BOOSTING CAUSAL DISCOVERY VIA ADAPTIVE SAMPLE REWEIGHTING

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ABSTRACT

Under stringent model type and variable distribution assumptions, score-based causal discovery methods learn the directed acyclic graph (DAG) from observational data by evaluating candidate graphs over an averaged score function. Despite the great success in low-dimensional linear systems, it has been observed that these approaches overly exploits easier-to-fit samples, thus inevitably learning spurious edges. Worse still, the common homogeneity assumption of most causal discovery methods can be easily violated due to the widespread existence of heterogeneous data in the real world, resulting in performance vulnerability when noise distributions vary. We propose a simple yet effective model-agnostic framework to boost causal discovery performance by dynamically learning the adaptive weights for the **Re**weighted **Score** function, **ReScore** for short, where the learned weights tailors quantitatively to the important degree of each samples. Intuitively, we leverage the bilevel optimization scheme to alternatively train a standard DAG learner first, then upweight the samples that the DAG learner fails to fit well and downweight the samples that the DAG learner easily extracts the causation information from. Extensive experiments on both synthetic and real-world datasets are carried out to validate the effectiveness of ReScore. We observe consistent and significant boosts in structure learning performance. We further visualize that ReScore concurrently mitigates the influence of spurious edges and generalizes to heterogeneous data. Finally, we perform theoretical analysis to guarantee the structure identifiability and the weight adaptive properties of ReScore. Our codes are available at https://anonymous.4open.science/r/ReScore-7631.

1 INTRODUCTION

Learning the causal structure from purely observational data (*i.e.,* causal discovery) is a fundamental but daunting task (Chickering et al., 2004; Shen et al., 2020). It strives to identify causal relationships between variables and encodes the conditional independencies as a directed acyclic graph (DAG). Differentiable score-based optimization is a crucial enabler of causal discovery (Vowels et al., 2021). Specifically, it is formulated as a continuous constraint optimization problem by minimizing the average score function and a smooth acyclicity constraint. To guarantee the structure is fully or partially identifiable (see Section 2), researchers impose stringent restrictions on model parametric family (*e.g.,* linear, additive) and common assumptions of variable distributions (*e.g.,* homogeneity data) (Peters et al., 2014; Ng et al., 2019a). Following this scheme, recent follow-on studies (Kalainathan et al., 2018; Ng et al., 2019b; Zhu et al., 2020; Khemakhem et al., 2021; Yu et al., 2021) extend the formulation to tackle general nonlinear problems by utilizing a variety of deep learning models.

However, upon careful inspections, we spot and justify two unsatisfactory behaviors of the current differentiable score-based methods:

- The score-based causal discovery is error-prone to learning spurious edges or reverse causal directions between variables, which derails the structure learning accuracy (He et al., 2021; Ng et al., 2022). We substantiate our claim with illustrative examples as shown in Figure 1. We find that even the fundamental structure, *i.e.,* chain, in a linear system, is easily misidentified by the state-of-the-art method, NOTEARS (Zheng et al., 2018).

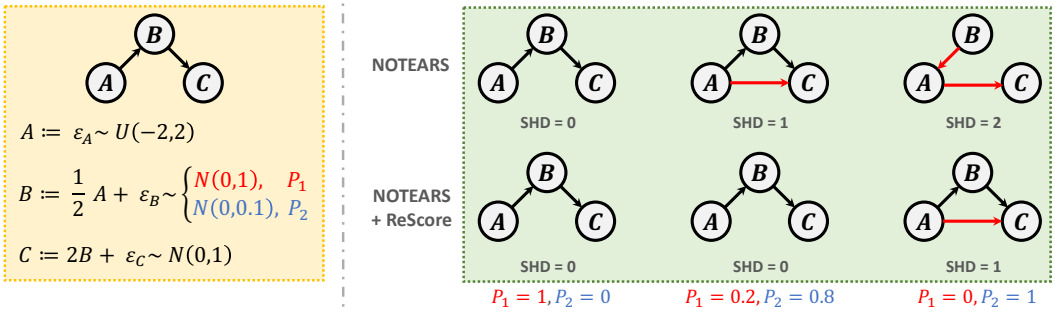


Figure 1: A simple example of basic chain structure that NOTEARS would learn spurious edges while ReScore can help to mitigate the bad influence.

- Despite being appealing in synthetic data, differentiable score-based causal discovery methods suffer from severe performance degradation when encountering heterogeneous data (Huang et al., 2020; 2019). Considering Figure 1, NOTEARS is susceptible to learning redundant causations when the distributions of noise variables vary.

Taking a closer look at this dominant score-based causal discovery scheme, *i.e.,* optimizing the DAG learner via an average score function under strict assumptions, we ascribe these undesirable behaviors to its inherent limitations:

- The collecting datasets naturally include an overwhelming number of easy samples and a small number of informative samples that might contain crucial causation information (Shrivastava et al., 2016). Averagely scoring the observational samples deprives the discovery process of differentiating sample importance, thus easy samples dominate the learning of DAG. As a result, prevailing score-based techniques fail to learn true causal relationship but instead exploit the easier-to-fit spurious edges.
- Noise distribution shifts are inevitable and common in real-world training, as the observations are typically collected at different periods, environments, locations, and so forth (Arjovsky et al., 2019). As a result, the strong assumption of noise homogeneity for differentiable DAG learner is easily violated in real-world data (Peters et al., 2016). A line of works (Ghassami et al., 2018; Wang et al., 2022) dedicated to heterogeneous data can successfully address this issue. However, they often require explicit domain annotations (*i.e.,* ideal partition according to heterogeneity underlying the data) for each sample, which are prohibitively expensive and hard to obtain (Creager et al., 2021), further limiting their applicability.

To reshape the optimization scheme and resolve these limitations, we propose to adaptively reweight the samples, which de facto concurrently mitigates the influence of spurious edges and generalizes to heterogeneous data. The core idea is to discover and upweight a set of less-fitted samples that offer additional insight to depict the causal edges, compared to the samples that can be easily fitted via the spurious edges. Focusing more on less-fitted samples enables the DAG learner to effectively generalize to heterogeneous data since in real-world scenarios, such samples typically come from disadvantaged domains. Due to the difficulty of accessing domain annotation, distinguishing such disadvantaged but informative samples and automatically assigning adaptive weights is challenging.

With the idea of adaptive sample reweighting, we present a simple yet effective model-agnostic optimization framework for DAG learner, coined **ReScore**, which alleviates the overfitting issue of easier-to-fit spurious edges. On the other hand, ReScore tackles heterogeneous data without knowing the domain annotation in advance by automatically learning the instance-wise adaptive weights. More precisely, we reformulate the adaptive weights learning as a bilevel optimization problem. The general model-agnostic bilevel scheme is designed below:

- In the inner loop, the DAG learner is evaluated by the reweighted score function to quantify the reliance on easier-to-fit samples and optimize the adaptive weights to achieve the worst-case.
- In the outer loop, any score-based causal discovery method can be deployed to obtain the optimal DAG learner on weighted observational data where the weights are determined by the inner loop.

The inner loop and outer loop are alternatively trained. Benefiting from this optimization scheme, our ReScore has three desirable properties. First, ReScore is a model-agnostic technique that is flexible enough to easily adapt to any score-based causal discovery method. Moreover, we theoretically reveal that the structure identifiability is inherited by ReScore from the original causal discovery method (*cf.* Theorem 1). Second, ReScore jointly lightens the negative effect of spurious edge learning and performance drop in heterogeneous data by auto-learnable adaptive weights. Theoretical analysis of adaptive properties for weights is provided in Section 3.3 (*cf.* Theorem 2). Third, our proposed ReScore strengthens the existing causal discovery methods by a large margin. Surprisingly, ReScore performs competitively or even outperforms CD-NOD (Huang et al., 2020) and DICD (Wang et al., 2022), which require domain annotation, on heterogeneous synthetic data (*cf.* Section 4.2).

2 Differentiable Causal Discovery

We begin with the preliminary of causal discovery, which includes the task formulation and description of the identifiability issue. We then present the differentiable score-based framework to solve and optimize the DAG learner.

2.1 Preliminaries of Causal Discovery

Task Formulation. Causal discovery aims to infer the Structural Causal Model (SCM) (Pearl, 2000; Pearl et al., 2016) from the observational data, which best describes the data generating procedure. Formally, let $\mathbf{X} \in \mathbb{R}^{n \times d}$ be a matrix of observational data, which consists of n independent and identically distributed (i.i.d.) random vectors $X = (X_1, \ldots, X_d) \in \mathbb{R}^d$. Given $\mathbf{X}$, we aim to learn a SCM $(P_X, \mathcal{G})$, which encodes a causal directed acyclic graph (DAG) with a structural equation model (SEM) to reveal the data generation from the distribution of variables X. Specifically, we denote the DAG by $\mathcal{G} = (V(\mathcal{G}), E(\mathcal{G}))$, where $V(\mathcal{G})$ is the variable set and $E(\mathcal{G})$ collects the causal directed edges between variables. We present the joint distribution over X as P_X, which is Markov *w.r.t.* $\mathcal{G}$. The probability distribution function of P_X is factored as $p(x) = \prod_{i=1}^{d} P(x_i | x_{pa(i)})$, where $pa(i) = \{j \in V(\mathcal{G}) : X_j \to X_i \in E(\mathcal{G})\}$ is the set of parents of variable X_i in $\mathcal{G}$ and $P(x_i | x_{pa(i)})$ is the conditional probability density function of variable X_i given $X_{pa(i)}$. As a result, the SEM can be formulated as a collection of d structural equations:

$$X_i = f_i(X_{pa(i)}, N_i), \quad i = 1, \ldots, d \tag{1}$$

where $f_i : \mathbb{R}^{|X_{pa(i)}|} \to \mathbb{R}$ can be any linear or nonlinear function, and $N = (N_1, \ldots, N_d)$ are jointly independent noise variables.

Identifiability Issue. In general, without further assumption on the SEM (*cf.* equation 1), it is not possible to uniquely learn the DAG $\mathcal{G}$ by only using the observations of P_X. This is the identifiability issue in causal discovery (Lachapelle et al., 2020). Nonetheless, with the assumption of the SEM, the DAG $\mathcal{G}$ is said to be identifiable over P_X, if no other SEM can encode the same distribution P_X with a different DAG under the same assumption. To guarantee the identifiability, most prior studies restrict the form of the structural equations to be additive *w.r.t.* to noises, *i.e.,* additive noise models (ANM). Assuming ANM, as long as the structural equations are linear with non-Gaussian errors (Shimizu et al., 2006; Loh & Bühlmann, 2014), linear Gaussian model with equal noise variances (Peters & Bühlmann, 2014), or nonlinear structural equation model with mild conditions (Hoyer et al., 2008; Zhang & Hyvarinen, 2009; Peters et al., 2014), then the DAG $\mathcal{G}$ is identifiable.

2.2 Solution to Causal Discovery

Prevailing causal discovery approaches roughly fall into two research lines: constraint-based and score-based methods (Spirtes & Zhang, 2016; Glymour et al., 2019). Specifically, constraint-based methods (Spirtes et al., 1995; Spirtes & Glymour, 1991; Colombo et al., 2012) determine up to the Markov equivalence class of causal graphs, according to conditional independent tests under certain assumptions. Score-based methods (Vowels et al., 2021), on the other hand, evaluate the candidate graphs with a predefined score function and search over the space of directed acyclic graphs for the optimal graph. In this work, we focus on the score-based line.

Score-based Causal Discovery. With a slight abuse of notation, $\mathcal{G}$ refers to a directed graph in the rest of the paper. Formally, score-based paradigm casts the task of DAG learning as a combinatorial optimization problem:

$$\begin{aligned} \min_{\mathcal{G}} \quad & S(\mathcal{G};\mathbf{X}) = \mathcal{L}(\mathcal{G};\mathbf{X}) + \lambda\mathcal{R}(\mathcal{G}) \\ \text{s.t.} \quad & \mathcal{G} \in \text{DAG}, \end{aligned} \tag{2}$$

where the score function $S(\mathcal{G};\mathbf{X})$ composes two terms: (1) the goodness-of-fit measure $\mathcal{L}(\mathcal{G};\mathbf{X}) = \frac{1}{n}\sum_{i=1}^{n} l(\mathbf{x}_i, f(\mathbf{x}_i))$, where $l(\mathbf{x}_i, f(\mathbf{x}_i))$ represents the fitting loss of observation $\mathbf{x}_i$; (2) the sparsity regularization term $\mathcal{R}(\mathcal{G})$ stipulates that the total number of edges in $\mathcal{G}$ should be penalized. λ is a regularization hyperparameter that can be selected via cross-validation in practice.

Now we elaborate on the two major components in Equation 2: the score function $S(\mathcal{G};\mathbf{X})$ and the combinatorial acyclicity constraint constraint $\mathcal{G} \in$ DAG.

In literature, various approaches have been proposed for the score function $S(\mathcal{G};\mathbf{X})$, such as penalized least-squares loss (Zheng et al., 2020; 2018; Ng et al., 2019b), Evidence Lower Bound (ELBO) (Yu et al., 2019), log-likelihood with complexity regularizers (Kalainathan et al., 2018; Van de Geer & Bühlmann, 2013; Ng et al., 2020), Maximum Mean Discrepancy (MMD) (Goudet et al., 2018), Bayesian Information Criterion (BIC) (Geiger & Heckerman, 1994; Zhu et al., 2020), Bayesian Dirichlet equivalence uniform (BDeu) score (Heckerman et al., 1995), Bayesian Gaussian equivalent (BGe) score (Kuipers et al., 2014), and others (Huang et al., 2018; Bach & Jordan, 2002; Sokolova et al., 2014).

Moreover, the combinatorial constraint $\mathcal{G} \in$ DAG enforces the directed graph $\mathcal{G}$ to be acyclic, thus becoming the main obstacle to the score-based causal structure learning. In literature, various approaches are proposed to search the acyclic space, such as greedy search (Chickering, 2002; Hauser & Bühlmann, 2012), hill-climbing (Gámez et al., 2011; Tsamardinos et al., 2006), dynamic programming (Silander & Myllymäki, 2006; Koivisto & Sood, 2004), A* (Yuan & Malone, 2013), and integer linear programming (Jaakkola et al., 2010; Cussens, 2011).

Differentiable Score-based Optimization. Different from those search approaches mentioned above, NOTEARS (Zheng et al., 2018) reframes the combinatorial optimizaiton problem as a continuous constrained optimization problem:

$$\min_{\mathcal{G}} \; S(\mathcal{G};\mathbf{X}) \quad \text{s.t.} \quad H(\mathcal{G}) = 0, \tag{3}$$

where $H(\mathcal{G}) = 0$ is a differentiable equality DAG constraint.

As for the DAG constraint $H(\mathcal{G}) = 0$, the prior effort (Zheng et al., 2018) turns to depict the "DAGness" of $\mathcal{G}$'s adjacency matrix $\mathcal{A}(\mathcal{G}) \in \{0,1\}^{d\times d}$. Specifically, $[\mathcal{A}(\mathcal{G})]_{ij} = 1$ if the causal edge $X_j \to X_i$ exists in $E(\mathcal{G})$, otherwise $[\mathcal{A}(\mathcal{G})]_{ij} = 0$. Prevailing implementations of DAGness constraints are $H(\mathcal{G}) = \text{Tr}(e^{\mathcal{A}\odot\mathcal{A}}) - d$ (Zheng et al., 2018), $H(\mathcal{G}) = \text{Tr}[(I + \alpha\mathcal{A}\odot\mathcal{A})^d] - d$ (Yu et al., 2019), and others (Wei et al., 2020; Kyono et al., 2020; Bello et al., 2022; Zhu et al., 2021). As a result, this optimization problem in Equation 3 can be further formulated via the augmented Lagrangian method as:

$$\min_{\mathcal{G}} \; S(\mathcal{G};\mathbf{X}) + \mathcal{P}_{\text{DAG}}(\mathcal{G}), \tag{4}$$

where $\mathcal{P}_{\text{DAG}}(\mathcal{G}) = \alpha H(\mathcal{G}) + \frac{\rho}{2}|H(\mathcal{G})|^2$ is the penalty term enforcing the DAGness on $\mathcal{G}$, and $\rho > 0$ is a penalty parameter and α is the Lagrange multiplier.

3 Methodology of ReScore

On the basis of differentiable score-based causal discovery methods, we devise our ReScore and present its desirable properties.

3.1 Bilevel Formulation of ReScore

We learn causal structure and DAG over large-scale observational data that is likely to be heterogeneous and contains a large proportion of easy observations. Standard score-based causal discovery

methods inherently rely on easy samples in order to obtain high average goodness-of-fit. Because of this, conventional score-based DAG learner that optimize average score functions tend to overly exploit easier-to-fit spurious edges and sacrifice causal relationship information from hard less-fitted samples. Suppose we know the importance score of each sample in advance. Then we can assign distinct weights to different samples and consider reweighted score function $S_{\mathrm{w}}(\mathcal{G};\mathbf{X})$, which is defined as

$$S_{\mathrm{w}}(\mathcal{G};\mathbf{X}) = \mathcal{L}_{\mathrm{w}}(\mathcal{G};\mathbf{X}) + \lambda\mathcal{R}_{sparse}(\mathcal{G}) = \sum_{i=1}^{n} w_i l(\mathbf{x}_i, f(\mathbf{x}_i)) + \lambda\mathcal{R}_{sparse}(\mathcal{G}), \tag{5}$$

where $\mathbf{w} = (w_1, \ldots, w_n)$ is a sample reweighting vector with length n indicating the importance of observational samples.

Then the problem comes to how to automatically learn appropriate sample reweighting vector $\mathbf{w}$. Intuitively, to remove the spurious edges and avoid the missing edges, easier-to-fit samples that the biased DAG learner largely depended on should be offered a relatively small importance score, whereas samples for which the existing causal discovery approaches fail to fit well are more likely to be informative and should be assigned a high importance score. In other words, upweighting the less-fitted and informative samples while downweighting the easy and non-informative samples. Thus we seek for the adaptive sample weights that maximizes the weighted score function. The overall framework of learning sample reweighting to boost causal discovery is formulated as the following bilevel optimization problem:

$$\begin{aligned} \min_{\mathcal{G}} \;\; & S_{\mathrm{w}^*}(\mathcal{G};\mathbf{X}) + \mathcal{P}_{DAG}(\mathcal{G}) \\ \text{s.t.} \;\; & \mathbf{w}^* \in \arg\max_{\mathbf{w}} \; S_{\mathrm{w}}(\mathcal{G};\mathbf{X}), \end{aligned} \tag{6}$$

where $\mathbf{w}$ has a constraint that $\mathbf{w} \in \mathbb{C}(\tau) := \{\mathbf{w} : 0 < \frac{\tau}{n} < w_1, \ldots, w_n < \frac{1}{\tau n}, \sum_{i=1}^{n} w_i = 1\}$ for some small constant $\tau > 0$. The deviation of the weight distribution from the uniform distribution is bound by the hyperparameter τ. The outer and inner objectives in this case can be any reweighted score function $S_{\mathrm{w}}(\mathcal{G};\mathbf{X})$ derived from the existing score functions $S(\mathcal{G};\mathbf{X})$ outlined in Section 2.

In the inner loop, we maximize the reweighted score function $S_{\mathrm{w}}(\mathcal{G};\mathbf{X})$ in order to automatically learn the adaptive weights w_i^* for each observation $\mathbf{x}_i$. In the outer loop, we minimize the reweighted objective function in score-based causal discovery under fixed weights $\mathbf{w}*$ to learn the optimal DAG learner. By alternatively training the inner and outer loops, the importance of samples is adaptively assigned as well as the score function is appropriately reweighted.

Moreover, our ReScore has the following desirable advantages:

- As shown in Section 3.2, under mild conditions, our ReScore inherits the identifiability property of the original score-based causal discovery method.
- ReScore is able to automatically select the more informative samples and assign adaptive weights to each observation through bilevel optimization, which is consistent with our theoretical analysis in Section 3.3 and empirical results in Section 4.2.
- ReScore is widely applicable to various types of data and models. In other words, ReScore is model-agnostic and can effectively handle heterogeneous data without knowing the domain annotation in advance. Detailed ReScore performance can be found in Section 4.

3.2 Theoretical Analysis on Identifiability

Graph identifiability issues are the primary challenges hindering the development of structure learning. As an optimization framework, the capacity of ReScore to ensure graph identifiability while substantially boosting the performance of the score-based DAG learner is the most desired property. We develop Theorem 1 that guarantees the identifiability of the DAG using ReScore.

Recall that to render a DAG theoretically identifiable, three standard steps are necessary (Zheng et al., 2020; Peters et al., 2014; Ng et al., 2022): Initially, the specific causal mechanism and data distribution of SEM for equation 1 are assumed. The second step is to theoretically prove the SEM's identifiability. Thirdly, developing an optimization algorithm with a predefined score function and showing the learned DAG asymptotically converges to the ground-truth DAG. Clearly, ReScore

naturally inherits the original identifiability of a specific SEM as stated in Section 2. The key concern arising is whether the DAG learned by our new optimization framework under reweighted score function $S_{\mathrm{w}}(\mathcal{G};\mathbf{X})$ can asymptotically converge to the ground-truth DAG. Fortunately, the following theorem demonstrates that, by guaranteeing the equivalence of optimization problems (2) and (6) in linear systems, the bounded weights will not affect the consistency results in identifiability analysis. See detailed proof in Appendix B.1.

Theorem 1. *Let* $\boldsymbol{w} \in \mathbb{C}\{\boldsymbol{w} : 0 < \frac{\tau}{n} < w_1, \ldots, w_n < \frac{1}{\tau n}, \sum_{i=1}^{n} w_i = 1\}$ *for some small* $\tau > 0$ *and the SEM in equation 1 is linear. The optimization problem* $\min_{\mathcal{G}} \left\{S(\mathcal{G};\boldsymbol{X}) + \mathcal{P}_{DAG}(\mathcal{G})\right\}$ *is equivalent to* $\min_{\mathcal{G}} \left\{S_{\mathrm{w}}(\mathcal{G};\boldsymbol{X}) + \mathcal{P}_{DAG}(\mathcal{G})\right\}$ *asymptotically in the following cases.*

a. Using the least-squares loss $\mathcal{L}(\mathcal{G};\boldsymbol{X}) = \frac{1}{2n}\|\boldsymbol{X} - f(\boldsymbol{X})\|_F^2$*;*

b. Using the negative log-likelihood loss with standard Gaussian noise.

Remark: The identifiability property of ReScore under two special but most common score functions, namely least-square loss and negative llog-likelihood loss, is proved in Theorem 1. Similar conclusions can be easily derived for other loss functions.

3.3 Oracle Property of Adaptive Weights

Our ReScore suggests assigning varying degrees of importance to observational samples. The less-fitted samples are fundamentally more important than the easier-to-fit samples as they contain the causation information the DAG learner fails to extract. That hard-to-learn causation information is the key to helping DAG learners mitigate the learning of spurious edges. The following theorem illustrates the adaptiveness property of ReScore, *i.e.,* instead of equally treating all the samples, ReScore tends to upweight the importance of informative and hard samples while downweighting the reliance on easier-to-fit samples.

Theorem 2. *Suppose that in the optimization phrase, the* i*-th observation has a larger error than the j-th observation in the sense that* $l(\boldsymbol{x}_i, f(\boldsymbol{x}_i)) > l(\boldsymbol{x}_j, f(\boldsymbol{x}_j))$*, where* $i, j \in \{1, \ldots, n\}$*. Then,*

$$w_i^* > w_j^*,$$

where $\boldsymbol{w}^* = (w_1^*, \ldots, w_n^*)$ *is the optimal weights in equation 6.*

See detailed proof in Appendix B.2. It is simple to infer that, following an inner loop for maximizing the reweighted score function $S_{\mathrm{w}}(\mathcal{G};\mathbf{X})$, the observations are ranked by learned adaptive weights $\mathbf{w}^*$. In other words, one observation equipped with a higher weight will have a stronger impact on the subsequent outer loop to dominate the DAG learning.

4 Experiments

We aim to answer the following research questions:

- **RQ1:** As a model-agnostic method, can ReScore widely strengthen the existing score-based causal discovery baselines?
- **RQ2:** How does ReScore perform when noise distribution varies? Can ReScore effectively learn the adaptive weights that successfully identify the important samples?

Baselines. To answer the first question (RQ1), we implement various backbone models including NOTEARS (Zheng et al., 2018) and GOLEM (Ng et al., 2020) in linear systems, and NOTEARS-MLP (Zheng et al., 2020) and GraN-DAG (Lachapelle et al., 2020) in nonlinear settings. To answer the second question (RQ2), we compare GOLEM+ReScore, NOTEARS-MLP+ReScore to a SOTA baseline CD-NOD (Huang et al., 2020) and a recently proposed approach DICD (Wang et al., 2022), which both require the ground-truth domain annotation. For a comprehensive comparison, extensive experiments are conducted on both homogeneous and heterogeneous synthetic datasets as well as a real-world benchmark dataset, *i.e.,* Sachs (Sachs et al., 2005). A detailed description of the employed baselines can be found in Appendix C.1.

Table 1: Results for ER graphs of 10 nodes on linear and nonlinear synthetic datasets.

	ER2				ER4			
	TPR ↑	FDR ↓	SHD ↓	SID ↓	TPR ↑	FDR ↓	SHD ↓	SID ↓
Random	$0.08_{\pm 0.07}$	$0.93_{\pm 0.18}$	$33.2_{\pm 7.3}$	$95.6_{\pm 12.2}$	$0.09_{\pm 0.17}$	$0.93_{\pm 0.09}$	$52.3_{\pm 16.7}$	$80.3_{\pm 17.7}$
NOTEARS	$0.85_{\pm 0.09}$	$\mathbf{0.07}_{\pm 0.07}$	$5.8_{\pm 2.2}$	$20.8_{\pm 5.2}$	$0.79_{\pm 0.11}$	$0.09_{\pm 0.05}$	$10.0_{\pm 5.2}$	$25.8_{\pm 9.9}$
+ ReScore	$\mathbf{0.89}_{\pm 0.07}^{+5\%}$	$0.08_{\pm 0.09}^{-12\%}$	$\mathbf{4.6}_{\pm 2.3}^{+26\%}$	$12.8_{\pm 7.0}^{+63\%}$	$\mathbf{0.85}_{\pm 0.04}^{+8\%}$	$\mathbf{0.05}_{\pm 0.04}^{+57\%}$	$\mathbf{7.2}_{\pm 1.9}^{+39\%}$	$\mathbf{24.2}_{\pm 8.4}^{+7\%}$
GOLEM	$0.87_{\pm 0.06}$	$0.22_{\pm 0.11}$	$6.5_{\pm 3.4}$	$13.0_{\pm 6.7}$	$0.63_{\pm 0.03}$	$0.16_{\pm 0.03}$	$17.2_{\pm 1.3}$	$48.0_{\pm 13.3}$
+ ReScore	$0.88_{\pm 0.06}^{+1\%}$	$0.21_{\pm 0.11}^{+2\%}$	$6.0_{\pm 3.4}^{+8\%}$	$\mathbf{12.4}_{\pm 6.3}^{+5\%}$	$0.66_{\pm 0.04}^{+5\%}$	$0.17_{\pm 0.01}^{-5\%}$	$16.2_{\pm 1.0}^{+6\%}$	$46.7_{\pm 13.3}^{+3\%}$
NOTEARS-MLP	$0.76_{\pm 0.17}$	$0.14_{\pm 0.09}$	$7.0_{\pm 3.5}$	$17.9_{\pm 10.0}$	$0.83_{\pm 0.05}$	$0.21_{\pm 0.04}$	$10.9_{\pm 1.9}$	$28.6_{\pm 12.0}$
+ ReScore	$0.73_{\pm 0.07}^{-4\%}$	$0.10_{\pm 0.09}^{+37\%}$	$6.8_{\pm 2.9}^{+3\%}$	$20.3_{\pm 9.7}^{-11\%}$	$0.94_{\pm 0.06}^{+14\%}$	$0.15_{\pm 0.06}^{+44\%}$	$6.80_{\pm 2.7}^{+60\%}$	$8.80_{\pm 12.4}^{+225\%}$
GraN-DAG	$0.88_{\pm 0.06}$	$0.02_{\pm 0.03}$	$2.7_{\pm 1.6}$	$8.70_{\pm 4.8}$	$0.98_{\pm 0.02}$	$0.12_{\pm 0.03}$	$5.4_{\pm 1.1}$	$3.70_{\pm 4.71}$
+ ReScore	$\mathbf{0.90}_{\pm 0.05}^{+2\%}$	$\mathbf{0.01}_{\pm 0.03}^{+35\%}$	$\mathbf{2.4}_{\pm 1.1}^{+13\%}$	$\mathbf{7.20}_{\pm 3.0}^{+21\%}$	$\mathbf{0.99}_{\pm 0.01}^{+1\%}$	$\mathbf{0.11}_{\pm 0.01}^{+12\%}$	$\mathbf{4.80}_{\pm 0.6}^{+13\%}$	$\mathbf{0.50}_{\pm 0.81}^{+640\%}$

Evaluation Metrics. To evaluate the quality of structure learning, four widely-used metrics are reported: True Positive Rate (TPR), False Discovery Rate (FDR), Structural Hamming Distance (SHD), and Structural Intervention Distance (SID) (Peters & Bühlmann, 2015), averaged over ten random trails.

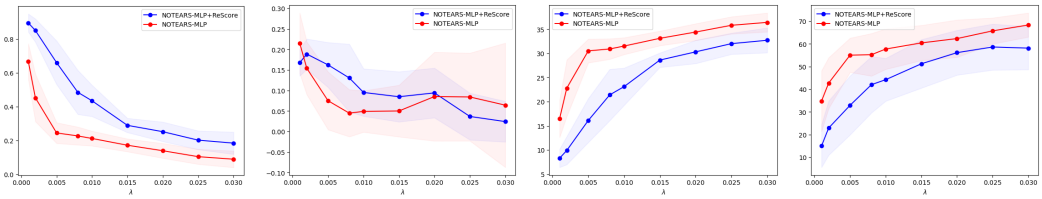
4.1 Overall Performance Comparison (RQ1)

4.1.1 Evaluations on Synthetic Data.

Simulations. The generating data differs along three dimensions: number of nodes, the degree of edge sparsity, and the type of graph. Two well-known graph sampling models, namely Erdos-Renyi (ER) and scale-free (SF) (Barabási & Albert, 1999) are considered with kd expected edges (denoted as ERk or SFk) and $d = \{10, 20, 50\}$ nodes. Specifically, in linear settings, similar to (Zheng et al., 2018; Gao et al., 2021), the coefficients are assigned following $U(-2, -0.5) \cup U(0.5, 2)$ with additive standard Gaussian noise. In nonlinear settings, following (Zheng et al., 2020), the ground-truth SEM in equation 1 is generated under the Gaussian process (GP) with radial basis function kernel of bandwidth one, where $f_i(\cdot)$ is additive noise models with N_i as an i.i.d. random variable following standard normal distribution. Both of these settings are known to be fully identifiable (Peters & Bühlmann, 2014; Peters et al., 2014). For each graph, 10 data sets of 2,000 samples are generated and the mean and standard deviations of the metrics are reported for a fair comparison.

Results. Tables 1, 2 and Tables in Appendix C.3 report the empirical results on both the linear and nonlinear synthetic data. The error bars depict the standard deviation across datasets over ten trails. The red and blue percentages separately refer to the increase and decrease of ReScore relative to the original score-based causal discovery methods in each metric. The best performing methods per task are bold. We observe that:

- **ReScore consistently and significantly strengthens the score-based methods for structure learning across all datasets.** In particular, it achieves substantial gains over the state-of-the-art baselines by around 3% to 60% in terms of SHD, revealing a lower number of missing, falsely detected, and reversed edges. We attribute the improvements to the dynamically learnable adaptive weights, which boost the quality of score-based DAG learners. With a closer look at the TPR and FDR, ReScore typically lowers FDR by eliminating spurious edges and enhances TPR by actively identifying more correct edges. This clearly demonstrates that ReScore effectively filters and upweights the more informative samples to better extract the causal relationship. Figure 4 also illustrates the clear trend that ReScore is excelling over NOTEARS-MLP as the sparsity penalty climbs. Additionally, as Table 10 indicates, ReScore only adds a negligible amount of computational complexity as compared to the backbone score-based DAG learners.
- **Score-based causal discovery baselines suffer from a severe performance drop on high-dimensional dense graph data.** Despite the advances, beyond linear, NOTEARS-MLP and GraN-DAG fail to scale to more than 50 nodes in SF4 and ER4 graphs, mainly due to difficulties in enforcing acyclicity in high-dimensional dense graph data (Varando, 2020; Lippe et al., 2022). Specifically, the TPR of GraN-DAG and NOTEARS-MLP in SF4 of 50 nodes is lower than 0.2, which indicates that they are not even able to accurately detect 40 edges out of 200 ground-truth edges. ReScore, as an optimization framework, relies heavily on the performance of the score-based backbone model. When the backbone model fails to infer DAG on its own as the number of nodes and edge density increase, adding ReScore will not be able to enhance the performance.



(a) TPR *w.r.t.* λ (b) FDR *w.r.t.* λ (c) SHD *w.r.t.* λ (d) SID *w.r.t.* λ

Figure 2: Performance comparison between NOTEARS-MLP and ReScore on ER4 graphs of 10 nodes on nonlinear synthetic datasets. The hyperparameter λ defined in equation 2 refers to the graph sparsity. See more results in Appendix C.3

Table 2: Results for ER graphs of 50 nodes on linear and nonlinear synthetic datasets.

	ER2				ER4			
	TPR ↑	FDR ↓	SHD ↓	SID ↓	TPR ↑	FDR ↓	SHD ↓	SID ↓
Random	0.04±0.02	0.90±0.03	397.3±12.7	1082.0±182.2	0.09±0.08	0.92±0.08	998.2±45.9	3399.1±489.2
NOTEARS	0.79±0.06	**0.09**±0.03	27.6±7.7	427.0±186.1	0.51±0.12	**0.27**±0.10	133.4±29.5	1643.8±172.2
+ ReScore	**0.88**±0.06 $^{+11\%}$	0.15±0.04 $^{-39\%}$	**26.2**±7.6 $^{+5\%}$	**266.0**±146.4 $^{+61\%}$	**0.52**±0.21 $^{+3\%}$	0.29±0.07 $^{-7\%}$	**130.2**±37.4 $^{+2\%}$	**1453.6**±336.5 $^{+13\%}$
GOLEM	0.80±0.09	0.35±0.09	68.6±19.7	433.5±215.6	0.31±0.11	0.68±0.06	150.6±25.1	1775.4±161.6
+ ReScore	0.82±0.15 $^{+3\%}$	0.33±0.14 $^{+5\%}$	63.4±27.9 $^{+8\%}$	430.2±155.5 $^{+1\%}$	0.39±0.06 $^{+24\%}$	0.66±0.06 $^{+3\%}$	146.3±26.3 $^{+3\%}$	1643.6±114.8 $^{+8\%}$
NOTEARS-MLP	0.32±0.04	0.13±0.08	69.5±4.7	884.4±172.8	0.17±0.02	**0.06**±0.04	167.0±4.1	1607.6±97.0
+ ReScore	0.51±0.08 $^{+59\%}$	**0.10**±0.07 $^{+30\%}$	53.5±8.7 $^{+30\%}$	628.1±120.6 $^{+41\%}$	0.26±0.04 $^{+52\%}$	0.11±0.05 $^{-51\%}$	154.4±6.4 $^{+8\%}$	1437.7±111.1 $^{+12\%}$
GraN-DAG	0.52±0.09	0.15±0.05	51.6±9.3	632.8±140.3	**0.32**±0.04	0.08±0.16	141.6±8.2	1379.0±91.3
+ ReScore	**0.53**±0.06 $^{+3\%}$	0.11±0.02 $^{+36\%}$	**46.0**±6.0 $^{+12\%}$	**581.0**±104.7 $^{+9\%}$	0.31±0.03 $^{-4\%}$	0.06±0.04 $^{+32\%}$	**138.8**±7.5 $^{+2\%}$	**1351.0**±98.2 $^{+2\%}$

4.1.2 Evaluations on Real Data.

A real-world dataset in cellular signaling networks provided by Sachs et al. (2005) is also covered in our experiments, which is a benchmark in graphical models. It contains the measurement of multiple phosphorylated protein and phospholipid components simultaneously in a large number of individual primary human immune system cells. We train all the baselines on 7,466 samples, where the ground-truth graph (11 nodes and 17 edges) is widely accepted by the biological community.

Table 3: The performance comparison on Sachs dataset.

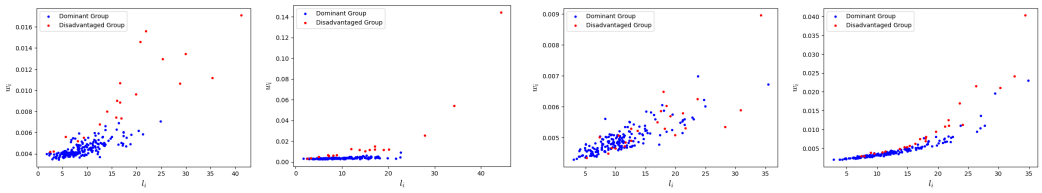
	TPR ↑	FDR ↓	SHD ↓	SID ↓	#Predicted Edges
Random	0.076	0.899	23	63	22
GOLEM	0.176	0.026	15	53	4
+ ReScore	0.294	0.063	**14**	49	6
NOTEARS-MLP	0.412	0.632	16	45	19
+ ReScore	0.412	0.500	**13**	43	14
GraN-DAG	0.294	0.643	16	60	14
+ ReScore	0.353	0.600	**15**	58	15

As Table 3 illustrates, ReScore steadily and prominently boosts all baselines *w.r.t.* SHD and SID metrics and successfully predicts more correct edges. This clearly shows the effectiveness of ReScore to better mitigate the reliance on easier-to-fit samples. With a closer look at the TPR, surprisingly, none of the causal discovery methods can achieve a performance of more than half correct, further highlighting the ineffectiveness of score-based causal discovery methods when dealing with real-world data. Our ReScore is a promising solution for enhancing the generalization and accuracy of DAG learning approaches. However, it is no doubt that integrating a strong backbone DAG learner with ReScore is the only way to truly advance in this field.

4.2 Performance on Heterogeneous Data (RQ2)

Motivations. It is commonplace to encounter heterogeneous data in real-world applications, of which the underlying causal generating process remain stable but the noise distribution may vary. Specific DAG learners designed for heterogeneous data are prone to assume strict conditions and require the knowledge of group annotation for each sample. Group annotations, however, are extremely costly and challenging to obtain. We conjecture that a robust DAG learner is able to successfully handle heterogeneous data without the information of group annotation.

Simulations. Synthetic heterogeneous data in both linear and nonlinear settings ($n = 1000$, $d = 20$, ER2) containing two distinct groups are also considered. 10% of observations come from the disadvantaged group, where half of the noise variables defined in equation 1 follow $\mathcal{N}(0, 1)$ and the remaining half of noise variables follow $\mathcal{N}(0, 0.1)$. 90% of observations, in contrast, are generated from the dominant group where the noise scale is flipped.



(a) Weights on linear data at the 1st and last epochs (b) Weights on nonlinear data at the 1st and last epochs

Figure 3: Illustration of adaptive weights learned by ReScore on linear and nonlinear synthetic data. For each dataset, the left and right plots correspond to the adaptive weights trained at the first and last epochs, respectively. The disadvantaged but more informative samples are represented by the red dots. The dominant and easy samples, in contrast, are depicted by the blue dots.

Table 4: Results on heterogeneous data.

Linear	TPR↑	FDR↓	SHD↓	Nonlinear	TPR↑	FDR↓	SHD↓
GOLEM	0.79	0.33	18.7	**NOTEARS-MLP**	0.46	0.44	31.6
+ ReScore	0.81	0.24	16.4	**+ ReScore**	0.50	0.41	29.0
CD-NOD	0.51	0.17	24.1	**CN-NOD**	0.56	0.51	30.2
DICD	0.82	0.28	16.7	**DICD**	0.67	0.31	25.1

Results. To evaluate whether ReScore can handle heterogeneous data without requiring the group annotation by automatically identifying and upweighting informative samples, we divide the whole observations into two subgroups. Obviously, samples from the disadvantaged group is more informative than those from the dominant group, as they offer additional insight to depict the causal edges. As Figure 3 shows, dots of different colours are mixed and scattered at the beginning of the training. After multiple iterations of training in inner and outer loops, the red dots from the disadvantaged group are gradually identified and assigned to relatively larger weights as compared to those blue dots with the same measure-of-fitness. This clearly validates the oracle property of adaptive weights proved in Theorem 2, which further illustrating the effectiveness of ReScore.

Table 4 indicates that ReScore drives impressive performance breakthroughs in heterogeneous data, achieving competitive or even lower SHD without group annotations compared to CD-NOD and DICD recognized as the lower bound. Specifically, both GOLEM and NOTEARS-MLP are struggling from notorious performance drop when homogeneity assumption is invalidated, and posing hurdle from being scaled up to real-world large-scale applications. We ascribe this hurdle to blindly scoring the observational samples evenly, rather than distilling the crucial group information from distribution shift of noise variables. In sheer contrast, benefiting from adaptive weights, ReScore can even extract group information from heterogeneous data that accomplish more profound causation understanding, leading to higher DAG learning quality. This validates that ReScore endows the backbone score-based DAG learner with better robustness against the heterogeneous data and alleviates the negative influence of spurious edges.

5 Conclusion

Today's score-based causal discovery approaches are still far from being able to accurately detect the causal structures, despite their great success on synthetic linear data. In this paper, we proposed ReScore, a simple-yet-effective model-agnostic optimization framework that simultaneously eliminates spurious edge learning and generalizes to heterogeneous data by utilizing learnable adaptive weights. Grounded by theoretical proof and empirical visualization studies, ReScore successfully identifies the informative samples and yields a consistent and significant boost in DAG learning. Extensive experiments verify that the remarkable improvement of ReScore on a variety of synthetic and real-world datasets indeed comes from adaptive weights.

Two aspects of ReScore's limitations will be covered in subsequent works. First, the performance of ReScore is highly related to the score-based causal discovery backbone methods, which leads to minor improvements when the backbone methods fail. Second, ReScore makes a basic assumption that no pure noise samples are involved in training progress, which restricts its applicability to clean data only. A generic ReScore technique is expected to substantially improve the DAG learning quality as well as able to distinguish between true informative samples and pure noise samples. However, we still believe that ReScore provides a promising research direction to diagnose the performance degradation for nonlinear and heterogeneous data in the structure learning challenge and will inspire more works in the future.

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A Related Work

Differentiable score-based causal discovery methods. Learning the directed acyclic graph (DAG) from purely observational data is challenging, owing mainly to the intractable combinatorial nature of acyclic graph space. A recent breakthrough, NOTEARS (Zheng et al., 2018), formulates the discrete DAG constraint into a continuous equality constraint, resulting in a differentiable score-based optimization problem. Recent subsequent works extends the formulation to deal with nonlinear problems by using a variety of deep learning models, such as neural networks (NOTEARS+ (Zheng et al., 2020), GraN-DAG (Lachapelle et al., 2020), CASTLE (Kyono et al., 2020), MCSL (Ng et al., 2019a), DARING (He et al., 2021)), generative autoencoder (CGNN (Goudet et al., 2018), Causal-VAE (Yang et al., 2021), ICL (Wang et al., 2020), DAG-GAN (Gao et al., 2021)), graph neural network (DAG-GNN (Gao et al., 2021), GAE (Ng et al., 2019b)), generative adversarial network (SAM (Kalainathan et al., 2018), ICL (Wang et al., 2020)), and reinforcement learning (RL-BIC (Zhu et al., 2020)).

Multi-domain causal structure learning. Most multi-domain causal structure learning methods are constraint-based and have diverse definition of domains. In our paper, the multi-domain or multi-group refers to heterogeneous data whose underlying causal generating process remain stable but the distributions of noise variables may vary. In literature, our definition of multi-domain is consistent with MC (Ghassami et al., 2018), CD-NOD (Huang et al., 2020), LRE (Ghassami et al., 2017), DICD (Wang et al., 2022), and others (Peters et al., 2016). In addition to the strict restriction of knowing the domain annotation in advance, the majority of structure learning models dedicated to heterogeneous data exhibit limited applicability, due to linear case assumption (Ghassami et al., 2018; 2017), causal direction identification only (Huang et al., 2019; Cai et al., 2020), and time-consuming (Huang et al., 2020).

B In-depth Analysis of ReScore

B.1 Proof of Theorem 1

Theorem 1. *Let* $\boldsymbol{w} \in \mathbb{C}\{\boldsymbol{w} : 0 < \frac{\tau}{n} < w_1, \ldots, w_n < \frac{1}{\tau n}, \sum_{i=1}^{n} w_i = 1\}$ *for some small* $\tau > 0$ *and the SEM in equation 1 is linear. The optimization problem* $\min_{\mathcal{G}} \left\{S(\mathcal{G}; \boldsymbol{X}) + \mathcal{P}_{DAG}(\mathcal{G})\right\}$ *is equivalent to* $\min_{\mathcal{G}} \left\{S_{\mathrm{w}}(\mathcal{G}; \boldsymbol{X}) + \mathcal{P}_{DAG}(\mathcal{G})\right\}$ *asymptotically in the following cases.*

a. Using the least-squares loss $\mathcal{L}(\mathcal{G}; \boldsymbol{X}) = \frac{1}{2n}\|\boldsymbol{X} - f(\boldsymbol{X})\|_F^2$*;*

b. Using the negative log-likelihood loss with standard Gaussian noise.

Proof. Let $B = (\beta_1, \ldots, \beta_d) \in \mathbb{R}^{d \times d}$ be the weighted adjacent matrix of a SEM, the linear SEM can be written in the matrix form:

$$X = XB + N \tag{7}$$

where $\mathbb{E}(N|X) = \overrightarrow{\mathbf{0}}$, $\mathrm{Var}(N|X) = diag(\sigma_1^2, \ldots, \sigma_d^2)$, and $B_{ii} = 0$ since X_i cannot be the parent of itself. Let $\mathbf{X} \in \mathbb{R}^{n \times d}$ be the observational data and $\mathbf{N} \in \mathbb{R}^{n \times d}$ be the corresponding errors, then

$$\mathbf{X} = \mathbf{X}B + \mathbf{N}.$$

The original and reweighted functions for optimization are

$$S(B; \mathbf{X}) + \mathcal{P}_{DAG}(B) = \mathcal{L}(B; \mathbf{X}) + \lambda \mathcal{R}_{sparse}(B) + \mathcal{P}(B),$$
$$S_{\mathrm{w}}(B; \mathbf{X}) + \mathcal{P}_{DAG}(B) = \mathcal{L}_{\mathrm{w}}(B; \mathbf{X}) + \lambda \mathcal{R}_{sparse}(B) + \mathcal{P}_{DAG}(B).$$

Comparing the above functions, only the first goodness-of-fit term are different, we will only consider this term.

For the least-squares loss case, the optimization problem is

$$\min_B \mathcal{L}_{\mathrm{w}}(B; \mathbf{X}) = \min_B \sum_{i=1}^{n} w_i l(\mathbf{x}_i, \mathbf{x}_i B),$$
$$s.t.\ B_{ii} = 0, \quad i = 1, \ldots, d.$$

Let $W = diag(w_1, \ldots, w_n)$ be the n-dimensional matrix, and rewrite the loss function as

$$\begin{aligned}
\mathcal{L}_{\mathrm{w}}(B; \mathbf{X}) &= \sum_{i=1}^{n} w_i \|\mathbf{x}_i - \mathbf{x}_i B\|_2^2 \\
&= \sum_{i=1}^{n} w_i (\mathbf{x}_i - \mathbf{x}_i B)(\mathbf{x}_i - \mathbf{x}_i B)^\top \\
&= \sum_{i=1}^{n} \sum_{j=1}^{d} w_i (\mathbf{X}_{ij} - \mathbf{x}_i \beta_j)^2 \\
&= \sum_{j=1}^{d} (\mathbf{x}^j - \mathbf{X}\beta_j)^\top W (\mathbf{x}^j - \mathbf{X}\beta_j),
\end{aligned}$$

where $\mathbf{x}^j$ is the j-th column in matrix $\mathbf{X}$. Let D_j be the d-dimensional identify matrix by setting j-th element as 0, for $j = 1, \ldots, d$. The above optimization is able to be written without the restriction:

$$\begin{aligned}
\min_B \tilde{\mathcal{L}}_{\mathrm{w}}(B; \mathbf{X}) &= \min_B \sum_{j=1}^{d} (\mathbf{x}^j - \mathbf{X} D_j \beta_j)^\top W (\mathbf{x}^j - \mathbf{X} D_j \beta_j) \\
&= \min_B \sum_{j=1}^{d} \big((\mathbf{x}^j)^\top W \mathbf{x}^j - 2(\mathbf{x}^j)^\top W \mathbf{X} D_j \beta_j + \beta_j^\top D_j^\top \mathbf{X}^\top W \mathbf{X} D_j \beta_j \big).
\end{aligned}$$

The partial derivative of the loss function with respect to β_j is

$$\begin{aligned}
\frac{\partial \tilde{\mathcal{L}}_{\mathrm{w}}(B; \mathbf{X})}{\partial \beta_j} &= \frac{\partial \Big[\sum_{j=1}^{d} \big((\mathbf{x}^j)^\top W X_j - 2(\mathbf{x}^j)^\top W \mathbf{X} D_j \beta_j + \beta_j^\top D_j^\top \mathbf{X}^\top W \mathbf{X} D_j \beta_j \big) \Big]}{\partial \beta_j} \\
&= \frac{\partial \big((\mathbf{x}^j)^\top W \mathbf{x}^j - 2(\mathbf{x}^j)^\top W \mathbf{X} D_j \beta_j + \beta_j^\top D_j^\top \mathbf{X}^\top W \mathbf{X} D_j \beta_j \big)}{\partial \beta_j} \\
&= -2 D_j^\top \mathbf{X}^\top W \mathbf{x}^j + 2 D_j^\top \mathbf{X}^\top W \mathbf{X} D_j \beta_j.
\end{aligned}$$

Setting the partial derivative to zero produces the optimal parameter:

$$\begin{aligned}
\hat{\beta}_j &= D_j^\top (\mathbf{X}^\top W \mathbf{X})^{-1} D_j D_j^\top \mathbf{X}^\top W \mathbf{x}^j \\
&= D_j^\top (\mathbf{X}^\top W \mathbf{X})^{-1} D_j D_j^\top \mathbf{X}^\top W (\mathbf{X} D_j \beta_j + \mathbf{N}^j) \\
&= D_j \beta_j + D_j (\mathbf{X}^\top W \mathbf{X})^{-1} \mathbf{X}^\top W \mathbf{N}^j, \qquad (8)
\end{aligned}$$

where $\mathbf{N}^j \in \mathbb{R}^n$ is the j-th column in matrix $\mathbf{N}$. In the above equation, the second equality holds because $\mathbf{x}^j = \mathbf{X} D_j \beta_j + \mathbf{N}^j$. Similarly, one is easy to obtain that the optimum parameter for ordinary mean-squared loss is

$$\tilde{\beta}_j = D_j \beta_j + D_j (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{N}^j. \qquad (9)$$

It is obvious that the difference between equation 8 and equation 9 is the second term. Compute the mean and variance matrix of that term, we can get

$$\begin{aligned}
\mathbb{E}\big[(\mathbf{X}^\top W \mathbf{X})^{-1} \mathbf{X}^\top W \mathbf{N}^j \big] &= \mathbb{E}\Big(\mathbb{E}\big[(\mathbf{X}^\top W \mathbf{X})^{-1} \mathbf{X}^\top W \mathbf{N}^j | \mathbf{X} \big] \Big) \\
&= \mathbb{E}\Big((\mathbf{X}^\top W \mathbf{X})^{-1} \mathbf{X}^\top W \cdot \mathbb{E}\big[\mathbf{N}^j | \mathbf{X} \big] \Big) \\
&= \overrightarrow{\mathbf{0}}; \\
\mathrm{Var}\big[(\mathbf{X}^\top W \mathbf{X})^{-1} \mathbf{X}^\top W \mathbf{N}^j \big] &= \mathbb{E}\Big(\mathrm{Var}\big[(\mathbf{X}^\top W \mathbf{X})^{-1} \mathbf{X}^\top W \mathbf{N}^j | \mathbf{X} \big] \Big) \\
&= \mathbb{E}\Big((\mathbf{X}^\top W \mathbf{X})^{-1} \mathbf{X}^\top W \cdot \mathrm{Var}\big[\mathbf{N}^j | \mathbf{X} \big] \cdot W \mathbf{X} (\mathbf{X}^\top W \mathbf{X})^{-1} \Big) \\
&= \sigma_j^2 \mathbb{E}\big[(\mathbf{X}^\top W \mathbf{X})^{-1} \mathbf{X}^\top W^2 \mathbf{X} (\mathbf{X}^\top W \mathbf{X})^{-1} \big].
\end{aligned}$$

Since $\mathrm{w} \in \mathbb{C}(\tau)$, it is easy to know that the variance matrix is finite. By the Kolmogorov's strong law of large numbers, the second term converges to zero, thus

$$\hat{\beta}_j \to D_j \beta_j,$$

which is same as the ordinary case. Since noise $N = (N_1, \ldots, N_d)$ are jointly independent, the previous process can be apply to the other $j \in \{1, \ldots, d\}$. Therefore, the convergence has been shown for 'case a.'.

Since the noise follows standard Gaussian distribution, i.e.

$$X - XB = N = (N_1, \ldots, N_d) \sim \mathcal{N}\big(\overrightarrow{\mathbf{0}}, diag(\sigma_1^2, \ldots, \sigma_d^2)\big),$$

the loss function (negative log-likelihood function) is

$$\begin{aligned}
\mathcal{L}_{\mathrm{w}}(B; \mathbf{X}) &= -\sum_{i=1}^{n} w_i \sum_{j=1}^{d} \left[\log\left(\frac{1}{\sigma_j \sqrt{2\pi}}\right) - \frac{(\mathbf{X}_{ij} - \mathbf{x}_i \beta_j)^2}{2\sigma_j^2} \right] \\
&= \sum_{j=1}^{d} \sum_{i=1}^{n} w_i \log\left(\sigma_j \sqrt{2\pi}\right) + \sum_{j=1}^{d} \sum_{i=1}^{n} \frac{w_i}{2\sigma_j^2} (\mathbf{X}_{ij} - \mathbf{x}_i \beta_j)^2 \\
&= \sum_{j=1}^{d} \sum_{i=1}^{n} w_i \log\left(\sigma_j \sqrt{2\pi}\right) + \sum_{j=1}^{d} \frac{1}{2\sigma_j^2} (\mathbf{x}^j - \mathbf{X}\beta_j)^\top W (\mathbf{x}^j - \mathbf{X}\beta_j). \qquad (10)
\end{aligned}$$

To minimize the loss function above w.r.t. B, it is equivalent to minimize the first term in equation 10:

$$\min_B \mathcal{L}_{\mathrm{w}}(B; \mathbf{X}) \quad \Longleftrightarrow \quad \min_B \sum_{j=1}^{d} \frac{1}{2\sigma_j^2} (\mathbf{x}^j - \mathbf{X}\beta_j)^\top W (\mathbf{x}^j - \mathbf{X}\beta_j).$$

It can be seen that the RHS above is similar to the loss function in case 1), except the coefficients $\frac{1}{2\sigma_j^2}, j = 1, \ldots, d$. Therefore, one can use same approaches to get the equivalence result for 'case b.', which will be omitted here.

Consequently, the proofs of the two special cases have been done. □

B.2 Proof of Theorem 2

Theorem 2. *Suppose that in the optimization phrase, the i-th observation has a larger error than the j-th observation in the sense that $l(\boldsymbol{x}_i, f(\boldsymbol{x}_i)) > l(\boldsymbol{x}_j, f(\boldsymbol{x}_j))$, where $i, j \in \{1, \ldots, n\}$. Then,*

$$w_i^* > w_j^*,$$

where $\boldsymbol{w}^* = (w_1^*, \ldots, w_n^*)$ is the optimal weights in equation 6.

Proof. We will show the theorem by contradiction. Without loss of generality, let $i = 1$, $j = 2$, and suppose $w_1^* \leq w_2^*$. Since $\mathrm{w}^* \in \mathbb{C}$ and $\mathbb{C}$ is an open set, one is able to find a small enough $\varepsilon > 0$ such that

$$\mathrm{w}^{**} = (w_1^* + \varepsilon, w_2^* - \varepsilon, w_3^* \ldots, w_n^*) \in \mathbb{C}.$$

Therefore,

$$\begin{aligned}
& S_{\mathrm{w}^*}(\mathcal{G}; \mathbf{X}) - S_{\mathrm{w}^{**}}(\mathcal{G}; \mathbf{X}) \\
= \; & \left[w_1^* \cdot l(\mathbf{x}_1, f(\mathbf{x}_1)) + w_2^* \cdot l(\mathbf{x}_2, f(\mathbf{x}_2)) \right] - \left[(w_1^* + \varepsilon) \cdot l(\mathbf{x}_1, f(\mathbf{x}_1)) + (w_2^* - \varepsilon) \cdot l(\mathbf{x}_2, f(\mathbf{x}_2)) \right] \\
= \; & \varepsilon \cdot \left[l(\mathbf{x}_2, f(\mathbf{x}_2)) - l(\mathbf{x}_1, f(\mathbf{x}_1)) \right] < 0,
\end{aligned}$$

which contradicts $\mathbf{w}^* \in \arg\max_{\mathrm{w}} \; S_{\mathrm{w}}(\mathcal{G}; \mathbf{X})$. □

C SUPPLEMENTARY EXPERIMENTS

C.1 BASELINES

We select six state-of-the-art causal discovery methods as baselines for comparison:

- **NOTEARS** (Zheng et al., 2018) is a breakthrough work that firstly recasts the combinatorial graph search problem as a continuous optimization problem in linear settings. NOTEARS estimates the true causal graph by minimizing the reconstruction loss with the continuous acyclicity constraint.
- **NOTEARS-MLP** (Zheng et al., 2020) is an extension of NOTEARS for nonlinear settings, approximating the generative SEM model by MLP while only applying the continuous acyclicity constraint to the first layer of the MLP.
- **GraN-DAG** (Lachapelle et al., 2020) adapts the continuous constrained optimization formulation to allow for nonlinear relationships between variables using neural networks and makes use of a final pruning step to remove spurious edges, thus achieving good results in nonlinear settings.
- **GOLEM** (Ng et al., 2020) improves on the least squares score function (Zheng et al., 2018) by proposing a score function that directly maximizes the data likelihood. They show the likelihood-based score function with soft sparsity regularization is sufficient to asymptotically learn a DAG equivalent to the ground-truth DAG.
- **DICD** (Wang et al., 2022) aims to discover the environment-invariant causation while removing the environment-dependent correlation based on ground truth domain annotation.
- **CD-NOD** (Huang et al., 2020) is a constrained-based causal discovery method that is designed for heterogeneous data, *i.e.,* datasets from different environments. CD-NOD utilizes the independent changes across environments to predict the causal orientations and proposes constrained-based and kernel-based methods to find the causal structure.

C.2 EXPERIMENTAL SETTINGS

For NOTEARS, we follow the original linear implementation. For GOLEM, we adopt the GOLEM-NV setting from the original repo. For NOTEARS-MLP, we follow the original non-linear implementation which consist a Multilayer Perceptron (MLP) comprising of two hidden layers with ten neurons each and ReLU activation functions (except for the Sachs dataset, which uses only one hidden layer, inherent the settings from Zheng et al. (2020)). For GranDAG, we employ the pns, training, and cam-pruning stages from the original code and tune three pipeline stages together for best performance. The ReScore adaptive weights learning model for all nonlinear baselines consists of two hidden layer and ReLU activation, and for linear baselines the layer size is reduced to one. All Experiments are conducted on a single Tesla V100 GPU. Detailed hyperparameter search space for different methods is shown in Table 5.

C.3 MORE EXPERIMENTAL RESULTS FOR RQ1

Discussions. More experimental results on both the linear and nonlinear synthetic data are reported in Figures 4 - 6 and Tables 6 - 8. The error bars depict the standard deviation across datasets over ten trails. The red and blue percentages separately refer to the increase and decrease of ReScore relative to the original score-based causal discovery methods in each metric. The best performing methods per task are bold.

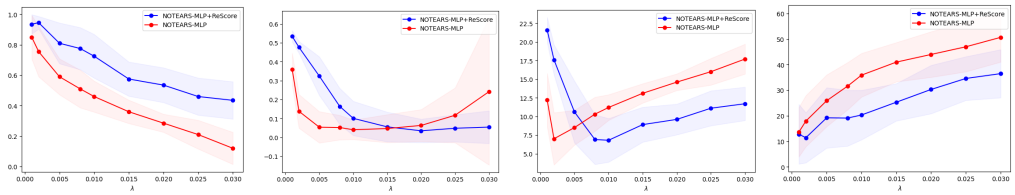
C.4 STUDY ON RESCORE

Sensitivity to Neural Network Complexity.

We also investigated the effect of number of hidden units in our adaptive weights learning model for ReScore. We plot the TPR, FDR, SHD, SID with varing number of hidden units ranging from 10 to 100 units in nonlinear settings, using $n = 600$ and $n = 2,000$ samples generated from GP model on ER4 graph with $d = 10$ nodes. Detailed results could be found in Figure 7. One can first observe

Table 5: Hyperparameter search spaces for each algorithm.

	Hyperparameter space
NOTEARS / NOTEARS+ReScore	$\lambda \sim U\{0.002, 0.005, 0.01, 0.015, 0.02, 0.03, 0.09, 0.1, 0.25\}$ $\tau \sim U\{0.1, 1, 5, 10, 20, 30, 40, 50, 100\}$ Final threshold $\sim U\{0.001, 0.003, 0.01, 0.03, 0.1, 0.3\}$ Constraint convergence tolerance $\sim U\{10^{-6}, 10^{-8}, 10^{-10}\}$ Log(learning rate of ReScore) $\sim U[-1, -5]$
GOLEM / GOLEM+ReScore	$\lambda \sim U\{0.002, 0.005, 0.01, 0.015, 0.02, 0.03, 0.09, 0.1, 0.25\}$ $\tau \sim U\{0.1, 1, 5, 10, 20, 30, 40, 50, 100\}$ GOLEM-λ^* $\sim U\{0.01, 0.1, 0.2, 1, 10, 100, 200, 500\}$ Log(learning rate of ReScore) $\sim U[-1, -5]$
NOTEARS-MLP / NOTEARS-MLP+ReScore	$\lambda \sim U\{0.002, 0.005, 0.01, 0.015, 0.02, 0.03, 0.09, 0.1, 0.25\}$ $\tau \sim U\{0.1, 1, 5, 10, 20, 30, 40, 50, 100\}$ # hidden units of ReScore $\sim U\{1, 10, 20, 50, 80, 100\}$ # hidden layers of ReScore $\sim U\{1, 2, 3, 4\}$ # hidden units of NOTEARS-MLP $\sim U\{1, 10, 20, 50, 80, 100\}$ # hidden layers of ReScore $\sim U\{1, 2, 3\}$ Final threshold $\sim U\{0.001, 0.003, 0.01, 0.03, 0.1, 0.3\}$ Constraint convergence tolerance $\sim U\{10^{-6}, 10^{-8}, 10^{-10}\}$ Log(learning rate of ReScore) $\sim U[-1, -5]$
GraN-DAG / GraN-DAG+ReScore	$\lambda \sim U\{0.002, 0.005, 0.01, 0.015, 0.02, 0.03, 0.09, 0.1, 0.25\}$ $\tau \sim U\{0.1, 1, 5, 10, 20, 30, 40, 50, 100\}$ # hidden units of ReScore $\sim U\{1, 10, 20, 50, 80, 100\}$ # hidden layers of ReScore $\sim U\{1, 2, 3, 4\}$ Log(learning rate of ReScore) $\sim U[-1, -5]$ PNS threshold $\sim U\{0.5, 0.75, 1, 2\}$ Log(Pruning cutoff) $\sim U\{0.001, 0.005, 0.01, 0.03, 0.1, 0.2, 0.3\}$



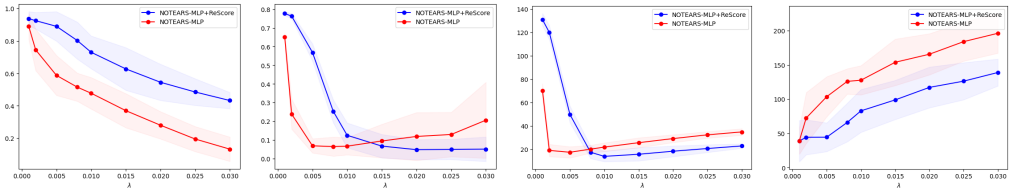
(a) TPR *w.r.t.* λ (b) FDR *w.r.t.* λ (c) SHD *w.r.t.* λ (d) SID *w.r.t.* λ

Figure 4: Performance comparison between NOTEARS-MLP and ReScore on ER2 graphs of 10 nodes on nonlinear synthetic datasets. The hyperparameter λ defined in equation 2 refers to the graph sparsity.

our model is stable when increasing the neurons, illustrating the insensitivity of ReScore *w.r.t.* the number of neurons in adaptive weights learning model. On the other hand, more observational samples to estimate the parameters could help the ReScore achieve higher performance, indicating rich samples bring benefit.

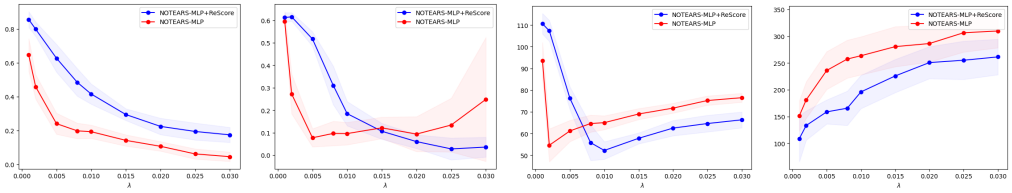
C.5 Training Costs

In terms of time complexity, as shown in Table 10, we report the time for each baseline and ReScore on Sachs. Compared with backbone methods, ReScore adds very little computing cost to training.



(a) TPR *w.r.t.* λ (b) FDR *w.r.t.* λ (c) SHD *w.r.t.* λ (d) SID *w.r.t.* λ

Figure 5: Performance comparison between NOTEARS-MLP and ReScore on ER2 graphs of 20 nodes on nonlinear synthetic datasets. The hyperparameter λ defined in equation 2 refers to the graph sparsity.



(a) TPR *w.r.t.* λ (b) FDR *w.r.t.* λ (c) SHD *w.r.t.* λ (d) SID *w.r.t.* λ

Figure 6: Performance comparison between NOTEARS-MLP and ReScore on ER4 graphs of 20 nodes on nonlinear synthetic datasets. The hyperparameter λ defined in equation 2 refers to the graph sparsity.

Table 6: Results for ER graphs of 20 nodes on linear and nonlinear synthetic datasets.

	ER2				ER4			
	TPR ↑	FDR ↓	SHD ↓	SID ↓	TPR ↑	FDR ↓	SHD ↓	SID ↓
Random	0.11±0.09	0.89±0.08	56.8±8.7	292.3±45.7	0.07±0.03	0.90±0.08	86.9±7.0	387.5±52.3
NOTEARS	0.85±0.08	**0.09**±0.03	9.2±3.8	55.4±31.1	0.74±0.02	**0.23**±0.03	39.4±7.9	185.8±38.1
+ ReScore	**0.87**±0.07 +2%	0.11±0.05 −17%	**8.8**±3.5 +5%	**50.6**±26.3 +9%	**0.79**±0.05 +7%	0.28±0.05 −17%	**36.8**±7.9 +7%	**180.8**±43.5 +3%
GOLEM	0.75±0.07	0.20±0.11	17.0±6.1	78.2±22.6	0.46±0.06	0.50±0.06	73.6±7.9	249.8±7.8
+ ReScore	0.76±0.06 +2%	0.20±0.10 +1%	15.8±5.8 +8%	77.0±21.5 +2%	0.48±0.06 +3%	0.43±0.06 +16%	70.2±8.3 +5%	246.2±11.4 +1%
NOTEARS-MLP	0.53±0.09	0.08±0.03	19.4±3.3	118.5±22.5	**0.44**±0.09	0.26±0.10	55.0±9.2	176.3±33.3
+ ReScore	0.70±0.11 +31%	0.16±0.05 −51%	15.7±5.1 +24%	88.7±23.3 +34%	0.41±0.07 −6%	0.17±0.08 +54%	**51.6**±6.4 +7%	179.9±33.7 −2%
GraN-DAG	**0.81**±0.15	0.08±0.08	9.3±5.4	53.4±24.4	0.20±0.07	0.18±0.08	57.4±4.6	131.5±21.4
+ ReScore	**0.81**±0.14 +0%	**0.05**±0.04 +64%	**8.5**±5.7 +9%	**51.0**±24.6 +5%	0.21±0.07 +5%	**0.17**±0.09 +8%	56.2±4.6 +2%	**125.4**±23.3 +5%

Table 7: Results for SF graphs of 10 nodes on linear and nonlinear synthetic datasets.

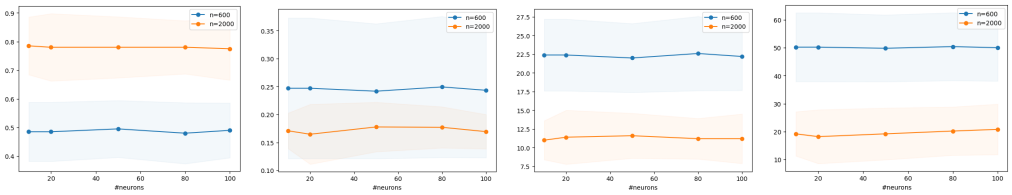
	SF2				SF4			
	TPR ↑	FDR ↓	SHD ↓	SID ↓	TPR ↑	FDR ↓	SHD ↓	SID ↓
Random	0.05±0.03	0.91±0.09	32.2±7.97	35.1±7.3	0.13±0.01	0.93±0.15	57.2±10.3	79.1±8.7
NOTEARS	0.98±0.02	**0.02**±0.03	0.8±0.5	**1.0**±2.0	0.95±0.03	0.03±0.02	12.2±1.2	6.2±5.3
+ ReScore	**0.99**±0.02 +1%	0.04±0.04 −45%	**0.4**±0.7 +100%	**1.0**±0.9 +0%	**0.97**±0.03 +2%	0.03±0.03 +27%	10.2±1.5 +20%	**3.0**±1.9 +107%
GOLEM	0.96±0.07	0.07±0.12	1.8±3.1	1.2±2.4	0.85±0.03	0.12±0.08	7.0±2.3	12.8±7.9
+ ReScore	0.97±0.07 +1%	0.07±0.12 +3%	1.4±2.9 +29%	1.2±2.4 +0%	0.87±0.06 +3%	**0.10**±0.08 +17%	**5.8**±2.9 +21%	9.8±8.2 +31%
NOTEARS-MLP	**0.84**±0.17	0.25±0.12	6.7±3.4	8.1±7.3	0.73±0.14	0.23±0.05	12.0±3.9	19.4±7.4
+ ReScore	0.82±0.22 −2%	0.17±0.08 +45%	5.8±3.3 +16%	**6.0**±3.8 +35%	**0.88**±0.09 +20%	0.27±0.07 −16%	11.0±3.4 +9%	12.8±9.3 +52%
GraN-DAG	0.69±0.20	0.05±0.05	5.9±3.0	12.0±8.2	0.82±0.11	**0.11**±0.08	8.7±1.8	8.4±4.1
+ ReScore	0.72±0.17 +4%	**0.04**±0.03 +28%	**5.3**±2.8 +11%	10.5±8.7 +14%	0.86±0.12 +5%	0.12±0.08 −12%	**8.1**±2.0 +7%	**7.0**±6.7 +20%

Table 8: Results for SF graphs of 20 nodes on linear and nonlinear synthetic datasets.

	SF2				SF4			
	TPR ↑	FDR ↓	SHD ↓	SID ↓	TPR ↑	FDR ↓	SHD ↓	SID ↓
Random	0.11±0.10	0.89±0.03	43.2±5.4	96.8±10.4	0.09±0.05	0.88±0.05	108.2±12.9	155.6±37.2
NOTEARS	0.90±0.06	**0.02**±0.01	4.0±1.9	19.8±12.8	0.90±0.05	0.12±0.06	45.2±7.0	28.6±20.2
+ ReScore	0.95±0.04 +6%	0.06±0.04 −70%	**3.6**±1.8 +11%	**9.8**±8.1 +102%	**0.93**±0.03 +3%	**0.02**±0.07 +624%	45.0±6.8 +0%	**25.6**±12.1 +12%
GOLEM	0.96±0.03	0.19±0.06	9.0±3.2	10.4±7.0	0.83±0.05	0.35±0.09	42.8±13.0	41.4±14.8
+ ReScore	**0.96**±0.02 +0%	0.18±0.06 +4%	8.6±3.1 +5%	10.4±7.0 +0%	0.85±0.43 +2%	0.34±0.09 +5%	**39.8**±14.0 +8%	37.6±12.8 +10%
NOTEARS-MLP	**0.42**±0.13	0.23±0.13	25.5±4.5	49.9±7.4	0.20±0.03	0.22±0.12	58.9±3.1	115.6±25.0
+ ReScore	0.41±0.13 −2%	**0.10**±0.10 +121%	**23.5**±4.5 +9%	**47.6**±9.4 +5%	**0.21**±0.04 +3%	**0.09**±0.09 +131%	**56.4**±2.2 +4%	**109.0**±21.8 +6%
GraN-DAG	0.03±0.15	0.24±0.17	27.1±4.15	77.0±28.0	0.20±0.06	0.18±0.12	56.8±4.5	133.4±21.0
+ ReScore	0.03±0.15 −6%	0.15±0.10 +63%	25.7±4.4 +5%	72.8±26.0 +6%	0.21±0.07 +2%	0.17±0.08 +8%	**56.4**±4.6 +1%	125.4±23.3 +6%

Table 9: Results for SF graphs of 50 nodes on linear and nonlinear synthetic datasets.

	SF2				SF4			
	TPR ↑	**FDR ↓**	**SHD ↓**	**SID ↓**	**TPR ↑**	**FDR ↓**	**SHD ↓**	**SID ↓**
Random	$0.10_{\pm 0.08}$	$0.89_{\pm 0.07}$	$334.2_{\pm 16.9}$	$1093.3_{\pm 145.4}$	$0.12_{\pm 0.11}$	$0.89_{\pm 0.04}$	$1023.5_{\pm 49.5}$	$1903.9_{\pm 194.3}$
NOTEARS	$0.82_{\pm 0.03}$	$\mathbf{0.07}_{\pm 0.05}$	$23.6_{\pm 6.2}$	$135.4_{\pm 47.5}$	$0.71_{\pm 0.18}$	$0.25_{\pm 0.07}$	$97.6_{\pm 36.9}$	$276.2_{\pm 131.0}$
+ ReScore	$\mathbf{0.94}_{\pm 0.03}^{+15\%}$	$0.15_{\pm 0.06}^{-55\%}$	$\mathbf{21.6}_{\pm 9.1}^{+9\%}$	$\mathbf{61.2}_{\pm 22.6}^{+121\%}$	$\mathbf{0.73}_{\pm 0.05}^{+3\%}$	$\mathbf{0.10}_{\pm 0.03}^{+138\%}$	$\mathbf{67.6}_{\pm 12.3}^{+44\%}$	$\mathbf{275.2}_{\pm 55.0}^{+0\%}$
GOLEM	$0.77_{\pm 0.07}$	$0.19_{\pm 0.11}$	$38.6_{\pm 16.7}$	$161.6_{\pm 53.2}$	$0.62_{\pm 0.17}$	$0.21_{\pm 0.09}$	$114.2_{\pm 37.5}$	$384.0_{\pm 107.4}$
+ ReScore	$0.79_{\pm 0.09}^{+2\%}$	$0.24_{\pm 0.12}^{-20\%}$	$32.2_{\pm 11.1}^{+20\%}$	$143.4_{\pm 63.0}^{+13\%}$	$0.68_{\pm 0.17}^{+9\%}$	$0.21_{\pm 0.09}^{+1\%}$	$113.7_{\pm 37.5}^{+0\%}$	$366.4_{\pm 107.0}^{+5\%}$
NOTEARS-MLP	$0.22_{\pm 0.04}$	$0.04_{\pm 0.04}$	$75.8_{\pm 4.0}$	$\mathbf{266.8}_{\pm 46.0}$	$0.11_{\pm 0.02}$	$\mathbf{0.03}_{\pm 0.02}$	$168.8_{\pm 3.8}$	$461.6_{\pm 54.9}$
+ ReScore	$\mathbf{0.23}_{\pm 0.05}^{+4\%}$	$0.07_{\pm 0.07}^{-47\%}$	$\mathbf{75.6}_{\pm 4.3}^{+0\%}$	$267.2_{\pm 36.6}^{-0\%}$	$\mathbf{0.13}_{\pm 0.04}^{+10\%}$	$0.07_{\pm 0.06}^{-52\%}$	$\mathbf{167.7}_{\pm 7.0}^{+1\%}$	$\mathbf{453.4}_{\pm 57.7}^{+2\%}$
GraN-DAG	$0.19_{\pm 0.03}$	$0.28_{\pm 0.05}$	$80.2_{\pm 3.5}$	$380.8_{\pm 56.1}$	$0.11_{\pm 0.03}$	$0.25_{\pm 0.11}$	$171.4_{\pm 6.3}$	$549.6_{\pm 84.9}$
+ ReScore	$0.20_{\pm 0.03}^{+5\%}$	$\mathbf{0.24}_{\pm 0.05}^{+17\%}$	$79.8_{\pm 0.3}^{+1\%}$	$349.2_{\pm 49.6}^{+9\%}$	$0.11_{\pm 0.02}^{+0\%}$	$0.24_{\pm 0.10}^{+5\%}$	$170.8_{\pm 4.0}^{+0\%}$	$548.0_{\pm 91.4}^{+0\%}$



(a) TPR *w.r.t.* neurons (b) FDR *w.r.t.* neurons (c) SHD *w.r.t.* neurons (d) SID *w.r.t.* neurons

Figure 7: Performance with varying neurons in ReScore model.

Table 10: Training cost on Sachs (seconds per iteration/in total).

NOTEARS	0.74 / 2.97
+ ReScore	3.8 / 15.3
NOTEARS-MLP	0.87 / 3.48
+ ReScore	4.3 / 17.0
GOLEM	13.4 / 53.5
+ ReScore	14.6 / 58.2
GraN-DAG	4.9 / 197.3
+ ReScore	5.5 / 221.6