ON LOW RANK DIRECTED ACYCLIC GRAPHS AND CAUSAL STRUCTURE LEARNING

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Paper under double-blind review

ABSTRACT

Despite several important advances in recent years, learning causal structures represented by directed acyclic graphs (DAGs) remains a challenging task in high dimensional settings when the graphs to be learned are not sparse. In this paper, we propose to exploit a low rank assumption regarding the (weighted) adjacency matrix of a DAG causal model to mitigate this problem. We demonstrate how to adapt existing methods for causal structure learning to take advantage of this assumption and establish several useful results relating interpretable graphical conditions to the low rank assumption. In particular, we show that the maximum rank is highly related to hubs, suggesting that scale-free networks which are frequently encountered in real applications tend to be low rank. We also provide empirical evidence for the utility of our low rank adaptations, especially on relatively large and dense graphs. Not only do they outperform existing algorithms when the low rank condition is satisfied, the performance is also competitive even though the true rank may not be as low as is assumed.

1 INTRODUCTION

An important goal in many sciences is to discover the underlying causal structures in various domains, both for the purpose of explaining and understanding phenomena, and for the purpose of predicting effects of interventions (Pearl, 2009). Due to the relative abundance of passively observed data as opposed to experimental data, how to learn causal structures from purely observational data has been vigorously investigated (Peters et al., 2017; Spirtes et al., 2000). In this context, causal structures are usually represented by directed acyclic graphs (DAGs) over a set of random variables.

For this task, existing methods can be roughly categorized into two classes: constraint- and score-based. The former use statistical tests to extract from data a number of constraints in the form of conditional (in)dependence and seek to identify the class of causal structures compatible with those constraints (Meek, 1995; Spirtes et al., 2000; Zhang, 2008). The latter employ a score function to evaluate candidate causal structures relative to data and seek to locate the causal structure (or a class of causal structures) with the optimal score. Due to the combinatorial nature of the acyclicity constraint (Chickering, 1996; He et al., 2015), most score-based methods rely on local heuristics to perform the search. A particular example is the greedy equivalence search (GES) algorithm (Chickering, 2002) that can find an optimal solution with infinite data and proper model assumptions.

Recently, Zheng et al. (2018) introduced a smooth acyclicity constraint w.r.t. graph adjacency matrix, and the task on linear data models was then formulated as a continuous optimization problem with least-squares loss. This change of perspective allows using deep learning techniques to model causal mechanisms and has already given rise to several new algorithms for causal structure learning with non-linear data, e.g., Yu et al. (2019); Ng et al. (2019b;a); Ke et al. (2019); Lachapelle et al. (2020); Zheng et al. (2020), among others. While these new algorithms represent the current state of the art in many settings, their performance generally degrades when the target DAG becomes large and relatively dense, as seen from the empirical results reported in the referred works and also in this paper. Of course this issue is a challenge to other approaches as well. Ramsey et al. (2017) proposed fast GES for impressively large problems, but it works reasonably well only when the large structure is very sparse. The max-min hill-climbing (MMHC) (Tsamardinos et al., 2006) relies on local learning methods that often do not perform well when the target node has a large neighborhood. How to improve the performance on relatively large and dense DAGs is therefore an important question.

In this work, we study the potential of exploiting a kind of *low rank* assumption on the DAG structure to help address this problem. The rank of a graph that concerns us is the algebraic rank of its associated weighted adjacency matrix. Similar to the role of a sparsity assumption on graph structures, we treat the low rank assumption as methodological and it is not restricted to a particular DAG learning method. However, unlike sparsity assumption, it is much less apparent when DAGs tend to be low rank and how low rank DAGs behave. Thus, besides demonstrating the utility of exploiting a low rank assumption in causal structure learning, another important goal is to improve our understanding of the low rank assumption by relating the rank of a graph to its graphical structure. Such a result also enables us to characterize the rank of a graph from several structural priors and helps to choose rank related hyperparameters for the learning algorithm. Our contributions are summarized as follows:

- We show how to adapt existing causal structure learning methods to take advantage of the low rank assumption, and provide a strategy to select rank related hyperparameters utilizing the lower and upper bounds on the true rank, if they are available.
- To improve our understanding of low rank DAGs, we establish some lower bounds on the rank of a DAG in terms of simple graphical conditions, which imply necessary conditions for DAGs to be low rank.
- We also show that the maximum possible rank of weighted adjacency matrices associated with a directed graph is highly related to hubs in the graph, which suggests that scale-free networks tend to be low rank. From this result, we derive several graphical conditions to bound the rank of a DAG from above, providing simple sufficient conditions for low rank.
- Empirically, we demonstrate that the low rank adaptations are indeed useful. Not only do they outperform the original algorithms when the low rank condition is satisfied, the performance is also very competitive even when the true rank is not as low as is assumed.

Related Work The low rank assumption is frequently adopted in graph-based applications (Smith et al., 2012; Zhou et al., 2013; Yao & Kwok, 2016; Frot et al., 2019), matrix completion and factorization (Recht, 2011; Koltchinskii et al., 2011; Cao et al., 2015; Davenport & Romberg, 2016), network sciences (Hsieh et al., 2012; Huang et al., 2013; Zhang et al., 2017) and so on, but to our best knowledge, has not been used on the DAG structures in the context of learning causal DAGs. Yet, we notice two related works Barik & Honorio (2019); Tichavskỳ & Vomlel (2018) that assume low rank conditional probability tables in learning Bayesian networks, which are different from ours.

Also related are existing works that studied the rank of real weighted matrices described by a given simple directed/undirected graph. However, most works only considered the zero-nonzero pattern of *off-diagonal* entries (see, e.g., Fallat & Hogben (2007); Hogben (2010); Mitchell et al. (2010)), whereas we also take into account the diagonal entries. This difference is crucial: if one only considers the off-diagonal entries, then the maximum rank over all possible weighted matrices is trivial and is always equal to the number of vertices. Consequently, many works focus on minimum ranks of a given graph, but to characterize exactly the minimum rank remains open, except for some special graph structures like trees (Hogben, 2010). Apart from these works, Edmonds (1967) studied algebraically the maximum rank for matrices with a common zero-nonzero pattern. In Section 4, we use this result to relate the maximum possible rank to a more interpretable graphical condition, which further implies several structural conditions of DAGs that may be easier to obtain in practice.

2 Preliminaries

2.1 Graph Terminology

A graph $\mathcal{G}$ is defined as a pair $(\mathbf{V}, \mathbf{E})$, where $\mathbf{V} = \{X_1, X_2, \cdots, X_d\}$ is the vertex set and $\mathbf{E} \subset \mathbf{V}^2$ denotes the edge set. We are particularly interested in directed (acyclic) graphs in the context of causal structure learning. For any $\mathbf{S} \subset \mathbf{V}$, we use $\mathrm{pa}(\mathbf{S}, \mathcal{G})$, $\mathrm{ch}(\mathbf{S}, \mathcal{G})$, and $\mathrm{adj}(\mathbf{S}, \mathcal{G})$ to denote the union of all parents, children, and adjacent vertices of the nodes of $\mathbf{S}$ in $\mathcal{G}$, respectively. A graph is called weighted if every edge in the graph is associated with a non-zero value. We will work with weighted graphs and treat unweighted graphs as a special case where the edge weights are set to 1. Weighted graphs can be treated algebraically via weighted adjacency matrices. Specifically, the weighted adjacency matrix of a weighted graph $\mathcal{G}$ is a matrix $W \in \mathbb{R}^{d \times d}$, where $W(i, j)$ is the weight of edge $X_i \to X_j$ and $W(i, j) \neq 0$ if and only if $X_i \to X_j$ exists in $\mathcal{G}$. The binary adjacency

matrix $A \in \{0,1\}^{d\times d}$ is such that $A(i,j)=1$ if $X_i \to X_j$ in $\mathcal{G}$ and $A(i,j)=0$ otherwise. The rank of a weighted graph is defined as the rank of the associated weighted adjacency matrix.

2.2 Causal Structure Learning and Recent Gradient-based Methods

A commonly used model in causal structure learning is the structural equation model (SEM) that describes data generating procedure. In a slight abuse of notation, we also use X_i to denote random variables associated with the nodes in a graph $\mathcal{G}$. Assuming $\mathcal{G}$ being a DAG, then the SEM is given by

$$X_i = f_i\left(\mathrm{pa}(X_i,\mathcal{G}),\epsilon_i\right), \;\; i=1,2,\ldots,d,$$

where f_i is a deterministic function and ϵ_i's are jointly independent noises. The SEM induces a marginal distribution $P(X)$ over $X=[X_1,X_2,\cdots,X_d]^T$, and $\mathcal{G}$ and $P(X)$ are said to form a causal Bayesian network (Pearl, 2009; Spirtes et al., 2000). The problem of causal structure learning is to infer the underlying causal DAG $\mathcal{G}$ based on the marginal distribution $P(X)$, or more practically, an empirical version consisting of a number of i.i.d. observations from $P(X)$.

We next briefly review recently developed gradient-based methods that rely on a smooth characterization of acyclicity of directed graphs. They aim to find a DAG that optimizes a score function and can be categorized into two classes. The first class of methods explicitly associates the target causal model with a weighted adjacency matrix W and then estimate W by solving optimization problems in the following form:

$$\min_{W,\phi} \mathbb{E}_{X\sim P(X)}\, \mathcal{S}\big(X, h(X;W,\phi)\big), \;\; \text{subject to } \mathrm{trace}\left(e^{W\circ W}\right)-d=0, \tag{1}$$

where $h:\mathbb{R}^d\to\mathbb{R}^d$ is a model function parameterized by W (and other possible parameter ϕ) that aims to reconstruct X, $\mathcal{S}(\cdot,\cdot)$ denotes a score function between the true and reconstructed variables, notation $\circ$ denotes the element-wise product, and e^M is the matrix exponential of a square matrix M. The constraint was proposed by Zheng et al. (2018), which is smooth and holds if and only if W indicates a DAG. Methods in this class include: NOTEARS (Zheng et al., 2018), which targets linear models, with $h(X;W,\phi)=W^TX$ and $\mathcal{S}(\cdot,\cdot)$ being the Frobenius norm or equivalently the least-squares loss; and DAG-GNN (Yu et al., 2019) and the graph autoencoder approach (Ng et al., 2019b), where neural networks are used for the function h with ϕ being the weights of neural networks, and the score function can be the evidence lower bound (Kingma & Welling, 2013). A sparsity inducing term may be further added when the causal graph is assumed to be sparse. We comment that these objectives are equivalent to or are variants of some well studied score functions like the penalized maximum likelihood. For technical issues such as statistical consistency and parameter optimization in these methods (and also for the methods described below), we refer the reader to the the cited works and references therein for details.

The second class uses certain functions, with parameter θ, to construct a weighted adjacency matrix $W(\theta)$ (or a binary one $A(\theta)$) to represent the causal structure. These methods can be summarized as

$$\min_{\theta,\,\phi} \mathbb{E}_{X\sim P(X)}\, \mathcal{S}\big(X, h(X;W(\theta),\phi)\big), \;\; \text{subject to } \mathrm{trace}\left(e^{W(\theta)\circ W(\theta)}\right)-d=0. \tag{2}$$

For example, GraN-DAG (Lachapelle et al., 2020) and NOTEARS-MLP (Zheng et al., 2020) respectively use neural network path products and partial derivatives between variables to construct $W(\theta)$. The binary matrix $A(\theta)$ can be obtained by sampling according to some distributions with learnable parameters, as used by Kalainathan et al. (2018); Ke et al. (2019); Ng et al. (2019a); Zhu et al. (2020).

3 Exploiting Low Rank Assumption in Causal Structure Learning

This section shows how to adapt existing gradient-based methods to take advantage of the low rank assumption, by providing a way for each class to utilize this assumption using techniques from the matrix completion literature. We remark that our adaptations with the low rank assumption are not restricted to a particular learning algorithm; other DAG learning methods may potentially combine one of the proposed modifications for learning low rank causal graphs, too.

Matrix Factorization Since the weighted adjacency matrix W is explicitly optimized in the first class of methods, we can then apply the matrix factorization technique. Specifically, with an estimate

$\hat{r}$ for the graph rank, we can factorize W as $W = UV^T$ with $U, V \in \mathbb{R}^{d\times\hat{r}}$. Problem (1) is then to optimize U and V that minimizes the score function under the DAG constraint, and has the same solution W (obtained from the product UV^T) as the original one if $\hat{r}$ is greater than or equal to the true rank. Furthermore, if $\hat{r} \ll d$, we have a much reduced number of parameters to optimize.

Nuclear Norm For the second class of methods, the adjacency matrix $W(\theta)$ is not an explicit parameter to be optimized. In such a case, we can adopt a commonly used technique to add a nuclear norm term $\lambda\|W(\theta)\|_*$, with $\lambda > 0$ being a tuning parameter, to the objective to induce low-rankness.

The optimization procedures in these recent structure learning methods can directly incorporate the two adaptations as they are all gradient-based, though some extra care needs to be taken. Appendix C provides a detailed description of the optimization procedure and our implementation. The second approach is also feasible for the first class of methods, but we find that it does not work as well as the matrix factorization approach, possibly due to the singular value decomposition to compute the (sub-)gradient w.r.t. W at each optimization step.

An acute reader may have noticed that we assumed a proper rank estimate $\hat{r}$ or a proper penalty parameter λ. Yet knowing exactly the rank of the graph to be learned can be difficult in practice. Similar to the sparsity assumption, one may determine the hyperparameters $\hat{r}$ and λ assisted by a validation dataset (or by cross-validation if the observed dataset is not sufficiently large). Alternatively, we can try different choices of the hyperparameters and then apply traditional score-based method where the search space is restricted to the resulting DAGs. However, since we are more concerned with relatively large and dense problems, the possible ranks may be too many to choose. As such, a lower bound r_l and an upper bound r_u on the graph rank would be beneficial—we need only consider ranks in $[r_l, r_u]$ in the matrix factorization method, while the bounds are still useful by providing qualitative information for the nuclear norm methods: the lower an upper bound, the higher the tuning parameter λ should be chosen. Moreover, a lower bound can also justifies the low rank assumption, i.e., if the lower bound is high, then the low rank assumption is likely to fail to hold.

4 Graphical Bounds on Ranks

Obtaining exact algebraic information of a DAG such as its rank and eigenvalues may be infeasible in practice, because it may require a full knowledge of the graph to be learned. On the other hand, we usually have access to some structural information, including graph connectivity, distributions of in-degrees and out-degrees, an estimate of number of hubs, etc. As such, this section is devoted to relating the rank of a graph to more easily interpretable graphical conditions, for the sake of a better understanding of what kinds of DAGs tend to satisfy the low rank assumption and for lower and upper bounds on the graph rank from certain structural priors.

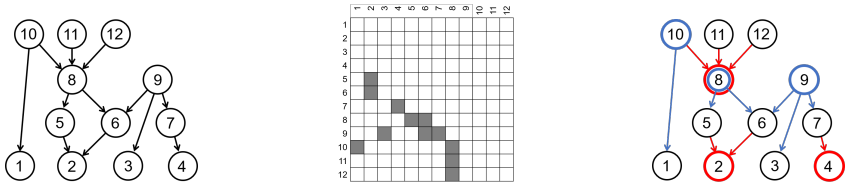
4.1 Problem Setting

Consider a DAG $\mathcal{G} = (\mathbf{V}, \mathbf{E})$ with weighted adjacency matrix W and binary adjacency matrix A. We aim to seek upper and lower bounds on $\mathrm{rank}(W)$ using only the graphical structure. Specifically, we focus on the weighted adjacency matrices with the same binary adjacency matrix A, i.e., $\mathcal{W}_A = \{W \in \mathbb{R}^{d\times d};\ \mathrm{sign}(|W|) = A\}$, where $\mathrm{sign}(\cdot)$ and $|\cdot|$ are point-wise sign and absolute value functions, respectively. Notice that there exist trivial upper bound $d-1$ and lower bound 0 for any DAG, but they are generally too loose for our purpose. In the following, we investigate the maximum rank $\max\{\mathrm{rank}(W); W \in \mathcal{W}_A\}$ and minimum rank $\min\{\mathrm{rank}(W); W \in \mathcal{W}_A\}$ to find tighter upper and lower bounds for any $W \in \mathcal{W}_\mathcal{A}$. Before introducing two useful graph concepts, we comment that low rank DAGs are not necessarily sparse and vice versa; see a discussion in Appendix A.

Definition 1 (Height)**.** *Given a DAG $\mathcal{G} = (\mathbf{V}, \mathbf{E})$ and a vertex $X_i \in \mathbf{V}$, the height of X_i, denoted by $l(X_i)$, is defined as the length of the longest directed path starting from X_i. The height of $\mathcal{G}$, denoted by $l(\mathcal{G})$, is defined as the longest directed path in $\mathcal{G}$.*

Definition 2 (Head-tail vertex cover)**.** *Let $\mathcal{G} = (\mathbf{V}, \mathbf{E})$ be a directed graph and $\mathbf{H}, \mathbf{T}$ be two subsets of $\mathbf{V}$. $(\mathbf{H}, \mathbf{T})$ is called a head-tail vertex cover of $\mathcal{G}$ if every edge in $\mathcal{G}$ has its head vertex in $\mathbf{H}$ or its tail vertex in $\mathbf{T}$. The size of a head-tail vertex cover $(\mathbf{H}, \mathbf{T})$ is defined as $|\mathbf{H}| + |\mathbf{T}|$.*

As an example, Figure 1c is a head-tail vertex cover of $\mathcal{G}$ in Figure 1a, where $\mathbf{H} = \{X_2, X_4, X_8\}$ (red nodes) and $\mathbf{T} = \{X_8, X_9, X_{10}\}$ (blue nodes). The size of this vertex cover is 6.



(a) A DAG $\mathcal{G}$ (b) Binary adjacency matrix (c) A head-tail vertex cover

Figure 1: A DAG $\mathcal{G}$ with 12 vertices, 12 edges and height 3, where $\mathbf{V}_0 = \{X_1, X_2, X_3, X_4\}$, $\mathbf{V}_1 = \{X_5, X_6, X_7\}$, $\mathbf{V}_2 = \{X_8, X_9\}$, and $\mathbf{V}_3 = \{X_{10}, X_{11}, X_{12}\}$.

4.2 Lower Bounds

We first study lower bounds on the rank of a weighted DAG. Define $\mathbf{V}_{-1} = \varnothing$ and $\mathbf{V}_s = \{X_i; l(X_i) = s\}$ for $s = 0, 1, \ldots, l(\mathcal{G})$. Denote by $\mathcal{G}_{s,s-1}$ the induced subgraph of $\mathcal{G}$ over $V_s \cup V_{s-1}$. Let $\mathcal{C}(\mathcal{G}_{s,s-1})$ be the set of non-singleton connected components of $\mathcal{G}_{s,s-1}$ and $|\mathcal{C}(\mathcal{G}_{s,s-1})|$ be the cardinality. We have the following lower bounds.

Theorem 1. *Let $\mathcal{G}$ be a DAG with binary adjacency matrix A. Then*

$$\min\{\mathrm{rank}(W)\,;\ W \in \mathcal{W}_A\} \geq \sum\nolimits_{s=1}^{l(\mathcal{G})} |\mathcal{C}(\mathcal{G}_{s,s-1})| \geq l(\mathcal{G}). \tag{3}$$

All the proofs in this paper are provided in Appendix B. Theorem 1 shows that $\mathrm{rank}(W)$ is greater than or equal to the sum of the number of non-singleton connected components in each $\mathcal{G}_{s,s-1}$. As $\mathcal{G}_{s,s-1}$ has at least one non-singleton connected component, we obtain the second inequality. In other words, the rank of a weighted DAG is at least as high as the length of the longest directed path. As an example, consider the graph shown in Figure 1. One can verify that $\min\{\mathrm{rank}(W); W \in \mathcal{W}_A\} = 6$, $|\mathcal{C}(\mathcal{G}_{1,0})| = 2$, $|\mathcal{C}(\mathcal{G}_{2,1})| = 1$, $|\mathcal{C}(\mathcal{G}_{3,2})| = 1$, and $l(\mathcal{G}) = 3$. Thus, we have $\min\{\mathrm{rank}(W); W \in \mathcal{W}_A\} = 6 > 2 + 1 + 1 = 4 > 3$. We remark the bounds in Theorem 1 may be loose in some cases. How to characterize the minimum rank exactly is still an on-going research problem (Hogben, 2010).

4.3 Upper Bounds

We turn to the more important issue for our purpose, regarding upper bounds on $\mathrm{rank}(W)$. The next theorem shows that $\max\{\mathrm{rank}(W); W \in \mathcal{W}_A\}$ can be characterized exactly in graphical terms.

Theorem 2. *Let $\mathcal{G}$ be a directed graph with binary adjacency matrix A. Then $\max\{\mathrm{rank}(W); W \in \mathcal{W}_A\}$ is equal to the minimum size of the head-tail vertex covers of $\mathcal{G}$, that is,*

$$\max\{\mathrm{rank}(W)\,;\ W \in \mathcal{W}_A\} = \min\{|\mathbf{H}| + |\mathbf{T}|\,;\ (\mathbf{H}, \mathbf{T}) \textit{ is a head-tail vertex cover of } \mathcal{G}\}.$$

We comment that Theorem 2 holds for all directed graphs (not only DAGs), which may be of independent interest to other applications. A head-tail vertex cover of minimum size is called a minimum head-tail vertex cover, which in general is not unique. For a head-tail vertex cover $(\mathbf{H}, \mathbf{T})$, the vertices in $\mathbf{H}$ cover all the edges pointing towards these vertices while the vertices in $\mathbf{T}$ cover the edges pointing away. A head-tail cover of a relatively small size then indicates the presence of hubs, that is, vertices with relatively high in-degrees or out-degrees. Therefore, Theorem 2 suggests that the maximum rank of a weighted DAG is highly related to the presence of hubs: a DAG with many hubs tends to have low rank. Intuitively, a hub of high in-degree (out-degree) is a common effect (cause) of a number of direct causes (effect variables), comprising many V-structures (inverted V-structures). For example, in Figure 1a, X_8 is a hub of V-structures and X_9 is a hub of inverted V-structures.

Such features are fairly common in real graph structures. Appendix A presents a real network, called *pathfinder*, which describes the causal relations among 109 variables (Heckerman et al., 1992) with the center node being the parent of a large number of other nodes. The famous scale-free (SF) graphs also tend to have hubs. A scale-free graph is one whose distribution of degree k follows a power law: $P(k) \sim k^{-\gamma}$, where γ is the power parameter typically within $[2, 3]$ and $P(k)$ denotes the fraction of nodes with degree k (Nikolova & Aluru, 2012). It is observed that many real-world networks are scale-free, and some of them may be viewed as causal networks (Guelzim et al., 2002; Barabasi & Oltvai, 2004; Hartemink, 2005; Eguíluz et al., 2005; Gao & en Ren, 2013; Ramsey et al., 2017).

Empirically, the ranks of scale-free graphs are relatively low, especially in comparison to Erdös-Rényi (ER) random graphs (Mihail & Papadimitriou, 2002). Figure 2 provides a simulated example where γ is chosen from $\{2, 3\}$ and each reported value is over 100 random runs. As graph becomes denser, the graph rank also increases. However, for scale-free graphs with a relatively large γ, the increase of their ranks is much slower than that of Erdös-Rényi graphs; indeed, their ranks tend to stay fairly low even when the graph degree is large.

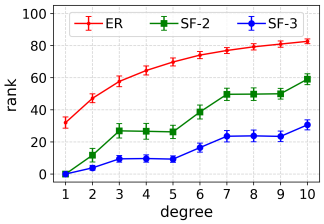


Figure 2: 100-node graphs.

Theorem 2 can also be used to generate a low rank graph, or more precisely, a random DAG with a given rank r and a properly specified graph degree. Here we briefly describe the idea and leave the detailed algorithm to Appendix C.1: first generate a graph with r edges and rank r; a random edge is sampled without replacement and would be added to the graph, if adding this edge does not increase the size of the minimum head-tail vertex cover; repeat the previous step until the pre-specified degree is reached or no edge could be added to the graph; finally, assign the edge weights randomly according to a continuous distribution and the weighted graph will have rank r with high probability.

The next two theorems report some looser but simpler upper bounds on $\mathrm{rank}(W)$.

Theorem 3. *Let $\mathcal{G}$ be a DAG with binary adjacency matrix A, and denote the set of vertices with at least one parent by $\mathbf{V}_{\mathrm{ch}}$ and those with at least one child by $\mathbf{V}_{\mathrm{pa}}$. Then we have*

$$\max\{\mathrm{rank}(W)\,;\; W \in \mathcal{W}_A\} \leq \begin{cases} \sum_{s=1}^{l(\mathcal{G})} \min\left(|\mathbf{V}_s|, |\mathrm{ch}(\mathbf{V}_s)|\right) \leq |\mathbf{V}_{\mathrm{pa}}|, \\ \sum_{s=0}^{l(\mathcal{G})-1} \min\left(|\mathbf{V}_s|, |\mathrm{pa}(\mathbf{V}_s)|\right) \leq |\mathbf{V}_{\mathrm{ch}}|, \\ |\mathbf{V}| - \max\{|\mathbf{V}_s|\,;\; 0 \leq s \leq l(\mathcal{G})\}. \end{cases} \tag{4}$$

Since $\mathbf{V}_{\mathrm{ch}}$ and $\mathbf{V}_{\mathrm{pa}}$ are the non-root and the non-leaf vertices, respectively, the first two inequalities of (4) indicate that the maximum rank is bounded from above by the number of non-root vertices and also by the number of non-leaf vertices. The last inequality of (4) is a generalization of the first two, which implies that the rank is likely to be low if most vertices have the same height.

Theorem 4. *Let $\mathcal{G}$ be a DAG with binary adjacency matrix A. Denote by* $\mathrm{skeleton(A)}$ *and* $\mathrm{moral(A)}$ *the binary adjacency matrices of the skeleton and moral graph of $\mathcal{G}$, respectively. Then we have*

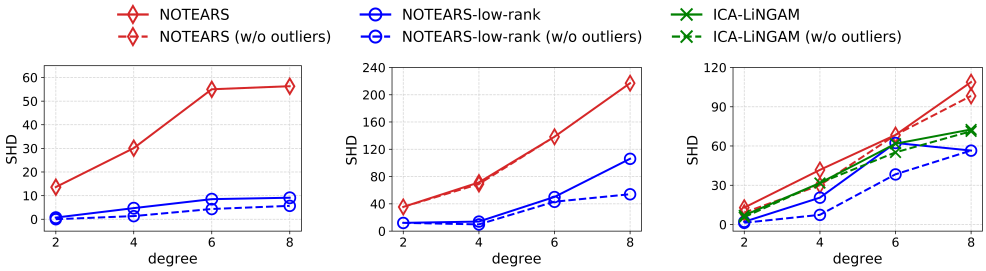
$$\begin{aligned} \max\{\mathrm{rank}(W)\,;\; W \in \mathcal{W}_A\} &\leq \max\{\mathrm{rank}(W)\,;\; \mathrm{sign}(|W|) = \mathrm{skeleton}(A)\} \\ &\leq \max\{\mathrm{rank}(W)\,;\; \mathrm{sign}(|W|) = \mathrm{moral}(A)\}. \end{aligned}$$

The skeleton of a DAG is the undirected graph obtained by removing all the arrowheads, and the moral graph is the undirected graph where two vertices are adjacent if they are adjacent or if they share a common child in the DAG. This is useful when the skeleton or the moral graph can be accurately estimated and the corresponding rank is low. However, we empirically find that the ranks of these two graphs are generally looser than the bounds given in Theorem 3.

5 Experiments

This section reports empirical results of the low rank adaptations of existing methods, compared with their original versions. We choose NOTEARS (Zheng et al., 2020) for linear SEMs by adopting the matrix factorization approach, denoted as NOTEARS-low-rank, and use the nuclear norm approach in combination with GraN-DAG (Lachapelle et al., 2020) for a non-linear data model. Again we remark that the two methods are only demonstrations of the utility of low rank assumption, which can be potentially combined with other methods as well. For more information, we also include several benchmark methods: fast GES (Ramsey et al., 2017), PC (Spirtes et al., 2000), MMHC (Tsamardinos et al., 2006), ICA-LiNGAM (Shimizu et al., 2006) specifically designed with non-Gaussian noises, for linear SEMs; and DAG-GNN (Yu et al., 2019), NOTEARS-MLP (Zheng et al., 2020), and CAM (Bühlmann et al., 2014) for the non-linear case. Their implementations are described in Appendix C.

We consider randomly sampled DAGs with specified ranks (the generating procedure was described in Section 4.3 and is given as Algorithm 1 in Appendix C.1), scale-free graphs, and a real network



(a) $d = 100$, Gaussian (b) $d = 300$, Gaussian (c) $d = 100$, Exponential

Figure 3: Average SHDs on rank-specified graphs. The models are linear SEMs with (a)-(b) Gaussian noises, and (c) exponential noises. The true rank is assumed to be known.

structure. For linear SEMs, the weights are uniformly sampled from $[-2, -0.5] \cup [0.5, 2]$ and the noises are either standard Gaussian or standard exponential. For non-linear SEMs, we use additive Gaussian noise model with functions sampled from Gaussian processes with RBF kernel of bandwidth one. These data models are known to be identifiable (Shimizu et al., 2006; Peters & Bühlmann, 2013; Peters et al., 2014). From each SEM, we then generate $n = 3,000$ observations. We repeat ten times over different seeds for each experiment setting. Detailed information about the setup can be found in Appendix C.3. Below we mainly report structural Hamming distance (SHD) which takes into account both false positives and false negatives, and a smaller SHD indicates a better estimate.

5.1 Linear SEMs with Rank-Specified Graphs

We first consider linear SEMs on rank-specified graphs, with number of nodes $d \in \{100, 300\}$, rank $r = \lceil 0.1d \rceil$, and degree $k \in \{2, 4, 6, 8\}$. The true rank is assumed to be known and is used as the rank parameter $\hat{r}$ in NOTEARS-low-rank. For a better visualization, Figure 3 only reports the average SHDs, while the true positive rate, false discovery rate, and running time are provided in Appendix D. We also show the results after using the interquartile range rule to remove outlier SHDs. We observe that the low rank assumption can greatly improve the performance of NOTEARS, reducing the SHDs by at least a half. For this data model, GES has much higher SHDs (see also Appendix D). PC is too slow (for example, it did not finish in 16 hours a dataset with 100 nodes and degree 6), because some nodes may have a high in-degree. For the same reason, the skeleton may not be well estimated by MMHC; its performance is similar to GES and is not reported.

Appendix D.1 studies graphs with higher ranks, where it is observed that the advantage of NOTEARS-low-rank over NOTEARS decreases when the rank of the underlying DAG increases. Nevertheless, NOTEARS-low-rank is still competitive when the true rank is $\lceil d/2 \rceil$, when the factorized matrix has the same number of parameters as NOTEARS. We also conduct an empirical analysis with different sample sizes in Appendix D.2, which shows that NOTEARS-low-rank performs reasonably well when the sample size is small and tends to have a better performance with a larger number of samples. Due to space limit, please find further details in the appendix.

5.2 Linear SEMs with Scale-Free Graphs

We next consider scale-free graphs with $d = 100$ nodes, average degree $k = 6$, and power $\gamma = 2.5$. For this experiment, the minimum, maximum, and mean ranks of generated graphs are 14, 24, and 18.7, respectively. Here we choose the rank parameter $\hat{r}$ from $\{20, 30, 40\}$ for NOTEARS-low-rank. As seen from Figure 4, NOTEARS-low-rank with rank parameter $\hat{r} = 20$ performs the best, even though there are graphs with ranks greater than 20.

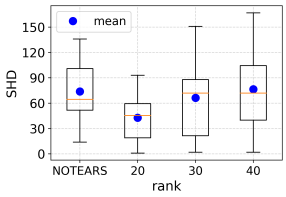


Figure 4: Scale-free graphs.

5.3 Sensitivity of Rank Parameters and Validation

So far we have assumed that the true rank or an accurate estimate is known. In this experiment, we conduct an empirical analysis with different rank parameters for linear Gaussian data model

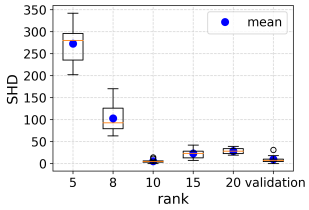


Figure 5: Different rank parameters.

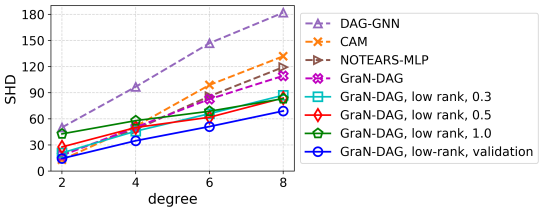


Figure 6: Non-linear SEMs.

on rank-specified graphs with 100 nodes, degree 8, and rank 10. We include the validation based approach where $2,000$ samples are chosen as training dataset and the rest for validation, and also use the derived lower and upper bounds in Theorems 1 and 3 to select 7 evenly distributed rank parameters, assuming that the corresponding structural priors are available. As seen from Figure 5, NOTEARS-low-rank performs the best when the rank parameter is identical to the true rank, while the rank parameter chosen by validation has almost the same performance. Compared with NOTEARS on the same datasets (cf. Figure 3), the low rank version performs well across a range of rank parameters.

5.4 Non-Linear SEMs

For non-linear data models, we pick rank-specified graphs with $d = 50$ nodes, rank 5, and degree $k \in \{2, 4, 6, 8\}$. To our knowledge, the selected benchmark methods CAM, NOTEARS-MLP, and GraN-DAG are current state-of-the-art methods on this data model. As a demonstration of the low rank assumption, we apply the nuclear norm approach to GraN-DAG and choose from $\{0.3, 0.5, 1.0\}$ as the penalty weights. For validation, we use the same splitting ratio as in Section 5.3 and consider more penalty weights ranging from 0.1 to 2, where the one with lowest validation error is chosen. As shown in Figure 6 (see Appendix D.5 for a more detailed result), adding a nuclear norm can improve the performance of GraN-DAG across a large range of weights when the graph is relatively dense. For degree 8, the low rank version with validation achieves an average SHD 77.4, while the SHDs of CAM, NOTEARS-MLP and original GraN-DAG are respectively 131.9, 119.4, and 109.4.

5.5 Real Network

We apply the proposed method to the *arth150* gene network, which is a DAG containing 107 genes and 150 edges. Its maximum rank is 40. Since the real dataset has only 22 samples, we instead use simulated data from linear Gaussian SEMs. We pick $\hat{r}$ from $\{36, 40, 44\}$ and use validation to pick the rank parameter. We also include NOTEARS with a sparsity inducing term, named NOTEARS-L1. Here the ℓ_1 penalty weight is chosen from $\{0.05, 0.1, 0.2\}$ and we treat this method favorably by reporting the lowest SHD. The mean and median SHDs are shown in Figure 7. The experimental result demonstrates again the utility of the low rank assumption, even when the true rank is not as low as is assumed.

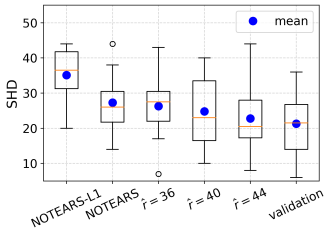


Figure 7: Real network.

6 Concluding Remarks

This paper studies the potential of low rank assumption in causal structure learning. Empirically, we show that the low rank adaptations perform noticeably better than existing algorithms when the low rank condition is satisfied, and also deliver competitive performances when the rank is not as low as is assumed. Theoretically, we provide an improved understanding of what kinds of graphs tend to be low rank and a possibility to obtain bounds on the true rank from several structural priors.

We treat the present work as our first step to incorporate low-rankness into causal DAG learning. A future direction is to approximate a high rank DAG with a low rank one. While there is a rich literature on low rank approximations of matrices, it is non-trivial to us to conclude under what conditions such an approximation is guaranteed to be effective to learn causal DAGs. Another direction is to investigate if a low rank DAG model implies any interesting and useful behavior in the data.

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Appendix

A EXAMPLES

We provide more examples and discussions in this section.

Minimum rank of the graph in Figure 1 We first show that the minimum rank of the DAG structure in Figure 1 is 6. It is clear that the 6-th to 10-th rows of A are always linearly independent, so it suffices to show that the 11-th row is linearly independent of the 6-th to 10-th rows. To see this, notice that if the 11-th row is a linear combination of the 6-th to 10-th rows, then $A(11, 1)$ would be non-zero, which is a contradiction.

The *pathfinder* and *arth150* networks Figure 8 visualizes the *pathfinder* and *arth150* networks that are mentioned in Sections 4.3 and 5, respectively. Both networks can be found at `http://www.bnlearn.com/bnrepository`. As one can see, these two networks contain hubs: the center note in the *pathfinder* network has a large number of children, while the *arth150* network contains many 'small' hubs, each of which has $5 \sim 10$ children. We also notice that nearly all the hubs in the two networks have high out-degrees.

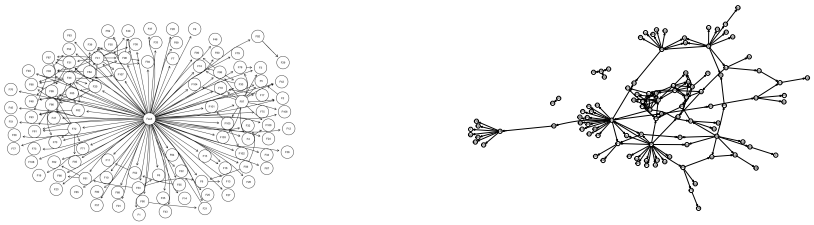
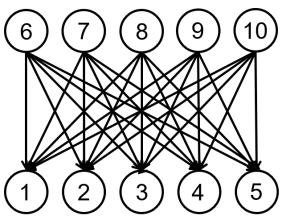


Figure 8: The *pathfinder* network (left) and the *arth150* network (right).

Sparse DAGs and low rank DAGs A sparse DAG does not necessarily indicate a low rank DAG, and vice versa. For example, a directed linear graph with d vertices has only $d - 1$ edges, while the rank of its binary adjacency matrix is $d - 1$. According to Theorems 1 and 2, the maximum and minimum ranks of a directed linear graph are equal to its number of edges. Thus, directed linear graphs are sparse but have high ranks. On the other hand, for some non-sparse graphs, we can assign the edge weights so that the resulting graphs have low ranks. A simple example would be a fully connected directed balanced bipartite graph, as shown in Figure 9. The definition of bipartite graphs can be found in Appendix B.1. A bipartite graph is called balanced if its two parts contain the same number of vertices. The rank of a fully connected balanced bipartite graph with d vertices is 1 if all the edge weights are the same (e.g., the binary adjacency matrix), but the number of edges is $d^2/4$.



(a) $\mathcal{G}$

	1	2	3	4	5	6	7	8	9	10
1										
2										
3										
4										
5										
6	1	1	1	1	1					
7	1	1	1	1	1					
8	1	1	1	1	1					
9	1	1	1	1	1					
10	1	1	1	1	1					

(b) binary adjacency matrix

Figure 9: A fully connected directed balanced bipartite graph $\mathcal{G}$ and its binary adjacency matrix.

We also notice that there exist some connections between the maximum rank and the graph degree, or more precisely, the total number of edges in the graph, according to Theorem 2. Intuitively, if the graph is dense, then we need more vertices to cover all the edges. Thus, the size of the minimum

head-tail vertex cover should be large. Explicitly providing a formula to characterize these two graph parameters is an interesting problem, which will be explored in the future.

B PROOFS

In this section, we present proofs for the theorems given in the main content.

B.1 PRELIMINARIES

A bipartite graph is a graph whose vertex set $\mathbf{V}$ can be partitioned into two disjoint subsets $\mathbf{V}_0$ and $\mathbf{V}_1$, such that the vertices within each subset are not adjacent to one another. $\mathbf{V}_0$ and $\mathbf{V}_1$ are called the parts of the graph. A matching of a graph is a subset of its edges where no two of them share a common endpoint. A vertex cover of a graph is a subset of the vertex set where every edge in the graph has at least one endpoint in the subset. The size of a matching (vertex cover) is the number of edges (vertices) in the matching (vertex cover). A maximum matching of a graph is a matching of the largest possible size and a minimum vertex cover is a vertex cover of the smallest possible size. An important result about bipartite graphs is König's theorem (Dénes, 1931), which states that the size of a minimum vertex cover is equal to the size of a maximum matching in a bipartite graph.

Based on the heights of vertices in $\mathbf{V}$, we can define a weak ordering among the vertices: $X_i \succ X_j$ if and only if $l(X_i) > l(X_j)$, and $X_i \sim X_j$ if and only if $l(X_i) = l(X_j)$. Given this weak ordering, we can group the vertices by their heights, and the resulting graph shows a hierarchical structure; see Figure 1 in the main text for an example. This hierarchical representation has some simple and nice properties. Let $\mathbf{V}_s = \{X_i; l(X_i) = s\}$, $s = 0, 1, \ldots, l(\mathcal{G})$, and let $\mathbf{V}_{-1} = \varnothing$. We have: (1) for any given $s \in \{0, 1, \ldots, l(\mathcal{G})\}$ and two distinct vertices $X_1, X_2 \in \mathbf{V}_s$, X_1 and X_2 are not adjacent, and (2) for any given $s \in \{1, 2, \ldots, l(\mathcal{G})\}$ and $X_i \in \mathbf{V}_s$, there is at least one vertex in $\mathbf{V}_{s-1}$ which is a child of X_i. If we denote the induced subgraph of $\mathcal{G}$ over $\mathbf{V}_s \cup \mathbf{V}_{s-1}$ by $\mathcal{G}_{s,s-1}$, then $\mathcal{G}_{s,s-1}$ is a bipartite graph with $\mathbf{V}_s$ and $\mathbf{V}_{s-1}$ as parts, and singletons in $\mathcal{G}_{s,s-1}$ (i.e., vertices that are not endpoints of any edge) only appear in $\mathbf{V}_{s-1}$.

For simplicity, we occasionally use index i to represent variable X_i in the following sections .

B.2 PROOF OF THEOREM 1

Proof. Let $\mathcal{G} = (\mathbf{V}, \mathbf{E})$. Consider an equivalence relation, denoted by $\sim$, among vertices in $\mathbf{V}$ defined as follows: for any $X_i, X_j \in \mathbf{V}$, $X_i \sim X_j$ if and only if $l(X_i) = l(X_j)$ and X_i and X_j are connected. Here, connected means that there is a path between X_i and X_j. Below we use $C(X_i)$ to denote the equivalence class containing X_i. Next, we define a weak ordering π on $\mathbf{V}/\sim$, i.e., the equivalence classes induced by $\sim$, by letting $C(X_i) \succeq_\pi C(X_j)$ if and only if $l(X_i) \geq l(X_j)$. Then, we extend $\succeq_\pi$ to a total ordering ρ on $\mathbf{V}/\sim$. The ordering ρ also induces a weak ordering (denoted by $\bar{\rho}$) on $\mathbf{V}$: $X_i \succeq_{\bar{\rho}} X_j$ if and only if $C(X_i) \succ_\rho C(X_j)$. Finally, we extend $\bar{\rho}$ to a total ordering γ on $\mathbf{V}$. It can be verified that γ is a topological ordering of $\mathcal{G}$, that is, if we relabel the vertices according to γ, then $X_i \in \mathrm{pa}(X_j, \mathcal{G})$ if and only if $i > j$ and X_i and X_j are adjacent, and the adjacency matrix of $\mathcal{G}$ becomes lower triangular.

Assume that the vertices of $\mathcal{G}$ are relabeled according to γ and we will consider the binary adjacency matrix A of the resulting graph throughout the rest of this proof. Note that relabelling is equivalent to applying a permutation onto the adjacency matrix, which does not change the rank. Let $\mathbf{V}_0 = \{1, 2, \ldots, k_1 - 1\}$ for some $k_1 \geq 2$. Then the k_1-th row of A, denoted by $A(k_1, \cdot)$, is the first non-zero row vector of A. Letting $S = \{A(k_1, \cdot)\}$, then S contains a subset of linearly independent vector(s) of the first k_1 rows of A. Suppose that we have visited the first m rows of A and $S = \{A(k_1, \cdot), A(k_2, \cdot), \ldots, A(k_t, \cdot)\}$ contains a subset of linearly independent vector(s) of the first m rows of A, where $k_1 \leq m < d$. If $X_{m+1} \nsim X_{k_t}$, then we add $A(m+1, \cdot)$ to S; otherwise, we keep S unchanged. We claim that the vectors in S are still linearly independent after the above step. Clearly, if we do not add any new vector, then S contains only linearly independent vectors. To show the other case, note that if $l(X_{m+1}) > l(X_{k_t}) \geq \cdots \geq l(X_{k_1})$, then there is an index $i \in \mathbf{V}_{l(X_{m+1})-1}$ such that $A(m+1, i) \neq 0$, by the definition of height. Since $l(X_{m+1}) > l(X_{k_t})$, we have $l(X_{k_t}) \leq l(X_{m+1}) - 1$ and thus $A(k_j, i) = 0$ for all $j = 1, 2, \ldots, t$. Therefore, $A(m+1, \cdot)$ cannot be linearly represented by $\{A(k_j, \cdot); j = 1, 2, \ldots, t\}$ and the vectors in S are linearly independent.

On the other hand, if $l(X_{m+1}) = l(X_{k_t})$, then the definition of the equivalence relation $\sim$ implies that X_{m+1} and X_{k_t} are disconnected, which means that X_{m+1} and X_{k_t} do not share a common child in $\mathbf{V}_{l(X_{m+1})-1}$. Consequently, there is an index $i \in \mathbf{V}_{l(X_{m+1})-1}$ such that $A(m+1, i) \neq 0$ but $A(k_t, i) = 0$. Similarly, we can show that $A(k_j, i) = 0$ for all $j = 1, 2, \ldots, t$. Thus, the vectors in S are still linearly independent.

After visiting all the rows in A, the number of vectors in S is equal to $\sum_{s=1}^{l(\mathcal{G})} |\mathcal{C}(\mathcal{G}_{s,s-1})|$ based on the definition of $\sim$. The second inequality can be shown by noting that $\mathcal{C}(\mathcal{G}_{s,s-1})$ has at least one elements. The proof is complete. □

B.3 Proof of Theorem 2

Proof. Denote the directed graph by $\mathcal{G} = (\mathbf{V}, \mathbf{E})$. Edmonds (1967, Theorem 1) shows that $\max\{\mathrm{rank}(W); W \in \mathcal{W}_A\}$ is equal to the maximum number of nonzero entries of A, no two of which lie in a common row or column. Therefore, it suffices to show that the latter quantity is equal to the size of the minimum head-tail vertex cover. Let $\mathbf{V}^{'} = \mathbf{V}_0' \cup \mathbf{V}_1'$, where $\mathbf{V}_0' = \mathbf{V} \times \{0\} = \{(X_i, 0); X_i \in \mathbf{V}\}$ and $\mathbf{V}_1' = \mathbf{V} \times \{1\} = \{(X_i, 1); X_i \in \mathbf{V}\}$. Now define a bipartite graph $\mathcal{B} = (\mathbf{V}^{'}, \mathbf{E}^{'})$ where $\mathbf{E}^{'} = \{(X_i, 0) \to (X_j, 1); (X_i, X_j) \in \mathbf{E}\}$. Denote by $\mathcal{M}$ a set of nonzero entries of A so that no two entries lie in the same row or column. Notice that $\mathcal{M}$ can be viewed as an edge set and no two edges in $\mathcal{M}$ share a common endpoint. Thus, $\mathcal{M}$ is a matching of $\mathcal{B}$. Conversely, it can be shown by similar arguments that any matching of $\mathcal{B}$ corresponds to a set of nonzero entries of A, no two of which lie in a common row or column. Therefore, $\max\{\mathrm{rank}(W), W \in \mathcal{W}_A\}$ equals the size of the maximum matching of $\mathcal{B}$, and further the size of the minimum vertex cover of $\mathcal{B}$ according to König theorem. Note that any vertex cover of $\mathcal{B}$ can be equivalently transformed to a head-tail vertex cover of $\mathcal{G}$, by letting $\mathbf{H}$ and $\mathbf{T}$ be the subsets of the vertex cover containing all variables in $\mathbf{V}_0'$ and of the vertex cover containing all variables in $\mathbf{V}_1'$, respectively. Thus, $\max\{\mathrm{rank}(W), W \in \mathcal{W}_A\}$ is equal to the size of the minimum head-tail vertex cover. □

B.4 Proof of Theorem 3

Proof. We start with the first inequality in Equation (4). Let $h_1, \ldots, h_p$ denote the heights where $|\mathbf{V}_s| < |\mathrm{ch}(\mathbf{V}_s)|$, and $t_1, \ldots, t_q$ the height where $|\mathbf{V}_s| > |\mathrm{ch}(\mathbf{V}_s)|$. Let $\mathbf{H} = \cup_{i=1}^{p} \mathbf{V}_{h_i}$ and $\mathbf{T} = \cup_{i=1}^{q} \mathbf{V}_{t_i}$. It is straightforward to see that $(\mathbf{H}, \mathbf{T})$ is a head-tail vertex cover. Thus, Equation (4) holds according to Theorem 2. The second inequality can be shown similarly and its proof is omitted. For the third inequality, let $m = \mathrm{argmax}\{|\mathbf{V}_s| : 0 \leq s \leq l(\mathcal{G})\}$, and define $\mathbf{H} = \cup_{i>m} \mathbf{V}_i$ and $\mathbf{T} = \cup_{i<m} \mathbf{V}_i$. Then $(\mathbf{H}, \mathbf{T})$ is also a head-tail vertex cover and the third inequality follows from Theorem 2, too. □

B.5 Proof of Theorem 4

Proof. Notice that Theorem 2 holds for all directed graphs. This theorem then follows by treating the skeleton and the moral graph as directed graphs with loops, i.e., an undirected edge $X_i - X_j$ is treated as two directed edges $X_i \to X_j$ and $X_j \to X_i$. □

C Implementation Details

In this section, we present an algorithm to generate a random DAG with a given rank, a low rank version of NOTEARS and GraN-DAG, and also a description of our experimental settings.

C.1 Generating Random DAGs

In Section 4.3, we briefly discuss the idea of generating a random DAG with a given rank. We now describe the detailed procedure in Algorithm 1. In particular, we aim to generate a random DAG with d nodes, average degree k, and rank r. The first part of Algorithm 1 after initialization is to sample a number N, representing the total number of edges, from a binomial distribution $\mathcal{B}(d(d-1)/2, p)$ where $p = k/(d-1)$. If $N < r$, Algorithm 1 would return FAIL since a graph with $N < r$ edges

Algorithm 1 Generating random DAGs

Require: Number of nodes d, average degree k, and rank r.
Ensure: A randomly sampled DAG with with number of nodes d, average degree k, and rank r.

```
Set M = empty graph, M_p = ∅, and R = {(i, j); i < j, i, j = 1, 2, ..., d}.
Set p = k/(d − 1).
Sample a number N ∼ B(d(d−1)/2, p), where B(n, p) is a binomial distribution with parameters
  n and p.
if N < r then
    return FAIL
end if
Sample r indices from 1, . . . , d − 1 and store them in M_p in descending order.
for each i in M_p do
    Sample an index j from i + 1 to d.
    Add edge (i, j) to M and remove (i, j) from R.
end for
while R ≠ ∅ and |M| < N do
    Sample an edge (i, j) from R and remove it from R.
    if adding (i, j) to M does not change the size of the minimum head-tail vertex cover of M
    then
        Add (i, j) to M.
    end if
end while
if |M| < N then
    return FAIL
end if
return M
```

could never have rank r. Otherwise, Algorithm 1 samples an initial graph with r edges and rank r, by choosing r edges such that no two of them share the same head points or the same tail points, i.e., each row and each column of the corresponding adjacency matrix have at most one non-zero entry. Then, Algorithm 1 sequentially samples an edge from R and checks whether adding this edge to the graph changes the size of the minimum head-tail vertex cover. If not, the edge will be added to the graph; otherwise, it will be removed from R. This is because if a graph $\mathcal{G}$ is a super-graph of another graph $\mathcal{H}$, then the size of the minimum head-tail cover of $\mathcal{G}$ is no less than that of $\mathcal{H}$. We repeat the above sampling procedure until there is no edge in R or the number of edges in the resulting graph reaches N. If the latter happens, the algorithm will return the generated graph; otherwise, it will return FAIL.

The theoretic basis of Algorithm 1 is Theorem 2. Note that the algorithm may not return a valid graph if the desired number N of edges cannot be reached. This could happen if the input rank is too low while the input average degree is too high. With our experiment settings, we find it rare for Algorithm 1 to fail to return a desired graph.

C.2 Optimization

For this part, we consider a dataset consisting of n i.i.d. observations from $P(X)$ and consequently the expectations in Problems (1) and (2) are replaced by empirical means. Denote the design matrix by $\mathbf{X} \in \mathbb{R}^{n \times d}$, where each row of $\mathbf{X}$ corresponds to a sample and each column of $\mathbf{X}$ corresponds to a variable. Here we use NOTEARS (Zheng et al., 2018) and Gran-DAG (Lachapelle et al., 2020) from each class of methods as examples and will describe their low rank versions in the following. Other gradient-based methods and their optimization procedures can be similarly modified to incorporate the low rank assumption.

C.2.1 NOTEARS with low rank assumption

Following Section 3, the optimization problem in our work can be written as

$$\min_{W} \frac{1}{2n} \left\| \mathbf{X} - \mathbf{X}UV^T \right\|_F^2, \quad \text{subject to } \operatorname{trace}\left(e^{UV^T \circ UV^T}\right) - d = 0, \tag{5}$$

Algorithm 2 Optimization procedure for NOTEARS-low-rank

Require: Design matrix $\mathbf{X}$, starting point (U_0, V_0, α_0), penalty parameter ρ, rate $c \in (0, 1)$, tolerance $\epsilon > 0$, and threshold $w > 0$.
Ensure: Locally optimal parameter W^*.
1: **for** $t = 1, 2, \ldots$ **do**
2: (Solve primal) $U_{t+1}, V_{t+1} \leftarrow \arg\min_{U,V} L_\rho(U, V, \alpha_t)$ with ρ such that $g(U_{t+1}V_{t+1}^T) < cg(U_tV_t^T)$.
3: (Dual ascent) $\alpha_{t+1} \leftarrow \alpha_t + \rho g(U_{t+1}V_{t+1}^T)$.
4: **if** $g(U_{t+1}V_{t+1}^T) < \epsilon$ **then**
5: Set $U^* = U_{t+1}$ and $V^* = V_{t+1}$.
6: **break**
7: **end if**
8: **end for**
9: (Thresholding) Set $W^* = U^*V^{*T} \circ \mathbf{1}(|U^*V^{*T}| > w)$.
10: **return** W^*

where $U, V \in \mathbb{R}^{d\times\hat{r}}$ and $\circ$ is the point-wise product. The constraint in Equation (5) holds if and only if UV^T is a weighted adjacency matrix of a DAG. This problem can then be solved by standard numeric optimization methods such as the augmented Lagrangian method (Bertsekas, 1999). In particular, the augmented Lagrangian is given by

$$L_\rho(U, V, \alpha) = \frac{1}{2n}\left\|\mathbf{X} - \mathbf{X}UV^T\right\|_F^2 + \alpha g(UV^T) + \frac{\rho}{2}|g(UV^T)|^2,$$

where $g(UV^T) := \operatorname{trace}\left(e^{UV^T\circ UV^T}\right) - d$, α is the Lagrange multiplier, and $\rho > 0$ is the penalty parameter. The optimization procedure is summarized in Algorithm 2, similar to Zheng et al. (2018, Algorithm 1). Notice that here we do not include the ℓ_1 penalty term (except for the last experiment in Section 5.5), for three reasons: (1) we are more concerned with relatively large and dense graphs, so a sparsity assumption may be harmful; (2) we consider relatively sufficient data for the experiments and NOTEARS has been shown in Zheng et al. (2018) to perform consistently well even when the graph is sparse; (3) the ℓ_1 penalty term requires a tuning parameter, which itself is not easy to choose.

Zheng et al. (2018) used L-BFGS to solve the unconstrained subproblem in Step 2. We alternatively use the Newton conjugate gradient method that is written in C. Empirically, these two optimizers behave similarly in terms of the estimate performance, while the latter can run much faster thanks to its C implementation. The DAG constraint may not be satisfied exactly using iterative numeric methods, so it is a common practice to pick a small tolerance, followed by a thresholding procedure on the estimate to obtain exact DAGs. In our implementation, we choose U_0 and V_0 to be $d \times d$ identity matrices. Other parameter choices are: $\alpha_0 = 0$, $c = 0.25$, $\epsilon = 10^{-6}$, and $w = 0.3$, similar to those used in related methods on the same datasets (e.g., Zheng et al. (2018); Yu et al. (2019); Zhu et al. (2020)). The chosen threshold $w = 0.3$ works well in our experiments and in the experiments of related works that use the same data model. In case the thresholded matrix is not a DAG, one may further increase the threshold until the matrix corresponds to a DAG.

After obtaining W^*, we add an additional pruning step: we use linear regression to refit the dataset based on the structure indicated by W^* and then apply another thresholding (with $w = 0.3$) to the refitted weighted adjacency matrix. Both the Newton conjugate gradient optimizer and the pruning technique are also applied to NOTEARS, which not only accelerate the optimization but also improve its performance by obtaining a much lower SHD, particularly for large and dense graphs. See Appendix D.3 for an empirical comparison.

C.2.2 GRAN-DAG WITH LOW RANK ASSUMPTION

We next consider a low rank version of GraN-DAG. The optimization problem can be written as

$$\begin{aligned} \min_{\theta} \quad & -\frac{1}{n}\sum_{l=1}^{n}\sum_{i=1}^{d}\log p\left(X_i^{(l)} \mid \mathrm{pa}(X_i, A(\theta))^{(l)}; \theta\right) + \lambda\|A(\theta)\|_* \\ \text{subject to} \quad & \operatorname{trace}\left(e^{A(\theta)}\right) - d = 0, \end{aligned} \tag{6}$$

where $X_i^{(l)}$ is the l-th sample of variable X_i and $\mathrm{pa}(X_i, A(\theta))^{(l)}$ means the l-th sample the X_i's parents indicated by the adjacency matrix $A(\theta)$. Here, θ denotes the parameters of neural networks and $A(\theta)$ is obtained from the neural network path products.

Problem (6) can be solved similarly using augmented Lagrangian. The procedure is similar to Algorithm 2 and is the same to that used by GraN-DAG, with slight modifications: (1) the subproblem in Step 2 is approximately solved using first-order method like Adam (Kingma & Ba, 2014); (2) the thresholding at Step 9 is replaced by a variable selection method proposed by Bühlmann et al. (2014). The same variable selection or pruning method is adopted by the three benchmarked methods CAM, NOTEARS-MLP, and GraN-DAG for non-linear data models in our experiment. Please refer to Lachapelle et al. (2020) and Bühlmann et al. (2014) for further details.

C.3 Experiment Setup

In our experiments, we consider three data models: linear Gaussian SEMs, linear non-Gaussian SEMs (linear exponential SEMs), and non-linear SEMs (Gaussian processes). Given a randomly generated DAG $\mathcal{G}$, the associated SEM is generated as follows:

Linear Gaussian A linear Gaussian SEM is given by

$$X_i = \sum_{X_j \in \mathrm{pa}(X_i, \mathcal{G})} W(j,i) X_j + \epsilon_i, \quad i = 1, 2, \ldots, d, \tag{7}$$

where $\mathrm{pa}(X_i, \mathcal{G})$ denotes X_i's parents in $\mathcal{G}$ and ϵ_i's are jointly independent standard Gaussian noises. In our experiments, the weights $W(i,j)$'s are uniformly sampled from $[-2, -0.5] \cup [0.5, 2]$.

Linear Exponential A linear exponential SEM is also generated according to Equation (7), where ϵ_i's are replaced by jointly independent $\mathrm{Exp}(1)$ random variables. The weights $W(i,j)$'s are sampled from $[-2, -0.5] \cup [0.5, 2]$ uniformly, too.

Gaussian Processes We consider the following additive noise model:

$$X_i = f_i(\mathrm{pa}(X_i, \mathcal{G})) + \epsilon_i, \quad i = 1, 2, \ldots, d, \tag{8}$$

where ϵ_i's are jointly independent standard Gaussian noises and f_i's are functions sampled from Gaussian processes with RBF kernel of bandwidth one.

We sample $3,000$ observations according the SEM. The reported results of each setting are summarized over 10 repetitions with different seeds. The experiments are run on a Linux workstation with 16-core Intel Xeon 3.20GHz CPU and 128GB RAM.

C.4 Benchmark Methods

Existing causal structure learning methods used in our experiments all have available implementations, as listed below:

- GES and PC: an implementation of both methods is available through the `py-causal` package at `https://github.com/bd2kccd/py-causal`. We note that, the implementation of `py-causal` package is based on the `CMU TETRAD` project, in which the version of GES is indeed the fast GES algorithm proposed by Ramsey et al. (2017).
- MMHC (Tsamardinos et al., 2006): an implementation is available in the `bnlearn` package at `https://CRAN.R-project.org/package=bnlearn`.
- CAM (Peters et al., 2014): its codes are available through the CRAN R package repository at `https://cran.r-project.org/web/packages/CAM`.
- NOTEARS (Zheng et al., 2018) and NOTEARS-MLP (Zheng et al., 2020): codes are available at the first author's github repository `https://github.com/xunzheng/notears`.
- GraN-DAG (Lachapelle et al., 2020): an implementation is available at the first author's github repository `https://github.com/kurowasan/GraN-DAG`. Note that for graphs of 50 nodes or more, GraN-DAG performs a preliminary neighborhood selection step to avoid overfitting.

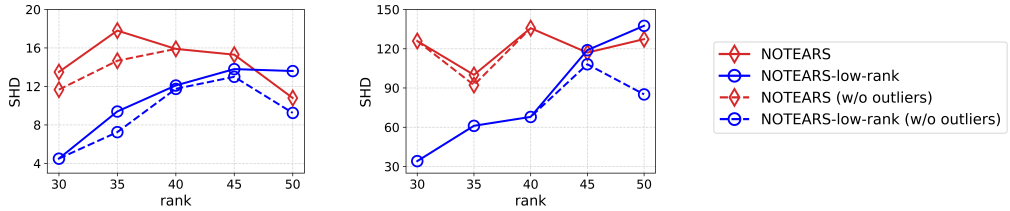
- DAG-GNN (Yu et al., 2019): the codes are available at the first author's github repository `https://github.com/fishmoon1234/DAG-GNN`.

In the experiments, we mostly use default hyperparameters unless otherwise stated.

D Additional Experimental Results

D.1 Linear SEMs with Higher Ranks

This experiment considers graphs of higher ranks. We use rank-specified random graphs with $d = 100$ nodes and rank $r \in \{30, 35, 40, 45, 50\}$ on linear Gaussian SEMs. The results are shown in Figures 10a and 10b with degrees 2 and 8, respectively. We observe that when the rank of the underlying graph becomes higher, the advantage of NOTEARS-low-rank over NOTEARS decreases. Nonetheless, NOTEARS-low-rank with rank $r = 50$ is still comparable to NOTEARS, and has a lower average SHD after removing outlier SHDs using the interquartile range rule.



(a) degree 2 (b) degree 8

Figure 10: Average SHDs on rank-specified graphs with higher ranks. The true rank is assumed to be known.

D.2 NOTEARS-Low-Rank with Different Sample Sizes

We next empirically study the consistency of NOTEARS-low-rank. Again, we use rank-specified random graphs (sampled according to Algorithm 1) with $d = 100$ nodes, degree $k = 8$, rank $r = 10$, and linear Gaussian SEMs. We also assume that the true rank is known. We fix the rank parameter $\hat{r} = 10$ and use different sample sizes ranging from 200 to $5,000$. From Figure 11, NOTEARS-low-rank performs reasonably well when the sample size is small and tends to have a better performance with a larger number of samples.

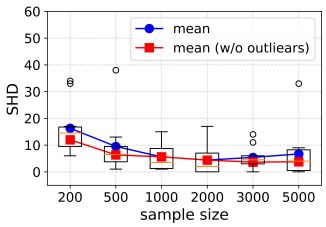


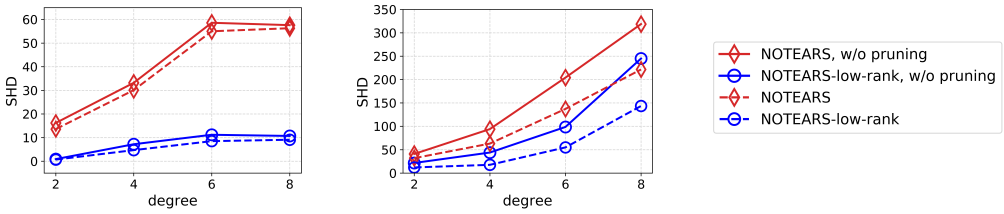
Figure 11: Different sample sizes.

D.3 Further Pruning

We compare the empirical results before and after applying the additional pruning technique described in Appendix C.2. The graphs are rank-specified with $d \in \{100, 300\}$ nodes, rank $r = \lceil 0.1d \rceil$, and degree $k \in \{2, 4, 6, 8\}$. We again use linear Gaussian data model with equal noise variances to generate the datasets. The average SHDs are reported in Figure 12. We see that applying an additional pruning step indeed improves the final performance of both NOTEARS and NOTEARS-low-rank, especially on relatively large and dense graphs.

D.4 Detailed Empirical Results for Experiment 1 with Linear Gaussian SEMs

Table 1 reports detailed results including true positive rates (TPRs), false discovery rates (FDRs), structural Hamming distances (SHDs), and running time on rank-specified graphs with linear Gaussian



(a) 100 nodes, rank 10 (b) 300 nodes, rank 30

Figure 12: Average SHDs before and after pruning.

data model. Here the true rank is assuming known and is used as the rank parameter in NOTEARS-low-rank. We also test (fast) GES, MMHC, and PC. However, PC is too slow since some nodes may have a high in-degree (i.e., hubs) in large, dense, and low rank graphs. For the same reason, the skeleton may not be correctly estimated by MMHC, which has a similar performance to that of GES. Therefore, we only include the results of GES for comparison. We treat GES favorably by regarding undireted edges as true positives if the true graph has a directed edge in place of the undirected ones.

Table 1: Detailed results for linear Gaussian data model with equal noise variances.

100 nodes, rank 10					
	Degree	2	4	6	8
NOTEARS-low-rank	TPR	0.99 ± 0.02	0.99 ± 0.03	0.99 ± 0.01	0.99 ± 0.01
	FDR	0.001 ± 0.003	0.01 ± 0.02	0.02 ± 0.04	0.02 ± 0.02
	SHD	0.7 ± 1.6	4.7 ± 10.2	8.5 ± 13.7	9.1 ± 11.5
	Time (mins.)	1.9 ± 0.2	5.7 ± 2.7	5.8 ± 2.6	7.5 ± 2.7
NOTEARS	TPR	0.90 ± 0.06	0.90 ± 0.04	0.87 ± 0.05	0.89 ± 0.03
	FDR	0.07 ± 0.03	0.06 ± 0.04	0.06 ± 0.02	0.04 ± 0.02
	SHD	13.6 ± 8.6	30.1 ± 13.2	55.0 ± 20.9	56.3 ± 15.2
	Time (mins.)	3.6 ± 1.6	6.6 ± 1.6	9.6 ± 1.5	7.3 ± 1.5
GES	TPR	0.3 ± 0.04	0.13 ± 0.02	0.08 ± 0.01	0.06 ± 0.00
	FDR	0.71 ± 0.03	0.82 ± 0.03	0.85 ± 0.01	0.87 ± 0.01
	SHD	141.6 ± 19.3	292.1 ± 26.0	412.5 ± 26.25	521.9 ± 22.3
	Time	< 10 seconds			

300 nodes, rank 30					
	Degree	2	4	6	8
NOTEARS-low-rank	TPR	0.99 ± 0.01	0.99 ± 0.01	0.99 ± 0.01	0.97 ± 0.05
	FDR	0.03 ± 0.03	0.02 ± 0.02	0.04 ± 0.02	0.06 ± 0.08
	SHD	12.0 ± 10.6	13.9 ± 14.8	50.0 ± 32.1	106.0 ± 169.5
	Time (mins.)	57.6 ± 43.2	76.5 ± 27.8	158.7 ± 94.7	262.9 ± 144.4
NOTEARS	TPR	0.94 ± 0.01	0.93 ± 0.02	0.93 ± 0.02	0.91 ± 0.02
	FDR	0.07 ± 0.02	0.06 ± 0.03	0.08 ± 0.04	0.09 ± 0.06
	SHD	35.4 ± 10.5	71.3 ± 29.9	138.3 ± 64.2	216.9 ± 102.6
	Time (mins.)	23.9 ± 5.8	42.0 ± 10.5	74.2 ± 37.9	104.2 ± 21.7
GES	TPR	0.31 ± 0.04	0.12 ± 0.01	0.07 ± 0.01	0.05 ± 0.01
	FDR	0.68 ± 0.05	0.83 ± 0.02	0.87 ± 0.01	0.89 ± 0.01
	SHD	427.0 ± 58.1	883.3 ± 60.5	1260.8 ± 59.8	1608.4 ± 67.5
	Time	< 30 seconds			

D.5 Detailed Results for Experiment 4 with Non-Linear SEMs

Table 2 reports the detailed SHDs for each method in Section 5.4. We also mark in bold the best results from methods with or without low rank modifications.

Table 2: Detailed SHDs for Experiment 4 with non-linear SEMs.

Degree	2	4	6	8
DAG-GNN	50.1 ± 8.2	96.8 ± 11.9	146.9 ± 10.6	182.0 ± 13.5
CAM	$\mathbf{12.9} \pm \mathbf{3.9}$	51.4 ± 19.3	98.9 ± 21.7	131.9 ± 27.1
NOTEARS-MLP	19.8 ± 6.4	$\mathbf{47.8} \pm \mathbf{20.4}$	86.0 ± 15.8	119.4 ± 23.9
GraN-DAG	17.9 ± 17.0	50.3 ± 51.7	$\mathbf{82.6} \pm \mathbf{75.8}$	$\mathbf{109.4} \pm \mathbf{102.4}$
GraN-DAG, low rank, 0.3	20.9 ± 23.2	45.8 ± 47.7	65.9 ± 59.1	87.1 ± 79.9
GraN-DAG, low rank, 0.5	27.7 ± 40.8	50.0 ± 53.4	$\mathbf{61.8} \pm \mathbf{66.7}$	83.9 ± 85.2
GraN-DAG, low rank, 1.0	42.7 ± 58.8	57.9 ± 67.6	68.7 ± 76.2	83.2 ± 76.9
GraN-DAG, low rank, validation	$\mathbf{16.0} \pm \mathbf{4.5}$	$\mathbf{44.4} \pm \mathbf{21.0}$	63.3 ± 24.7	$\mathbf{77.4} \pm \mathbf{28.8}$