2, all v-structures are correctly identified on the event E'. Let's consider all node triplets i-k-j in \mathcal{T} . If the ground truth is $i \to k \leftarrow j$, we know that $\rho_{ij} = 0$ and then on E' we have $|\hat{\rho}_{ij}| \leq \gamma' \leq \rho_{crit}$. This means the v-structure is identified by Algorithm 2. In contrast, if the ground truth is $i \leftarrow k \leftarrow j$ or $i \leftarrow k \to j$ or $i \to k \to j$, Corollary 3.2 implies that $|\rho_{ij}| = |\rho_{ik}| |\rho_{kj}| \geq \rho_{\min}^2$, and then on E' there holds $|\hat{\rho}_{ij}| \geq |\rho_{ij}| - \gamma' \geq \rho_{\min}^2 - \gamma' > \rho_{crit}$. This means this triplet is correctly identified as a non-v-structure. In sum, we know that on the event E', we identify all the v-structures exactly. Then the CPDAG of T can be exactly recovered by Algorithm 2 as guaranteed in Meek (1995).

Finally, we have

$$\mathbb{P}(\hat{C}(X^{(1:n)}) \neq C_T) \leq \mathbb{P}((E')^c) \leq C_1 \binom{p}{2} (n-2) \exp\left((n-4) \log\left(\frac{4-\gamma'^2}{4+\gamma'^2}\right)\right).$$

Then, we know that $\mathbb{P}(\hat{C}(\boldsymbol{X}^{(1:n)}) \neq C_T) \leq \delta$ under the sample size condition $\frac{n-4}{\frac{2}{\gamma'^2} + \frac{1}{2}} - \log n > \log \frac{3p^2}{2\delta(1-\rho_{\max})^{7/2}}$ by the same argument in Theorem 3.6.

3.3 Sub-Gaussian case

We now move to the sub-Gaussian case for the linear polytree SEM (2.2). To be concrete, in addition to Assumption 1, we relax Assumption 2 to the following sub-Gaussian assumption imposed on the independent noise variables.

Assumption 3. $\epsilon_1, \ldots, \epsilon_p$ are independent mean-zero sub-Gaussian random variables satisfying

$$\mathbb{E}[e^{\lambda \epsilon_i}] \le e^{\frac{1}{2}\lambda^2 \kappa \omega_{ii}}, \quad \forall \lambda \in \mathbb{R},$$

where κ is some constant and $\omega_{ii} = var(\epsilon_i)$. That is, the squared sub-Gaussian parameter of ϵ_i is upper bounded by $\kappa\omega_{ii}$.

Remark 5. As an example, if ϵ_i is a mean-zero Gaussian random variable, then $\kappa = 1$.

Remark 6. Assumption 3 actually implies the linear invariance for the parameter κ . In fact, any linear combination $X := a_1 \epsilon_1 + a_2 \epsilon_2 + \ldots + a_p \epsilon_p$ satisfies

$$\mathbb{E}[e^{\lambda X}] = \mathbb{E}[e^{\lambda(a_1\epsilon_1 + \dots + a_p\epsilon_p)}]$$

$$= \mathbb{E}[e^{\lambda(a_1\epsilon_1)}] \dots \mathbb{E}[e^{\lambda(a_p\epsilon_p)}]$$

$$\leq \exp\left[\frac{\lambda^2 \kappa}{2} \left(a_1^2 \omega_{11} + \dots + a_p^2 \omega_{pp}\right)\right]$$

$$= e^{\frac{\lambda^2 \kappa}{2} var(X)}, \quad \forall \lambda \in \mathbb{R},$$

which implies that X is a sub-Gaussian random variable whose sub-Gaussian parameter is controlled by $\kappa var(X)$. This fact can be applied to the components of the feature variables $\mathbf{X} = (\mathbf{I} - \mathbf{B})^{-\top} \boldsymbol{\epsilon}$ and their standardized counterparts $\tilde{\mathbf{X}} = \mathbf{D}^{-1} (\mathbf{I} - \mathbf{B})^{-\top} \boldsymbol{\epsilon}$. As before, \mathbf{D} is a diagonal matrix whose diagonal entries are the standard deviations of X_1, \ldots, X_p .

Lemma 3.8 (Harris and Drton (2013), Lemma 7). Let (X,Y) be a bivariate random vector with mean zero and covariance matrix Σ . Denote the empirical covariance matrix with $\hat{\Sigma}_n$ from an i.i.d. sample of size n. If Σ is positive definite with $\Sigma_{11}, \Sigma_{22} \geq 1$ and $\|\hat{\Sigma}_n - \Sigma\|_{\text{max}} < t < 1$, where $\|\cdot\|_{\text{max}}$ represents the elementwise maximum absolute value of a matrix, then for the population and sample correlation between X and Y, we have

$$|\hat{\rho}_{XY} - \rho_{XY}| < \frac{2t}{1-t}.$$

Lemma 3.9. Assume X_i and X_j are jointly distributed mean-zero sub-Gaussian random variables whose sub-Gaussian parameters are controlled by $\kappa Var(X_i)$ and $\kappa Var(X_j)$, respectively. Assume we have i.i.d. samples from their joint distribution as $(X_i^{(1)}, X_j^{(1)}), \ldots, (X_i^{(n)}, X_j^{(n)})$. Then, for any $0 < \gamma \le 2$, their population and sample correlation coefficients satisfy

$$\mathbb{P}(|\hat{\rho}_{ij} - \rho_{ij}| > \gamma) \le 8 \exp\left\{-\frac{n}{2} \min\left\{\frac{\gamma^2}{128\kappa^2(2+\gamma)^2}, \frac{\gamma}{8\kappa(2+\gamma)}\right\}\right\}.$$

Proof. Notice that both population and sample correlation coefficients are scaling invariant. Therefore, WLOG, we can assume that $Var(X_i) = Var(X_j) = 1$. Remark 6 implies that their sub-Gaussian parameters are both controlled by κ .

It is known that X_i^2 is sub-Exponential with parameters $(32\kappa^2, 4\kappa)$ (Honorio and Jaakkola, 2014). In other words, it holds that

$$\mathbb{E}[e^{\lambda(X_i^2 - \mathbb{E}[X_i^2])}] \le e^{16\kappa^2}, \quad \forall |\lambda| \le \frac{1}{4\kappa}.$$

Note that our assumption give $\mathbb{E}[X_i^2] = \text{Var}(X_i) = 1$. By sub-Exponential tail bound, for any t > 0,

$$\mathbb{P}\left(\left|\frac{1}{n}\sum_{l=1}^{n}(X_{i}^{(l)})^{2}-\operatorname{Var}(X_{i})\right|>t\right)\leq2\exp\left\{-\frac{n}{2}\min\left\{\frac{t^{2}}{32\kappa^{2}},\frac{t}{4\kappa}\right\}\right\}.$$

Similarly, we have

$$\mathbb{P}\left(\left|\frac{1}{n}\sum_{l=1}^{n}(X_{j}^{(l)})^{2}-\operatorname{Var}(X_{j})\right|>t\right)\leq2\exp\left\{-\frac{n}{2}\min\left\{\frac{t^{2}}{32\kappa^{2}},\frac{t}{4\kappa}\right\}\right\}.$$

For the covariance term between X_i and X_j , note that $X_iX_j = \frac{(X_i + X_j)^2 - (X_i - X_j)^2}{4}$. Since X_i and X_j are sub-Gaussian variables, we have that $X_i \pm X_j$ are both sub-Gaussian with parameter 4κ .

Then, the sub-Exponential tail bound can be applied to $(X_i \pm X_j)^2$ to obtain the following result.

$$\mathbb{P}\left(\left|\frac{1}{n}\sum_{l=1}^{n}X_{i}^{(l)}X_{j}^{(l)} - \operatorname{Cov}(X_{i}, X_{j})\right| > t\right) \\
\leq \mathbb{P}\left(\left|\frac{1}{4n}\sum_{l=1}^{n}(X_{i}^{(l)} + X_{j}^{(l)})^{2} - \frac{1}{4}\mathbb{E}(X_{i}^{(1)} + X_{j}^{(1)})^{2}\right| > \frac{t}{2}\right) \\
+ \mathbb{P}\left(\left|\frac{1}{4n}\sum_{l=1}^{n}(X_{i}^{(l)} - X_{j}^{(l)})^{2} - \frac{1}{4}\mathbb{E}(X_{i}^{(1)} - X_{j}^{(1)})^{2}\right| > \frac{t}{2}\right) \\
\leq 4\exp\left\{-\frac{n}{2}\min\left\{\frac{t^{2}}{128\kappa^{2}}, \frac{t}{8\kappa}\right\}\right\}.$$

Denote by Σ^{ij} and $\widehat{\Sigma}_n^{ij}$ the population and sample covariance matrices of X_i and X_j , respectively. A union bound gives

$$\mathbb{P}(\|\widehat{\mathbf{\Sigma}}_n^{ij} - \mathbf{\Sigma}^{ij}\|_{\max} > t) \le 8 \exp\left\{-\frac{n}{2} \min\left\{\frac{t^2}{128\kappa^2}, \frac{t}{8\kappa}\right\}\right\}.$$

Applying Lemma 3.8 and setting $t = \frac{\gamma}{2+\gamma}$ for some $0 < \gamma \le 2$, we have

$$\mathbb{P}(|\hat{\rho}_{ij} - \rho_{ij}| > \gamma) \leq \mathbb{P}\left(\|\widehat{\mathbf{\Sigma}}_{n}^{ij} - \mathbf{\Sigma}^{ij}\|_{\max} > \frac{\gamma}{2+\gamma}\right) \\
\leq 8 \exp\left\{-\frac{n}{2} \min\left\{\frac{\gamma^{2}}{128\kappa^{2}(2+\gamma)^{2}}, \frac{\gamma}{8\kappa(2+\gamma)}\right\}\right\}.$$

It is obvious that Lemma 3.9 is a counterpart of Lemma 3.4 in the Gaussian case. With this tool as well as correlation relations in Corollary 3.2, we can establish the following CPDAG exact recovery result analogous to Theorem 3.7. Given the proof is exactly the same as that of Theorem 3.7, we skip the detailed argument and directly give the statement.

Theorem 3.10. Consider the sub-Gaussian linear polytree SEM (2.2) with Assumptions 1 and 3 satisfied. Denote by $\hat{C}(\mathbf{X}^{(1:n)})$ the estimate from the entire algorithm in Sections 2.3.1 and 2.3.2, and by C_T the true CPDAG from the polytree T. Denote $\gamma' = \min\left\{\frac{\rho_{\min}}{3}, \frac{1-\rho_{\max}}{2}\right\}\rho_{\min}$. For any $\delta \in (0,1)$, we have

$$\mathbb{P}(\hat{C}(\boldsymbol{X}^{(1:n)}) \neq C_T) < \delta,$$

if

C1
$$\gamma' \le \rho_{crit} \le \rho_{\min}^2 - \gamma';$$

$$C2 \ n > 2 \max\{\frac{128\kappa^2(2+\gamma')^2}{\gamma'^2}, \frac{8\kappa(2+\gamma')}{\gamma'}\}\log\frac{4p^2}{\delta}.$$

3.4 Inverse Correlation Matrix Estimation

In this section, let's consider the linear polytree SEM (2.2) with Assumptions 1 and 3 imposed. Moreover, let's consider the event that the CPDAG of T has been already exactly recovered by using the method described in Algorithms 1 and 2. We choose one realization form the equivalent class represented by this CPDAG, and still refer to it as T without loss of generality. In this case, we want to study how well we can estimate the inverse correlation matrix of X.

For this purpose, we can just estimate the model parameters for the companion standardized linear polytree SEM (3.1). Due to scaling invariance of population and sample correlations, without loss of generality, we can simply assume that all X_i have unit variances. Then the inverse correlation matrix is

$$\Theta := \Sigma^{-1} = (I - B)\Omega^{-1}(I - B^{\top}). \tag{3.8}$$

Our discussion in this section relies on the following notations: For each node j, denote by $Ch(j) := \{k : j \to k \in T\}$ its children set, and by $coPa(j) := \{i : \exists k, s.t. \ i \to k \leftarrow j \in T\}$ its co-parent set. We use d_i^{in} to denote the in-degree of node j.

By Eq. (3.8), the elements in the inverse correlation matrix Θ are given by

$$\theta_{ij} = \begin{cases} -\beta_{ij}/\omega_{jj} & \text{if } i \to j \in T \\ -\beta_{ji}/\omega_{ii} & \text{if } j \to i \in T \\ \beta_{ik}\beta_{jk}/\omega_{kk} & \text{if } i \to k \leftarrow j \in T \\ 0 & \text{otherwise,} \end{cases}$$
 for $i \neq j$

$$\theta_{jj} = \frac{1}{\omega_{jj}} + \sum_{k \in Ch(j)} \frac{\beta_{jk}^2}{\omega_{kk}}, \text{ for } j = 1, \dots p.$$

Notice that the k in $i \to k \leftarrow j \in T$ must be unique in a polytree.

It has been verified in Section 3.1 that for each $i \to j \in T$, β_{ij} is actually the correlation coefficient ρ_{ij} between X_i and X_j , so we also have

$$\theta_{ij} = \begin{cases} -\rho_{ij}/\omega_{jj} & \text{if } i \to j \in T \\ -\rho_{ji}/\omega_{ii} & \text{if } j \to i \in T \\ \rho_{ik}\rho_{jk}/\omega_{kk} & \text{if } i \to k \leftarrow j \in T \\ 0 & \text{otherwise,} \end{cases}$$
 for $i \neq j$

$$\theta_{jj} = \frac{1}{\omega_{jj}} + \sum_{k \in Ch(j)} \frac{\rho_{jk}^2}{\omega_{kk}}, \text{ for } j = 1, \dots p.$$

where
$$\omega_{jj} = 1 - \sum_{i \in Pa(j)} \beta_{ij}^2$$
 for $j = 1, \dots, p$.

These equations indicate that how we should estimate the elements of Θ by the sample correlations $\hat{\rho}_{ij}$ for any $i-j \in \mathcal{T}$, where \mathcal{T} is the skeleton of T. Then we can estimate θ_{ij} by simple

substitution, that is

$$\hat{\theta}_{ij} = \begin{cases} -\hat{\rho}_{ij}/\hat{\omega}_{jj} & \text{if } i \to j \in T \\ -\hat{\rho}_{ji}/\hat{\omega}_{ii} & \text{if } j \to i \in T \\ \hat{\rho}_{ik}\hat{\rho}_{jk}/\hat{\omega}_{kk} & \text{if } i \to k \leftarrow j \in T \\ 0 & \text{otherwise,} \end{cases}$$
 for $i \neq j$

$$\hat{\theta}_{jj} = \frac{1}{\hat{\omega}_{jj}} + \sum_{k \in Ch(j)} \frac{\hat{\rho}_{jk}^2}{\hat{\omega}_{kk}}, \text{ for } j = 1, \dots p,$$
 (3.9)

where
$$\hat{\omega}_{jj} = 1 - \sum_{i \in Pa(j)} \hat{\rho}_{ij}^2$$
 for $j = 1, \dots, p$.

Recall that we can only recover CPDAG(T) when the sample size is large enough, so it is necessary to show that the inverse correlation estimates (3.9) only depend on CPDAG(T). To this end, we first introduce a fact about the nodes in CPDAG(T) without proof.

Lemma 3.11. Denote by C_T the true CPDAG from the polytree T. We denote V_m the collection of nodes j such that there is at least one undirected edge i-j in C_T . On the other hand, we denote V_d the collection of nodes j such that all its neighbors are connected to it with a directed edge in C_T . Then we know that V_m and V_d is a partition of V. Moreover, we have the following properties

- 1. For each $j \in V_m$, there is no i such that $i \to j \in C_T$.
- 2. For each $j \in V_m$, In each polytree T' corresponding to C_T , j has at most one parent.
- 3. For each $j \in V_d$, Given the set of parents of j are kept the same for any T' according to C_T , we know that $\hat{\omega}_{jj} = 1 \sum_{i \in Pa(j)} \hat{\rho}_{ij}^2$ is well-defined.
- 4. Combining the third property and the contrapositive of the first property, we know for each $i \to j \in C_T$, we have $j \in V_d$, and $\hat{\omega}_{jj}$ is thereby well-defined.

We omit the proof since this result can be directly implied by the fact that v-structures are kept unchanged in all polytrees corresponding to C_T . With this result, we can easily obtain the following result that shows (3.9) only relies on C_T .

Lemma 3.12. The estimate of the inverse correlation matrix in (3.9) only depends on the CPDAG of T. In particular, by denoting by C_T the true CPDAG from the polytree T, we have

$$\hat{\theta}_{ij} = \begin{cases} -\hat{\rho}_{ij}/\hat{\omega}_{jj} & \text{if } i \to j \in C_T \\ -\hat{\rho}_{ji}/\hat{\omega}_{ii} & \text{if } j \to i \in C_T \\ -\hat{\rho}_{ij}/(1-\hat{\rho}_{ij}^2) & \text{if } i - j \in C_T \\ \hat{\rho}_{ik}\hat{\rho}_{jk}/\hat{\omega}_{kk} & \text{if } i \to k \leftarrow j \in C_T \\ 0 & \text{otherwise,} \end{cases}$$
 for $i \neq j$

and

$$\hat{\theta}_{jj} = \begin{cases} \frac{1}{\hat{\omega}_{jj}} + \sum\limits_{j \to k \in C_T} \frac{\hat{\rho}_{jk}^2}{\hat{\omega}_{kk}}, & j \in V_d, \\ 1 + \sum\limits_{j - k \in C_T} \frac{\hat{\rho}_{jk}^2}{1 - \hat{\rho}_{jk}^2} + \sum\limits_{j \to k \in C_T} \frac{\hat{\rho}_{jk}^2}{\hat{\omega}_{kk}}, & j \in V_m. \end{cases}$$

Here $\hat{\omega}_{jj} = 1 - \sum_{i \in Pa(j)} \hat{\rho}_{ij}^2$ is defined for $j \in V_d$.

The result can be obtained relatively straightforward by the facts listed in Lemma 3.11. The formula of $\hat{\theta}_{jj}$ for $j \in V_m$ may not be obvious. One needs to verify this formula for two different cases of $T' \in C_T$: j has no parent, and j has one parent. It turns out that these two cases lead to the same formula. We omit the detailed argument for the proof.

Theorem 3.13. Consider the linear polytree SEM (2.2) where X_j has unit variance for each $j \in V$. Denote by $\hat{C}(\mathbf{X}^{(1:n)})$ the estimated CPDAG and by C_T the true CPDAG from the polytree T. We impose a uniform lower bound of the variances of the noise variables $\epsilon_1, \ldots, \epsilon_p$: there exists $\omega_{\min} \in (0,1)$ such that $\omega_{jj} \geq \omega_{\min}$ for $j=1,\ldots,p$. For any $\varepsilon > 0$ satisfying $2d_*\varepsilon < \omega_{\min}$, consider the events $E_{\rho}(\varepsilon) = \{|\hat{\rho}_{ij} - \rho_{ij}| \leq \varepsilon, \forall i \to j \in T\}$ and $E_{C_T} = \{\hat{C}(\mathbf{X}^{(1:n)}) = C_T\}$. Then on the event $E_{\rho}(\varepsilon) \cap E_{C_T}$, the estimated inverse correlation matrix (3.9) satisfies

$$\sum_{j=1}^{p} \sum_{i=1}^{p} |\hat{\theta}_{ij} - \theta_{ij}| \le \frac{p\varepsilon(7 + 8d_* + 2d_*^2)}{(\omega_{\min} - 2d_*\varepsilon)\omega_{\min}}.$$

Recall that we use d_* to denote the maximum in-degree over the polytree.

Remark 7. Under Gaussian or sub-Gaussian cases, the event $E_{\rho}(\varepsilon) \cap E_{C_T}$ occurs with high probability. Taking Theorem 3.7 for instance, when the sample size is large enough, $E_{\rho}(\varepsilon) \cap E_{C_T}$ occurs with high probability with $\varepsilon = \min \left\{ \frac{\rho_{\min}}{3}, \frac{1-\rho_{\max}}{2} \right\} \rho_{\min}$.

Remark 8. Previously we have shown that $\hat{\theta}_{ij}$ only relies on C_T . In fact, we can also show that d_* and ω_{\min} only depend on C_T . Note that for each $j \in V_m$ and any $T' \in C_T$, we have $d_j^{in} \leq 1$. Therefore, we actually have the identity $d_* = \max\{d_j^{in} : j \in V_d\} \vee 1$. As for ω_{\min} , one can actually show that the set of $\{\omega_{jj} : j \in V_m\}$ is the same as $\{1 - \rho_{ij} : i - j \in C_T\} \cap 1$. Then, we actually have

$$\omega_{\min} = \min\{\omega_{jj} : j \in V_d\} \land \min\{1 - \rho_{ij} : i - j \in C_T\},\$$

which only relies on C_T .

Proof. In the sequel, we only consider directed edges in T rather than in C_T . For any noise variable ϵ_j , we can control the estimation error of its variance by

$$|\hat{\omega}_{jj} - \omega_{jj}| = |\sum_{i \in Pa(j)} (\hat{\rho}_{ij}^2 - \rho_{ij}^2)| \le \sum_{i \in Pa(j)} |\hat{\rho}_{ij}^2 - \rho_{ij}^2| \le 2 \sum_{i \in Pa(j)} |\hat{\rho}_{ij} - \rho_{ij}| \le 2d_j^{in} \varepsilon.$$

Notice that for each node j, we can divide $\sum_{i=1}^{p} |\hat{\theta}_{ij} - \theta_{ij}|$ into four parts:

$$\sum_{i=1}^{p} |\hat{\theta}_{ij} - \theta_{ij}| = \underbrace{|\hat{\theta}_{jj} - \theta_{jj}|}_{I} + \underbrace{\sum_{i \in Pa(j)} |\hat{\theta}_{ij} - \theta_{ij}|}_{II} + \underbrace{\sum_{k \in Ch(j)} |\hat{\theta}_{kj} - \theta_{kj}|}_{III} + \underbrace{\sum_{l \in coPa(j)} |\hat{\theta}_{lj} - \theta_{lj}|}_{IV}.$$

We will control each part in the sequel:

I.

$$\begin{aligned} |\hat{\theta}_{jj} - \theta_{jj}| &= \left| \frac{1}{\hat{\omega}_{jj}} - \frac{1}{\omega_{jj}} + \sum_{k \in Ch(j)} \left(\frac{\hat{\rho}_{jk}^2}{\hat{\omega}_{kk}} - \frac{\rho_{jk}^2}{\omega_{kk}} \right) \right| \\ &\leq \left| \frac{1}{\hat{\omega}_{jj}} - \frac{1}{\omega_{jj}} \right| + \sum_{k \in Ch(j)} \left[\frac{|\hat{\rho}_{jk}^2 - \rho_{jk}^2|}{\hat{\omega}_{kk}} + \rho_{jk}^2 \left| \frac{1}{\hat{\omega}_{kk}} - \frac{1}{\omega_{kk}} \right| \right] \\ &\leq \frac{2d_j^{in} \varepsilon}{(\omega_{jj} - 2d_j^{in} \varepsilon) \omega_{jj}} + \sum_{k \in Ch(j)} \left[\frac{2\varepsilon}{\omega_{kk} - 2d_k^{in} \varepsilon} + \rho_{\max}^2 \frac{2d_k^{in} \varepsilon}{(\omega_{kk} - 2d_k^{in} \varepsilon) \omega_{kk}} \right] \\ &\leq \frac{2d_j^{in} \varepsilon}{(\omega_{jj} - 2d_j^{in} \varepsilon) \omega_{jj}} + \sum_{k \in Ch(j)} \frac{2\varepsilon(\omega_{kk} + \rho_{\max}^2 d_k^{in})}{(\omega_{kk} - d_k^{in} \varepsilon) \omega_{kk}}. \end{aligned}$$

II.

$$\sum_{i \in Pa(j)} |\hat{\theta}_{ij} - \theta_{ij}| = \sum_{i \in Pa(j)} \left| \frac{\hat{\rho}_{ij}}{\hat{\omega}_{jj}} - \frac{\rho_{ij}}{\omega_{jj}} \right|$$

$$\leq \sum_{i \in Pa(j)} \frac{1}{\hat{\omega}_{jj}} |\hat{\rho}_{ij} - \rho_{ij}| + |\rho_{ij}| \left| \frac{1}{\hat{\omega}_{jj}} - \frac{1}{\omega_{jj}} \right|$$

$$\leq d_j^{in} \frac{\varepsilon(\omega_{jj} + 2\rho_{\max}d_j^{in})}{(\omega_{jj} - 2d_j^{in}\varepsilon)\omega_{jj}}.$$

III.

$$\sum_{k \in Ch(j)} |\hat{\theta}_{kj} - \theta_{kj}| = \sum_{k \in Ch(j)} \left| \frac{\hat{\rho}_{jk}}{\hat{\omega}_{kk}} - \frac{\rho_{jk}}{\omega_{kk}} \right|$$

$$\leq \sum_{k \in Ch(j)} \frac{1}{\hat{\omega}_{kk}} |\hat{\rho}_{jk} - \rho_{jk}| + |\rho_{jk}| \left| \frac{1}{\hat{\omega}_{kk}} - \frac{1}{\omega_{kk}} \right|$$

$$\leq \sum_{k \in Ch(j)} \frac{\varepsilon(\omega_{kk} + 2\rho_{\max}d_k^{in})}{(\omega_{kk} - 2d_k^{in}\varepsilon)\omega_{kk}}.$$

IV. For any $l \in coPa(j)$, let k_l denote the v-node such that $j \to k_l \leftarrow l$ is a v-structure in T.

$$\begin{split} \sum_{l \in coPa(j)} |\hat{\theta}_{lj} - \theta_{lj}| &= \sum_{l \in coPa(j)} \left| \frac{\hat{\rho}_{lk_l} \hat{\rho}_{jk_l}}{\hat{\omega}_{k_l k_l}} - \frac{\rho_{lk_l} \rho_{jk_l}}{\omega_{k_l k_l}} \right| \\ &\leq \sum_{l \in coPa(j)} \frac{1}{\hat{\omega}_{k_l k_l}} |\hat{\rho}_{lk_l} \hat{\rho}_{jk_l} - \rho_{lk_l} \rho_{jk_l}| + |\rho_{lk_l} \rho_{jk_l}| \left| \frac{1}{\hat{\omega}_{k_l k_l}} - \frac{1}{\omega_{k_l k_l}} \right| \\ &\leq \sum_{l \in coPa(j)} \frac{(2\rho_{\max} + \varepsilon)\varepsilon\omega_{k_l k_l} + 2\rho_{\max}^2 d_{k_l}^{in}\varepsilon}{(\omega_{k_l k_l} - 2d_{k_l}^{in}\varepsilon)\omega_{k_l k_l}}. \end{split}$$

Combining I, II, III, and IV together, we have

$$\sum_{i=1}^{p} |\hat{\theta}_{ij} - \theta_{ij}| \leq \frac{(3 + 2d_j^{in})d_j^{in}\varepsilon}{(\omega_{\min} - 2d_j^{in}\varepsilon)\omega_{\min}} + \sum_{k \in Ch(j)} \frac{(3 + 4d_k^{in})\varepsilon}{(\omega_{\min} - 2d_j^{in}\varepsilon)\omega_{\min}} + \sum_{l \in coPa(j)} \frac{(2 + 2d_{k_l}^{in} + \varepsilon)\varepsilon}{(\omega_{\min} - 2d_{k_l}^{in}\varepsilon)\omega_{\min}}.$$

Then

$$\sum_{j=1}^{p} \sum_{i=1}^{p} |\hat{\theta}_{ij} - \theta_{ij}| \leq \frac{6(p-1)\varepsilon + 2\varepsilon \sum_{j=1}^{p} (d_j^{in})^2 + 4\varepsilon \sum_{j=1}^{p} \sum_{k \in Ch(j)} d_k^{in}}{(\omega_{\min} - 2d_*\varepsilon)\omega_{\min}} + \sum_{j=1}^{p} \sum_{l \in coPa(j)} \frac{(2 + 2d_{kl}^{in} + \varepsilon)\varepsilon}{(\omega_{\min} - 2d_{kl}^{in}\varepsilon)\omega_{\min}}.$$

Changing the order of summation gives

$$\sum_{j=1}^{p} \sum_{k \in Ch(j)} d_k^{in} = \sum_{k=1}^{p} \sum_{j \in Pa(k)} d_k^{in} = \sum_{k=1}^{p} (d_k^{in})^2.$$

The facts $\sum_{j=1}^p d_j^{in} = p-1$ and $0 \le d_j^{in} \le d_*$ imply that $\sum_{j=1}^p (d_j^{in})^2 \le pd_*$. Moreover, by counting the number of v-structures, there hold

$$\sum_{j=1}^{p} \sum_{l \in coPa(j)} d_{k_l}^{in} = 2 \sum_{j: d_i^{in} \ge 2} d_j^{in} \binom{d_j^{in}}{2} \le p d_*^2$$

and

$$\sum_{j=1}^{p} \sum_{l \in coPa(j)} 1 = 2 \sum_{j: d_i^{in} \ge 2} {d_j^{in} \ge 2 \choose 2} \le pd_*.$$

Taking all of these inequalities together, and by the assumption $2\varepsilon d_* < \omega_{\min} \leq 1$, we get the following result:

$$\sum_{j=1}^{p} \sum_{i=1}^{p} |\hat{\theta}_{ij} - \theta_{ij}| \le \frac{p\varepsilon(7 + 8d_* + 2d_*^2)}{(\omega_{\min} - 2d_*\varepsilon)\omega_{\min}}.$$

4 Experiments

To illustrate the performance of the polytree learning method, we implement Algorithms 1 and 2 in Python and perform simulations on synthetic data as well as applying to the widely used benchmark datasets ASIA and ALARM. All codes are available at https://github.com/huyu00/linear-polytree-SEM.

4.1 Polytree synthetic data

Here we generate i.i.d. samples from a Gaussian linear SEM with a polytree structure. We first generate an undirected tree with p nodes from a Prufer sequence obtained by sampling p-2 numbers with replacement from $1, 2, \ldots, p$, which has a one-to-one correspondence to all the trees. Next the polytree is obtained by randomly orienting the edges of the undirected tree. We can also ensure

that one of the node has a specified large in-degree $d_{\text{max}}^{\text{in}}$. This is done by making the node i occur at least $d_{\text{max}}^{\text{in}} - 1$ times in the Prufer sequence, so the node will have degree at least $d_{\text{max}}^{\text{in}}$ in the tree. We then select $d_{\text{max}}^{\text{in}}$ of the edges connected to i to be in-coming edges (the rest of the edges are oriented randomly as before).

In the next step, we choose the value of the standardized β_{ij} corresponding to the correlation matrix Eq. (3.1). Note that once β_{ij} 's are given, ω_{ii} are determined by Eq. (3.3). Motivated by the theoretical conditions on n, p such as that in Theorems 3.6 and 3.7, we choose β_{ij} according to some pre-specified values ρ_{\min} and ρ_{\max} to study their effects on the recovery accuracy. To avoid ill-conditioned cases, we require that $\omega_{ii} \geq \omega_{\min}$. This adds constraints on β_{ij} , $\sum_{j=1}^{p} \beta_{ij}^2 \leq 1 - \omega_{\min}$, in addition to $\rho_{\min} \leq |\beta_{ij}| \leq \rho_{\max}$. We sample β_{ij}^2 uniformly among the set of values that satisfy the inequality constraints above. This sampling is implemented by drawing β_{ij}^2 (corresponding to all the edges) sequentially in a random order as $\max(\rho_{\max}^2, \rho_{\min}^2 + v_j x)$, where x is drawn from the beta distribution $B(1, \tilde{d}_j^{\text{in}})$. Here \tilde{d}_j^{in} is the number of incoming edges to node j whose β_{ij}^2 has not yet been chosen, and $v_j = 1 - \omega_{\min} - d_j^{\text{in}} \rho_{\min}^2 - \sum_k \beta_{kj}^2$ where β_{kj}^2 are incoming edges to j whose value have been chosen, d_j^{in} is the number of incoming edges to j. The beta distribution used here is based on the fact of the order statistics of independent uniformly distributed random variables. As an exception, we particularly set two $|\beta_{ij}|$ values before choosing the rest as described above to attain equality with ρ_{\min} and ρ_{\max} . For ρ_{\max} , we randomly choose a node i that satisfies $\rho_{\min}^2(d_i^{\text{in}}-1)+\rho_{\max}^2\leq 1-\omega_{\min},\ d_i^{\text{in}}>0,\ \text{and set one of its incoming edges to have } |\beta_{ji}|=\rho_{\max}.$ For ρ_{\min} , we choose a node among the rest nodes with $d_k^{\text{in}} > 0$ and set $|\beta_{lk}| = \rho_{\min}$ for one of its incoming edges. Lastly, a positive or negative sign is given to each β_{ij} with equal probability. After the β_{ij} (i.e., matrix **B**) are chosen, the zero mean Gaussian samples **X** are drawn according to Eq. (2.3).

We assess the inference result by comparing the true and inferred CPDAGs G and G. On the skeleton level, there can be edges in the true graph that are missing in the inferred, and vice versa the inferred graph can have extra edges. For the CPDAG, we consider a directed edge to be correct if it is present and is directed with the same direction in both CPDAGs. For an undirected edge, it needs to be undirected in both CPDAGs. Any other edges that occur in both CPDAGs are considered to have a wrong direction. With these notions, we can calculate the False Discovery Rate (FDR) for the skeleton as $\frac{|\text{extra}|}{|\hat{G}|}$, and for the CPDAG as $\frac{|\text{extra}|+|\text{wrong direction}|}{|\hat{G}|}$. Here |extra| is the number of extra edges, and $|\hat{G}|$ is the number of edges in \hat{G} , other notations are defined similarly. To quantify the overall similarity, we calculate the Jaccard indices, which are $\frac{|\text{correct}| + |\text{wrong direction}|}{|G \cup \hat{G}|} = \frac{|\text{correct}| + |\text{wrong direction}|}{|\text{missing}| + |\hat{G}|} \text{ for the skeleton, and } \frac{|\text{correct}|}{|G| + |\hat{G}| - |\text{correct}|} \text{ for the CPDAG.}$ In these simulations and all other inferences, we set the threshold ρ_{crit} in Algorithm 2 for rejecting a pair of node to be independent based on hypothesis testing of zero correlation. Specifically, $\rho_{crit} =$ $\sqrt{1-\frac{1}{1+t_{\alpha/2}^2/(n-2)}}$, where $t_{\alpha/2}$ is the $1-\alpha/2$ quantile of a t-distribution with n-2 degree-of-freedom, and we use $\alpha = 0.1$. The results of our simulation is summarize in Fig. 1. For comparison, we also run the same data using the hill-climbing Gámez et al. (2011), a common score-based algorithm, as a comparison (implemented in R package bnlearn using all the default parameters/options). We see that the polytree learning has a smaller FDR and Jaccard index than the hill-climbing. The performance of the polytree learning drops as ρ_{\min} decreases, or as the maximum in-degree increases, whereas the hill-climbing is little affected. The computational time of the polytree learning is much shorter than the hill-climbing: 0.0093 vs 1.15 seconds on a 2019 i7 quad-core CPU desktop computer.

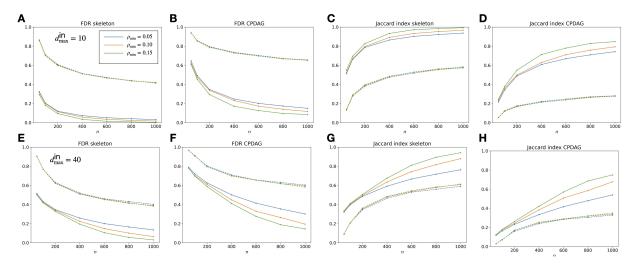


Figure 1: Performance on the polytree synthetic data. The solid lines are from the polytree learning and the dashed lines are from the hill-climbing. Colors correspond to different values of ρ_{\min} dim $d_{\max}^{in}=10$ for A-D and $d_{\max}^{in}=40$ for E-H. Each data point (n=50,100,200,400,600,800,1000) is averaged across 100 realizations of randomly generating the synthetic data (see text). The rest of the parameters are the same for all curves: p=100, $\rho_{\max}=0.8$, $\omega_{\min}=0.1$.

4.2 DAG benchmark data

The Asia dataset Lauritzen and Spiegelhalter (1988) is a synthetic dataset of a small DAG with 8 nodes. With n = 500 samples, the polytree learning recovered 5.76 ± 0.88 edges out of the 8 edges of the true graph (mean \pm sd from inference results on 1000 bootstrap samples). With more samples n = 5000, the algorithm can recover all but one edge and with an wrong direction edge in 22% of the cases Fig. 2. Note this is the best possible result since any polytree has to miss at least one edge, and the V-structure involving B, E, D cannot be identified once missing the edge ED, leading to BD being undirected. Overall, in 81% of the cases, the inferred polytree has good agreement with the true DAG with no more than 2 missing edges and 3 wrong direction edges.

The ALARM dataset Beinlich et al. (1989) is widely used in benchmarking the structural learning of DAGs. The true model (Fig. 3A) is a DAG with 37 nodes and 46 edges, hence there has to be at least 10 edges missing in the inferred polytree. Interestingly, the polytree learning performs reasonably for n = 500 with 14 missing edges, 4 extra edges, 4 wrong direction edges, leading to a FDR of 0.11 for the skeleton, 0.22 for the CPDAG, and a Jaccard index of 0.64 for the skeleton and 0.52 for the CPDAG. At n = 5000 (Fig. 3B), it even achieves the best possible accuracy for the skeleton.

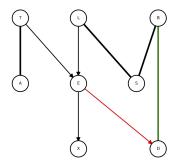


Figure 2: The inferred polytree with n=5000 samples. There is one edge in the true DAG that is missing (red) and the directed edge from B to D is inferred as undirected (green). This graph is the most likely result occurring 22% across bootstraps.

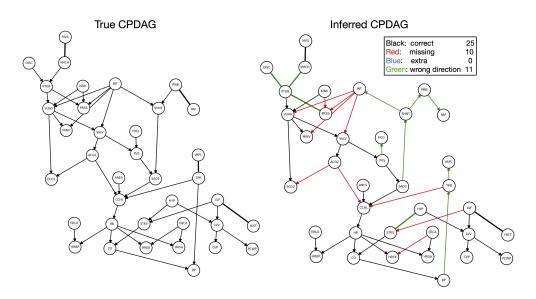


Figure 3: Comparing the true CPDAG of the ALARM data and the one inferred using the polytree learning algorithm at sample size n = 5000. There are 37 nodes and 46 edges in the true CPDAG. The inferred graph has a FDR of 0 for the skeleton and 0.31 for the CPDAG, and a Jaccard index of 0.78 for the skeleton and 0.44 for the CPDAG.

5 Discussions

This paper studies the problem of polytree learning, a special case of DAG learning where the skeleton of the directed graph is a tree. This model has been widely used in the literature for both prediction and structure learning. We consider the linear polytree model, and consider the Chow-Liu algorithm (Chow and Liu, 1968) that has been proposed in Rebane and Pearl (1987) for polytree learning.

In theory, our major contribution is to study the sample size conditions under which the algorithm considered is able to recover the skeleton and the CPDAG. Roughly speaking, under certain mild assumptions on the correlation coefficients, we show that the skeleton can be exactly recovered

with high probability if the sample size satisfies $n > O(\frac{1}{\rho_{\min}^2} \log \frac{p}{\sqrt{\delta}})$, and the CPDAG of the polytree can be exactly recovered with high probability if the sample size satisfies $n > O(\frac{1}{\rho_{\min}^4} \log \frac{p}{\sqrt{\delta}})$.

Under the event of exact recovery of CPDAG, we also establish the estimation error rate for the estimation of the inverse correlation matrix. Under the ℓ_1 metric, we specify how the estimation error relies on the estimation error of pairwise correlations, the minimum noise variance ω_{\min} , and the maximum in-degree d_* .

There are a number of remaining questions to study in future. It would be interesting to study how to relax the polytree assumption. In fact, the benchmark data analysis (Section 4.2) is very insightful, since it shows that the considered Chow-Liu based CPDAG recovery algorithm, which seemingly relies heavily on the polytree assumption, could lead to reasonable and accurate structure learning result when the ground truth deviates from a polytree significantly. This inspires us to consider the robustness of the proposed approach against such structural assumptions. For example, if the ground truth can only be approximated by a polytree, can the structure learning method described in Sections 2.3.1 and 2.3.2 lead to an approximate recovery of the ground truth CPDAG with theoretical guarantees?

When the ground truth DAG is a polytree, our result on the estimation of the inverse correlation matrix stated in Theorem 3.13 relies on the assumption that the ground truth of the CPDAG must be exactly recovered. Naturally, we wonder whether this is necessary. In other words, if the sample size is not large enough and the CPDAG is thereby not recovered exactly, can we still obtain an accurate estimate of the inverse correlation matrix? Which method should be used to achieve such estimate?

As aforementioned, polytree modeling is usually used in practice only as initialization, and post-processing could give better structural recovery result. A well-known method of this type is given in Cheng et al. (2002) without theoretical guarantees. An interesting future research direction is to consider such post processing steps in our theoretical analysis, such that our structural learning results in Theorems 3.7 and 3.10 for more general sparse DAGs.

References

- Anandkumar, A., Hsu, D. J., Huang, F., and Kakade, S. M. (2012a). Learning mixtures of tree graphical models. In *NIPS*, pages 1061–1069.
- Anandkumar, A., Tan, V. Y., Huang, F., Willsky, A. S., et al. (2012b). High-dimensional structure estimation in ising models: Local separation criterion. *The Annals of Statistics*, 40(3):1346–1375.
- Beinlich, I., Suermondt, H. J., Chavez, R. M., and Cooper, G. (1989). The ALARM Monitoring System: A Case Study with two Probabilistic Inference Techniques for Belief Networks. *Proc.* 2nd European Conference on Artificial Intelligence in Medicine, pages 247–256.
- Bresler, G., Karzand, M., et al. (2020). Learning a tree-structured ising model in order to make predictions. *Annals of Statistics*, 48(2):713–737.
- Cheng, J., Greiner, R., Kelly, J., Bell, D., and Liu, W. (2002). Learning bayesian networks from data: An information-theory based approach. *Artificial intelligence*, 137(1-2):43–90.
- Chickering, D. M. (2002). Optimal structure identification with greedy search. *Journal of machine learning research*, 3(Nov):507–554.

- Chow, C. and Liu, C. (1968). Approximating discrete probability distributions with dependence trees. *IEEE transactions on Information Theory*, 14(3):462–467.
- Cover, T. M. (1999). Elements of information theory. John Wiley & Sons.
- Dasgupta, S. (1999). Learning polytrees. In *Proceedings of the Fifteenth conference on Uncertainty in artificial intelligence*, pages 134–141.
- Drton, M. and Maathuis, M. H. (2017). Structure learning in graphical modeling. *Annual Review of Statistics and Its Application*, 4:365–393.
- Foygel, R., Draisma, J., and Drton, M. (2012). Half-trek criterion for generic identifiability of linear structural equation models. *The Annals of Statistics*, pages 1682–1713.
- Gámez, J. A., Mateo, J. L., and Puerta, J. M. (2011). Learning Bayesian networks by hill climbing: Efficient methods based on progressive restriction of the neighborhood. *Data Mining and Knowledge Discovery*, 22(1-2):106–148.
- Ghassami, A., Yang, A., Kiyavash, N., and Zhang, K. (2020). Characterizing distribution equivalence and structure learning for cyclic and acyclic directed graphs. In *International Conference on Machine Learning*, pages 3494–3504. PMLR.
- Harris, N. and Drton, M. (2013). Pc algorithm for nonparanormal graphical models. *Journal of Machine Learning Research*, 14(11).
- Heinemann, U. and Globerson, A. (2014). Inferning with high girth graphical models. In *International Conference on Machine Learning*, pages 1260–1268. PMLR.
- Heinze-Deml, C., Maathuis, M. H., and Meinshausen, N. (2018). Causal structure learning. *Annual Review of Statistics and Its Application*, 5:371–391.
- Honorio, J. and Jaakkola, T. (2014). Tight bounds for the expected risk of linear classifiers and pac-bayes finite-sample guarantees. In *Artificial Intelligence and Statistics*, pages 384–392. PMLR.
- Huete, J. F. and de Campos, L. M. (1993). Learning causal polytrees. In *European Conference on Symbolic and Quantitative Approaches to Reasoning and Uncertainty*, pages 180–185. Springer.
- Kalisch, M. and Bühlman, P. (2007). Estimating high-dimensional directed acyclic graphs with the pc-algorithm. *Journal of Machine Learning Research*, 8(3).
- Katiyar, A., Hoffmann, J., and Caramanis, C. (2019). Robust estimation of tree structured gaussian graphical model. arxiv e-prints, page. arXiv preprint arXiv:1901.08770.
- Koller, D. and Friedman, N. (2009). Probabilistic graphical models: principles and techniques. MIT press.
- Kruskal, J. B. (1956). On the shortest spanning subtree of a graph and the traveling salesman problem. *Proceedings of the American Mathematical society*, 7(1):48–50.
- Lauritzen, S. L. and Spiegelhalter, D. J. (1988). Local computations with probabilities on graphical structures and their application to expert systems. *Journal of the Royal Statistical Society. Series B (Methodological)*, 50(2):157–224.

- Meek, C. (1995). Causal inference and causal explanation with background knowledge. In *Proceedings of the Eleventh conference on Uncertainty in artificial intelligence*, pages 403–410.
- Netrapalli, P., Banerjee, S., Sanghavi, S., and Shakkottai, S. (2010). Greedy learning of markov network structure. In 2010 48th Annual Allerton Conference on Communication, Control, and Computing (Allerton), pages 1295–1302. IEEE.
- Nikolakakis, K. E., Kalogerias, D. S., and Sarwate, A. D. (2019). Learning tree structures from noisy data. In *The 22nd International Conference on Artificial Intelligence and Statistics*, pages 1771–1782. PMLR.
- Nowzohour, C., Maathuis, M. H., Evans, R. J., Bühlmann, P., et al. (2017). Distributional equivalence and structure learning for bow-free acyclic path diagrams. *Electronic Journal of Statistics*, 11(2):5342–5374.
- Ouerd, M., Oommen, B. J., and Matwin, S. (2004). A formal approach to using data distributions for building causal polytree structures. *Information Sciences*, 168(1-4):111–132.
- Pearl, J. (2009). Causality. Cambridge university press.
- Rebane, G. and Pearl, J. (1987). The recovery of causal poly-trees from statistical data. In *Proceedings of the Third Conference on Uncertainty in Artificial Intelligence*, pages 222–228.
- Sachs, K., Perez, O., Pe'er, D., Lauffenburger, D. A., and Nolan, G. P. (2005). Causal protein-signaling networks derived from multiparameter single-cell data. *Science*, 308(5721):523–529.
- Spirtes, P., Glymour, C. N., Scheines, R., and Heckerman, D. (2000). Causation, prediction, and search. MIT press.
- Tan, V. Y., Anandkumar, A., and Willsky, A. S. (2010). Learning gaussian tree models: Analysis of error exponents and extremal structures. *IEEE Transactions on Signal Processing*, 58(5):2701–2714.
- Tavassolipour, M., Motahari, S. A., and Shalmani, M.-T. M. (2018). Learning of tree-structured gaussian graphical models on distributed data under communication constraints. *IEEE Transactions on Signal Processing*, 67(1):17–28.
- Verma, T. and Pearl, J. (1991). Equivalence and synthesis of causal models. UCLA, Computer Science Department.
- Verma, T. and Pearl, J. (1992). An algorithm for deciding if a set of observed independencies has a causal explanation. In *Uncertainty in artificial intelligence*, pages 323–330. Elsevier.
- Wright, S. (1960). Path coefficients and path regressions: alternative or complementary concepts? *Biometrics*, 16(2):189–202.
- Zhang, B., Gaiteri, C., Bodea, L.-G., Wang, Z., McElwee, J., Podtelezhnikov, A. A., Zhang, C., Xie, T., Tran, L., Dobrin, R., et al. (2013). Integrated systems approach identifies genetic nodes and networks in late-onset alzheimer's disease. *Cell*, 153(3):707–720.