



Identifiability of Gaussian linear structural equation models with homogeneous and heterogeneous error variances

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Abstract

In this work, we consider the identifiability assumption of Gaussian linear structural equation models (SEMs) in which each variable is determined by a linear function of its parents plus normally distributed error. It has been shown that linear Gaussian structural equation models are fully identifiable if all error variances are the same or known. Hence, this work proves the identifiability of Gaussian SEMs with both homogeneous and heterogeneous unknown error variances. Our new identifiability assumption exploits not only error variances, but edge weights; hence, it is strictly milder than prior work on the identifiability result. We further provide a structure learning algorithm that is statistically consistent and computationally feasible, based on our new assumption. The proposed algorithm assumes that all relevant variables are observed, while it does not assume causal minimality and faithfulness. We verify our theoretical findings through simulations and real multivariate data, and compare our algorithm to state-of-the-art PC, GES and GDS algorithms.

Keywords Bayesian network · Causal inference · Directed acyclic graphical model · Identifiability · Structural equation model

1 Introduction

Learning the causal structure of a set of random variables from joint distribution is an important problem in many areas (Kephart and White 1991; Friedman et al. 2000; Doya 2007; Peters and Bühlmann 2014). This problem becomes more crucial when the causal graph is of interest but interventional experiments are impossible. However, learning causal graphical models from only observational data is a notoriously difficult problem due to non-identifiability. Hence, a number of prior works have addressed

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the question of identifiability for different classes of joint distribution by placing further restrictions on distribution $P(G)$. Spirtes et al. (2000), Chickering (2003), Tsamardinos and Aliferis (2003), Zhang and Spirtes (2016) and many other works show that directed acyclic graphical (DAG) models are recoverable up to the Markov equivalence class (MEC) under the faithfulness or related assumptions. However, since many MECs contain more than one graph, a true causal graph cannot be determined.

Recent works prove a number of fully identifiable classes of DAG models by placing a different type of restrictions on $P(G)$: (i) Shimizu et al. (2006) shows that linear non-Gaussian models where each variable is determined by a linear function of its parents plus an independent non-Gaussian error term are identifiable; (ii) Hoyer et al. (2009), Mooij et al. (2009), Peters et al. (2012) relax the assumption of linearity, and prove the identifiability of nonlinear additive noise models where each variable is determined by a non-linear function of its parents and an error term; (iii) Peters and Bühlmann (2014), Loh and Bühlmann (2014) prove that Gaussian linear structural equation models with equal or known error variances are identifiable; and (iv) Park and Raskutti (2018), Park and Park (2019) prove the identifiability of DAG models where the variance of the conditional distribution of each node given its parents is a non-concave function of the mean.

In this article, we prove the identifiability of a new class of DAG models: Gaussian linear structural equation models with unknown error variances that can be different. Our approach exploits an uncertainty level of conditional distribution by considering both error variances and edge weights. We show that the new identifiability assumption is strictly milder than the equal error variance assumption for the Gaussian linear structural equation models in Peters and Bühlmann (2014).

In addition, we develop a statistically consistent and computationally feasible algorithm to recover a graph based on our new identifiability condition. We compare our algorithm against state-of-the-art PC (Spirtes et al. 2000) greedy equivalence search (GES) (Chickering 2003), and greedy DAG search (GDS) (Peters and Bühlmann 2014) algorithms in Sect. 4. Our algorithm performs better than the comparisons because our algorithm is not a heuristic search, but exploits a relaxed identifiability condition. Lastly, we emphasize that the new condition enables the proposed algorithm to be a polynomial-time complete search, and hence, it can learn large-scale graphs.

The remainder of this paper is structured as follows. Section 2 summarizes the necessary notations and problem settings, discusses Gaussian SEMs, and proves their identifiability. In Sect. 3, we introduce a practical graph-learning algorithm based on our theoretical findings. Section 4 provides an evaluation of our algorithm against other state-of-the-art DAG learning algorithms when recovering the graphs. Lastly, Sect. 5 compares our algorithm to the PC, GES, and GDS algorithms by analyzing a real mathematics marks data.

2 Gaussian structural equation models and identifiability

We first introduce some necessary notations and definitions for Gaussian structural equation models (SEMs) and directed acyclic graphical (DAG) models. Then, we give a detailed description of the previous work on the identifiability of Gaussian SEMs

in Peters and Bühlmann (2014), Loh and Bühlmann (2014), Ghoshal and Honorio (2017). Lastly, we propose a new identifiability condition.

2.1 Problem set-up and notations

A DAG $G = (V, E)$ consists of a set of nodes $V = \{1, 2, \dots, p\}$ and a set of directed edges $E \subset V \times V$ with no directed cycles. A directed edge from node j to k is denoted by (j, k) or $j \rightarrow k$. The set of *parents* of node k denoted by $\text{Pa}(k)$ consists of all nodes j such that $(j, k) \in E$. If there is a directed path $j \rightarrow \dots \rightarrow k$, then k is called a *descendant* of j and j is an *ancestor* of k . The set $\text{De}(k)$ denotes the set of all descendants of node k . The *non-descendants* of node k are $\text{Nd}(k) := V \setminus (\{k\} \cup \text{De}(k))$. An important property of DAGs is that there exists a (possibly non-unique) *ordering* $\pi = (\pi_1, \dots, \pi_p)$ of a directed graph that represents directions of edges such that for every directed edge $(j, k) \in E$, j comes before k in the ordering.

We consider a set of random variables $X := (X_j)_{j \in V}$ with a probability distribution taking values in probability space \mathcal{X}_V over the nodes in the graph G . Suppose that a random vector X has a joint probability density function $P(G) = P(X_1, X_2, \dots, X_p)$. For any subset S of V , let $X_S := \{X_j : j \in S \subset V\}$ and $\mathcal{X}(S) := \times_{j \in S} \mathcal{X}_j$ where \mathcal{X}_j is a sample space of X_j . For any node $j \in V$, $P(X_j | X_S)$ denotes the conditional distribution of a variable X_j given a random vector X_S . Then, a DAG model has the following factorization Lauritzen (1996):

$$P(G) = P(X_1, X_2, \dots, X_p) = \prod_{j=1}^p P(X_j | X_{\text{Pa}(j)}), \quad (1)$$

where $P(X_j | X_{\text{Pa}(j)})$ is the conditional distribution of variable X_j given its parents $X_{\text{Pa}(j)} := \{X_k : k \in \text{Pa}(j) \subset V\}$.

A important concept in this paper is *identifiability* for a family of probability distributions defined by the factorization provided above. Intuitively identifiability addresses the question of what condition on the conditional distributions $P(X_j | X_{\text{Pa}(j)})$ enables us to uniquely determine the structure of that DAG G given the joint distribution $P(G)$.

For the precise definition of identifiability, let \mathcal{P} denote the set of conditional distributions $P(X_j | X_{\text{Pa}(j)})$ for all $j \in V$. In addition for a graph G , define the class of joint distributions with respect to graph G and class of distributions \mathcal{P} by

$$\mathcal{F}(G; \mathcal{P}) := \{P(G) = \prod_{j \in V} P(X_j | X_{\text{Pa}(j)}) ; \text{ where } P(X_j | X_{\text{Pa}(j)}) \in \mathcal{P} \forall j \in V\}.$$

Next, let \mathcal{G}_p be the set of p -node DAGs. Now, we define identifiability for the class \mathcal{P} over the space of DAGs \mathcal{G}_p .

Definition 1 (Identifiability in Park and Raskutti 2018) A class of conditional distributions \mathcal{P} is *identifiable* over \mathcal{G}_p if $G \neq G'$ where $G, G' \in \mathcal{G}_p$, there exists no $P(G) \in \mathcal{F}(G; \mathcal{P})$ and $P(G') \in \mathcal{F}(G'; \mathcal{P})$ such that $P(G) = P(G')$.

Throughout the paper, we assume causal sufficiency that all variables have been observed. Causal sufficiency is assumed in most DAG model learning methods including Gaussian SEMs with identical errors in Peters and Bühlmann (2014), Loh and Bühlmann (2014), Ghoshal and Honorio (2017), Park and Park (2019). In addition, although learning a DAG model is deeply involved with causal inference, we present the main statement without using causal terminology.

2.2 Gaussian structural equation models

The Gaussian structural equation model (SEM) we consider is a special case of Gaussian DAG models where the joint distribution is defined by the following linear structural equations:

$$X_j = \beta_{j0} + \sum_{k \in \text{Pa}(j)} \beta_{jk} X_k + \epsilon_j, \quad \forall j \in V \quad (2)$$

where $(\epsilon_j)_{j \in V}$ are independent, but not identical Gaussian distributions, $N(0, \sigma_j^2)$.

It can be restated in the following matrix form:

$$(X_1, X_2, \dots, X_p)^T = B_0 + B(X_1, \dots, X_p)^T + (\epsilon_1, \dots, \epsilon_p)^T \quad (3)$$

where $B_0 \in \mathbb{R}^p$ is an intercept vector, and $B \in \mathbb{R}^{p \times p}$ is an edge weight matrix or an auto regression matrix with each element $[B]_{jk} = \beta_{jk}$, in which β_{jk} is the weight of an edge from X_k to X_j . Furthermore, $\epsilon = (\epsilon_1, \epsilon_2, \dots, \epsilon_p)^T \sim N(\mathbf{0}_p, \Sigma_\epsilon)$ where $\mathbf{0}_p = (0, 0, \dots, 0)^T \in \mathbb{R}^p$, and Σ_ϵ is a diagonal matrix with unknown variances $\sigma_1^2, \sigma_2^2, \dots, \sigma_p^2$.

The edge weight matrix B encodes the structure under the *non-zero edge weights condition* where β_{jk} is non-zero if $k \in \text{Pa}(j)$; otherwise, $\beta_{jk} = 0$, as in other linear structural equation models (see details in Spirtes 1995; Peters and Bühlmann 2014). It is a natural condition that is in accordance with the intuitive understanding of causal relationships among variables. In our linear structural equation settings, Theorem 1 to 3 in Pearl (2014) and Lemma 4 in Peters and Bühlmann (2014) prove that the condition of the non-zero edge weights (β_{jk}) implies the widely held Markov and *causal minimality* conditions in many causal DAG models learning approaches (see e.g. Pearl 2014; Spirtes et al. 2000; Peters et al. 2012). Causal minimality means that a joint distribution is not Markov with respect to a strict sub-graph of the true graph. In our settings, it means the following for any node $j \in V$ and one of its parents $k \in \text{Pa}(j)$:

$$X_j \not\perp\!\!\!\perp X_k \mid X_S, \quad \forall \text{Pa}(j) \setminus \{k\} \subset S \subset \text{Nd}(j) \setminus \{k\}.$$

Hence, causal minimality is a weak form of faithfulness (Spirtes et al. 2000). As we discussed, faithfulness is commonly assumed for learning the Markov equivalence graph, such as in the PC (Spirtes et al. 2000), the GES (Chickering 2003), and the max-min hill-climbing (Tsamardinos et al. 2006) algorithms. However, in practice, it cannot be tested, and might be very restrictive in finite sample settings (Uhler et al. 2013).

Without loss of generality, we assume that $\mathbb{E}(X_j) = 0$ for all $j \in V$. Then, the distribution of the Gaussian SEM in Equation (3) is as follows:

$$X \sim N(0, \Sigma_X) = N(0, (I_p - B)^{-1} \Sigma_\epsilon (I_p - B)^{-T}),$$

where $I_p \in \mathbb{R}^{p \times p}$ is the identity matrix, and Σ_ϵ is a covariance matrix for errors ϵ . Then, its density can be parameterized by the inverse covariance or concentration matrix $\Theta = (I_p - B)^T \Sigma_\epsilon^{-1} (I_p - B) \succ 0$, and can be restated as

$$f_G(x_1, x_2, \dots, x_p; \Theta) = \frac{1}{\sqrt{(2\pi)^p \det(\Theta^{-1})}} \exp\left(-\frac{1}{2}(x_1, \dots, x_p)\Theta(x_1, \dots, x_p)^T\right). \quad (4)$$

As discussed, Peters and Bühlmann (2014) shows that Gaussian SEMs are identifiable under the non-zero edge weights and the same error variances assumptions. In other words, if the data are generated by a Gaussian SEM with different unknown error variances, it is not guaranteed to find the correct graph. The assumption of the same error variances might be reasonable for applications with variables from a similar domain like biology data and is commonly used in time series models. However, the exact same error variances assumption could be unrealistic for many real-world data. Therefore, the main focus of this paper is to propose a strictly milder identifiability condition, which allows heterogeneous error variances, by utilizing not only the scale of error variances but that of edge weights (β_{jk}). We discuss the details of the new identifiability assumption in the next section.

2.3 Identifiability

In this section, we prove that how Gaussian DAG models with both homogeneous or heterogeneous error variances are identifiable. To provide intuition, we explain how Gaussian SEMs are identifiable from only the distribution using bivariate Gaussian SEMs illustrated in Fig. 1: $G_1 : X_1 \sim N(0, \sigma_1^2)$ and $X_2 | X_1 \sim N(\beta_1 X_1, \sigma_2^2)$, $G_2 : X_2 \sim N(0, \sigma_2^2)$ and $X_1 | X_2 \sim N(\beta_2 X_2, \sigma_1^2)$, and $G_3 : X_1 \sim N(0, \sigma_1^2)$ and $X_2 \sim N(0, \sigma_2^2)$, where X_1 and X_2 are independent.

Now, we show how to determine if the underlying graph is either G_1 , G_2 , or G_3 . For G_1 ,

$$\text{Var}(X_2) = \mathbb{E}(\text{Var}(X_2 | X_1)) + \text{Var}(\mathbb{E}(X_2 | X_1)) = \sigma_2^2 + \beta_1^2 \sigma_1^2 > \sigma_1^2 = \text{Var}(X_1),$$

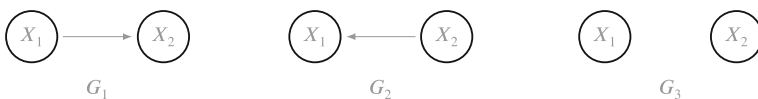


Fig. 1 Bivariate directed acyclic graphs of G_1 , G_2 , and G_3

if $\sigma_2^2/\sigma_1^2 > (1 - \beta_1^2)$. This condition holds under the same error variances and non-zero parameter β_1 , which is the identifiability condition in Peters and Bühlmann (2014). Therefore, we can determine the true ordering (1, 2). In the same manner, G_2 satisfies $\text{Var}(X_1) > \text{Var}(X_2)$ as long as $\sigma_1^2/\sigma_2^2 > (1 - \beta_2^2)$, and hence we can choose the true ordering (2, 1). Lastly for G_3 , there is no guarantee as to which marginal variance is bigger. However, either choice of ordering is fine since both (1, 2) and (2, 1) are correct orderings of G_3 . Therefore, we can recover the orderings of G_1 , G_2 , and G_3 by testing which marginal variance is bigger.

Finding the skeleton procedure can be performed using the dependence relationships between variables. For G_1 and G_2 , X_1 and X_2 are dependent under the minimality condition that is implied by the non-zero edge weights assumption. Combined with the ordering, we can distinguish G_1 and G_2 . For G_3 , X_1 and X_2 are independent under the Markov condition, and therefore, we can recover the graph.

The only required condition we exploited for identifiability of the bivariate graphs is the variance ratio condition, $\sigma_{\pi_2}^2/\sigma_{\pi_1}^2 > 1 - \beta_{\pi_1}^2$, instead of the equal variance assumption. As we explained, if $\sigma_{\pi_1}^2 = \sigma_{\pi_2}^2$, then the above variance ratio condition is always satisfied as long as $\beta_{\pi_1} \neq 0$. We also note that our condition is satisfied with any values of error variances as long as the edge weight is $\beta_{\pi_1}^2 > 1$. Hence, for the bivariate case, we can see that our condition is strictly milder. We also explain how a 3-node DAG model can be recovered in Appendix.

Now, we generalize this idea to p -variate Gaussian SEMs with unknown error variances. The key idea to extending model identifiability from the bivariate to the multivariate involves the comparisons of the (conditional) node variances.

Theorem 2 (Identifiability) *Let $P(X)$ be generated from a Gaussian SEM (4) with directed acyclic graph G . Suppose that π is a true ordering of graph G , and let $X_{1,2,\dots,j} = \{X_{\pi_1}, X_{\pi_2}, \dots, X_{\pi_j}\}$. In addition, for any node $m \in V$, let $j = \pi_m$ and $k \in V \setminus \text{Nd}(j)$. If the conditional variance of X_j given its parents is smaller than the conditional variance of X_k given the variables before j in the ordering π ,*

$$\sigma_j^2 < \sigma_k^2 + \mathbb{E}(\text{Var}(\mathbb{E}(X_k \mid X_{\text{Pa}(k)}) \mid X_{1:(j-1)})),$$

then the Gaussian SEM is identifiable.

Theorem 2 claims that Gaussian SEMs are identifiable if the uncertainty level of a node j is smaller than that of its descendant, $\text{De}(j)$, given the non-descendant, $\text{Nd}(j)$. The main idea of the proof is that the level of uncertainty increases as relevant variables are not provided. The detailed proof is provided in Appendix.

Compared to the previous identifiability result of Gaussian SEMs in Peters and Bühlmann (2014), the assumption in Theorem 2 is strictly weaker. That is because, under the same error variances, our identifiability assumption is equivalent to $\mathbb{E}(\text{Var}(\mathbb{E}(X_k \mid X_{\text{Pa}(k)}) \mid X_{1:(j-1)})) > 0$, which is implied by the non-zero edge weights assumption. In addition, we note that it is analogous to the identifiability assumption for DAG models with some exponential family distributions in Park and Raskutti (2018). While Park and Raskutti (2018) applies a mean-variance relationship, it proves that a graph is identifiable if all parents of node j contribute to its variability.

In Sects. 4.1 and 4.2, we provide numerical experiments on Gaussian SEMs with homogeneous and heterogeneous error variances to support Theorem 2.

It is worth noting that many works have attempted to relax the equal or known variance assumption for the model identifiability. Peters and Bühlmann (2014) and Ghoshal and Honorio (2017) only provide simulation results that Gaussian SEMs with heterogeneous error variances can be recovered in low and high dimensional settings, respectively. In addition, Loh and Bühlmann (2014) tries to theoretically explain how a Gaussian SEM with different error variances can be learned using 2 and 3 node DAG models. However, their method still requires almost the same error variances, because what Loh and Bühlmann (2014) considers is how sensitive their method is to the heterogeneous error variances, rather than finding the identifiability condition for Gaussian SEM with different error variances.

Lemma 3 (Lemma 11 of Loh and Bühlmann 2014) *Consider the two-variable Gaussian SEM G_1 in Fig. 1 where $X_1 \sim N(0, \sigma_1^2)$ and $X_2 = \beta_1 X_1 + \epsilon_2$ where $\epsilon_2 \sim N(0, \sigma_2^2)$. Suppose that the error variance ratio is $r = \sigma_2^2 / \sigma_1^2$. Then, the graph is identifiable if the following conditions hold:*

$$\beta_1^2 \geq \begin{cases} r^2((r^2 - 1) + \sqrt{r^4 - 1}), & \text{if } r \geq 1, \\ (1 - r^2) + \sqrt{1 - r^4}, & \text{if } r \leq 1. \end{cases}$$

In contrast, Theorem 2 implies the following corollary.

Corollary 4 *Consider the two-variable Gaussian SEM G_1 in Fig. 1 where $X_1 \sim N(0, \sigma_1^2)$ and $X_2 = \beta_1 X_1 + \epsilon_2$ where $\epsilon_2 \sim N(0, \sigma_2^2)$. Suppose that the error variance ratio is $r = \sigma_2^2 / \sigma_1^2$. Then, the graph is identifiable if $\beta_1^2 \geq 1 - r^2$.*

Corollary 4 shows that when $r > 1$, the graph is always identifiable with any value of β_1 while Lemma 3 claims that the graph is identifiable when $\beta_1^2 > r^2((r^2 - 1) + \sqrt{r^4 - 1})$. In addition when $r < 1$, we need $\beta_1^2 \geq 1 - r^2$ while Loh and Bühlmann (2014) requires a $\beta_1^2 \geq (1 - r^2) + \sqrt{1 - r^4}$ that is strictly bigger than $1 - r^2$. Hence, the identifiability condition in Corollary 4 is strictly milder than the condition in Lemma 3.

3 Algorithm

To verify our theoretical result, we present the algorithm for learning a Gaussian SEM (4). As shown in brief pseudo-code below, Algorithm 1 consists of two steps: (1) ordering estimation using the conditional variances; and (2) parent estimation using the (conditional) independence relations between variables. Our algorithm runs with any conditional variance estimation method and independence test.

Now, we present our choice of method for each step. Regarding the ordering estimation in Step (1), Algorithm 1 requires computation of conditional variances. Hence, we use a consistent estimator for the error variances using linear regression or inverse covariance matrix. More precisely, for $\text{Var}(X_j \mid X_S)$, we first regress X_j over X_S , and then, estimate $\text{Var}(X_j \mid X_S)$ using the residuals, that is $\widehat{\text{Var}}(X_j \mid X_S) = X_j^T (I - X_S(X_S^T X_S)^{-1} X_S^T) X_j / (n - |S|)$. Under the assumption in

Theorem 2, the conditional variance of the correct element of the ordering π_j given π_1, \dots, π_{j-1} is strictly smaller than that of the other nodes in population. Hence, we can choose the correct element of the ordering with the smallest conditional variance. For the next element of the ordering π_{j+1} , we compute all conditional variances given π_1, \dots, π_j . Therefore, the ordering is determined one node at a time by selecting the node with the minimum conditional variance and updating the condition set. Similar strategies of element-wise ordering learning can be found in many existing algorithms (e.g., Shimizu et al. 2011; Park and Raskutti 2015; Park and Park 2019). We point out that since we move from population to finitely many sample settings, our algorithm possibly chooses an incorrect element of the ordering if sample size is not enough to estimate the conditional variances precisely.

Estimating the set of parents of a node j in Step (2) boils down to selecting the parents among all elements before a node j in the ordering. Hence, given the estimated ordering from Step (1), Step (2) is reduced to a neighborhood selection problems using conditional dependence relations like the PC algorithm. However, unlike the PC algorithm which requires the faithfulness assumption, in our case, causal minimality is sufficient due to the ordering estimation in Step (1). As discussed, we do not assume causal minimality, but it is naturally mounted in our settings. We empirically verify that our algorithm does not need the faithfulness assumption in Sect 4.3.

As discussed, any appropriate conditional independence test can be applied such as Fisher's exact independence test, Fisher's z-transform of the partial correlation test, and mutual information. Since each step of Algorithm 1 consistently recovers the ordering and edges, we can conclude that our algorithm consistently recover the graph.

Compared to the greedy DAG search algorithm in Peters and Bühlmann (2014), another novelty of our algorithm is a polynomial-time complexity. More precisely, Peters and Bühlmann (2014) exploits the ℓ_0 -penalized regression, and hence, computational cost grows super-exponentially as the number of nodes increases. In contrast, our method applies linear regression without any penalty terms, and conditional independence tests. Therefore, by decoupling the ordering estimation or parents search, we gain significant computational improvements. Similar ideas on reducing computational complexity by separating estimation of the ordering with the parents were applied in some existing algorithms (e.g., Bühlmann et al. 2014; Park and Raskutti 2018). We present the average run-time of both algorithms in Sect. 4.4.

4 Numerical experiments

We provide simulation results to support our main theoretical results in Theorem 2 with various settings: (1) the same error variances, (2) different error variances, and (3) non-faithful distributions. We compared Algorithm 1 to state-of-the-art DAG learning PC, GES, and GDS algorithms in terms of the Hamming distance between the true and estimated graphs as in Peters and Bühlmann (2014). The Hamming distance is the total number of errors that is the number of missing edges plus the number of extra edges in the estimated graph. As we discussed, the PC and GES algorithms can learn only up to the MEC under the faithfulness assumption. Hence, we also report the Hamming distance between the true and estimated MECs.

Algorithm 1: Conditional Variance Scoring Algorithm**Input** : n i.i.d. samples from a Gaussian Linear SEM, $X^{1:n}$ **Output**: Estimated causal graph, $\hat{G} = (V, \hat{E})$

Step (1): Ordering Estimation (Forward Selection);

Set $\hat{\pi}_0 = \emptyset$;**for** $m = \{1, 2, \dots, p\}$ **do**Set $S = \{\hat{\pi}_0, \dots, \hat{\pi}_{m-1}\}$;**for** $j \in \{1, 2, \dots, p\} \setminus S$ **do**Estimate conditional variance $\hat{\sigma}_{j|S}^2$;**end**The m -th element of the ordering $\hat{\pi}_m = \arg \min_j \hat{\sigma}_{j|S}^2$ **end**

Step (2): Parents Estimation;

for $m = \{2, \dots, p\}$ **do****for** $j = \{1, \dots, m-1\}$ **do**Perform an independence test between $\hat{\pi}_m$ and $\hat{\pi}_j$;If dependent, include j into $\hat{\text{Pa}}(\hat{\pi}_m)$;**end****end**Estimate the edge set $\hat{E} := \cup_{m \in V} \cup_{k \in \hat{\text{Pa}}(\hat{\pi}_m)} (k, m)$;

Step (2) of Algorithm 1 and the PC algorithm were implemented using a consistent Fisher's exact independence test. In addition, we always set the significance level of statistical tests to $\alpha = 1\%$ by ignoring multiple testing issues as in most constrained based graph learning methods (e.g., Kalisch and Bühlmann 2007; Tsamardinos et al. 2006). The GES algorithm exploits the BIC-regularized maximum likelihood of Gaussian SEMs. Lastly, for GDS, we set the initial graph to the empty graph. Since the GDS algorithm uses a greedy search, and its accuracy relies on the initial graph, we acknowledge that GDS can be better with prior information of an initial graph. Lastly, all algorithms were run on Xeon E5-2650 v4, 2.2 GHz, and 128 GB RAM with Windows, and R program were used.

4.1 Random Gaussian SEMs with homogeneous error variances

We conducted simulations using 100 realizations of p -node Gaussian SEMs (4) with a randomly generated underlying DAG structure. The set of parameters $\beta_{jk} \in \mathbb{R}$ in Eq. (4) was generated uniformly at random in the range $\beta_{jk} \in [-2, 2]$, and was then set to 0 if $\beta_{jk} \in (-0.25, 0.25)$. Hence, the graphs we considered may not be sparse. Lastly, all noise variances were set to 1.

In Fig. 2, we compare our algorithm to state-of-the-art PC, GES, and GDS algorithms by varying sample size $n \in \{100, 200, \dots, 1000\}$ and node size $p \in \{20, 50\}$. As expected, Fig. 2 shows that our algorithm and GDS consistently recover the true graph, and hence, we empirically verify that Gaussian SEMs with identical errors are identifiable. In addition, our method outperforms the GDS algorithm, on average, even with the same error variances, because our method is a complete search-based and exploits the weaker identifiability assumption in Theorem 2. Lastly, the PC and

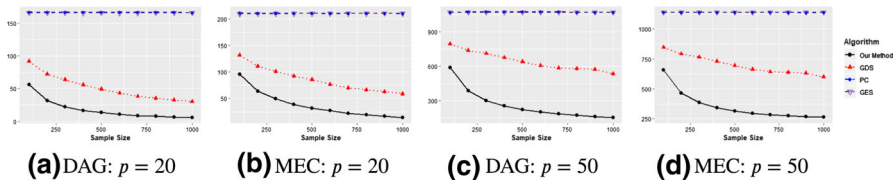


Fig. 2 Average Hamming distances between the estimated and true graphs, and the estimated and true MECs, when error variances are the same

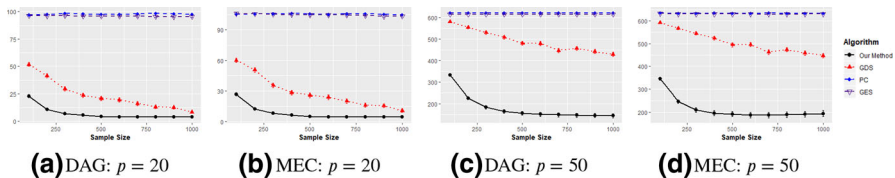


Fig. 3 Average Hamming distances between the estimated and true graphs, and the estimated and true MECs, when error variances are different

GES algorithms seem to fail to recover both directed graphs and the MECs. It is worth noting that the PC and GES algorithms are not consistent, and often fail to recover the MEC if a true graph is not sparse due to the very strong faithfulness assumption in finite samples Uhler et al. (2013).

4.2 Random Gaussian SEMs with heterogeneous error variances

We generated 100 sets of samples with the same procedure specified in Sect. 4.1, except that randomly chosen error variances, $\sigma_j^2 \in [1, 3]$, and the range of parameters, $\beta_{jk} \in [-2, 2]$ and was set to 0 if $\beta_{jk} \in (-1, 1)$. We note that this range of parameters, β_{jk} , forces the graphs to be sparser and ensures that our identifiability assumption in Theorem 2 is satisfied with any values of error variances.

In Fig. 3, we evaluated Algorithm 1 and the comparison methods by varying sample size $n \in \{100, 200, \dots, 1000\}$ and node size $p \in \{20, 50\}$. Fig. 3 shows that our algorithm consistently recovers the true graph, and therefore, confirms our theoretical findings that Gaussian SEMs are identifiable, even with different error variances. Fig. 3 also shows that the GDS algorithm recovers graphs more accurately as a sample size increases. This robustness to non-identical errors is not a surprising result, according to Section 5.3 in Peters and Bühlmann (2014), although they do not provide legitimate reasons. Lastly, the PC and GES algorithms still show poor performances when learning MECs in our settings.

4.3 Non-faithful Gaussian SEMs with heterogeneous error variances

In Sect. 3, we proved that Gaussian SEMs are identifiable even when the distributions are non-faithful. Hence, in this section, we empirically verify this phenomenon. We generated 100 sets of samples from the following non-faithful directed graphical models:

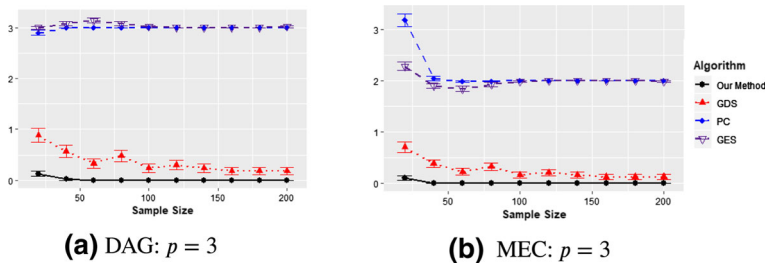


Fig. 4 Average Hamming distances between the estimated and true graphs, and the estimated and true MECs, when the distribution is non-faithful and error variances are different

$$X_1 = \epsilon_1, \quad X_2 = X_1 + \epsilon_2, \quad X_3 = X_1 + X_2 + \epsilon_3,$$

where $\epsilon_j \sim N(0, \sigma_j^2)$ has $\sigma_1^2 = 2.25$ and $\sigma_2^2 = \sigma_3^2 = 1.5$. The violation of the faithfulness assumption can be verified from the inverse covariance matrix Ω where $\Omega_{13} = 0$ since it implies that X_1 and X_2 are conditionally independent given X_3 . We emphasize that it is not a very favorable setting for our algorithm, since $\sigma_1^2 > \sigma_j^2$ for all $j \in \{2, 3\}$.

Figure 4 compares the DAG learning algorithm as a function of sample size $n \in \{20, 40, \dots, 200\}$. As we can see in Fig. 4, it confirms that our algorithm and GDS do not require the faithfulness assumption to recover the underlying graphs of Gaussian SEMs. Fig. 4 also shows that our algorithm performs better than the comparison algorithms on average.

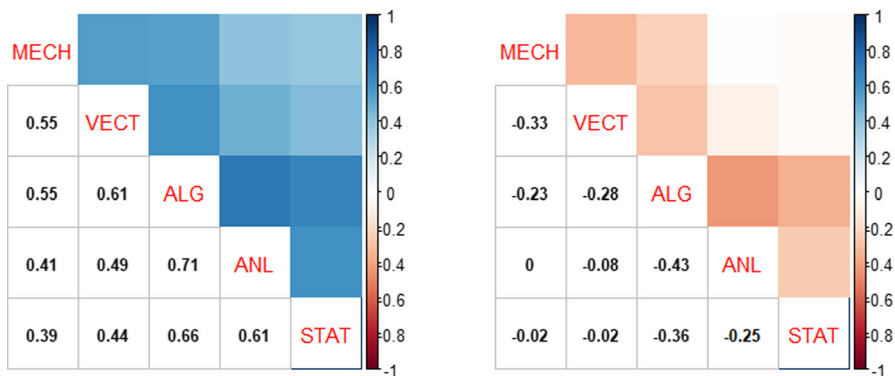
4.4 Computational complexity

One of the important issues in learning DAG models is computational complexity due to the super-exponentially growing size of the space of DAGs in the number of nodes (Harary 1973). Hence, it is in general NP-hard to search DAG space (Chickering et al. 1994; Chickering 1996), and many existing algorithms, such as PC, GES, MMHC, and GDS, are inevitably heuristic, which may not guarantee recovering the true graph. Hence, we now investigate the run-time of our algorithm using the random Gaussian DAG models with identical errors discussed in Sect. 4.1.

Table 1 compares the run-time of Algorithm 1 to GDS for learning Gaussian SEMs by varying sample size $n \in \{100, 200, \dots, 1000\}$ and node size $p \in \{20, 50, 80\}$. Table 1 shows that our algorithm is computationally feasible, even in large-scale graphs learning. In particular, our algorithm is almost 400 times faster than GDS when $p = 20$. As the node size gets bigger, our algorithm is even faster than GDS, and is approximately 800 times faster when $p = 50$. We do not apply GDS when $p = 80$ due to a very long run-time that takes more than a day if implemented. Again, we emphasize that our mild identifiability assumption enables our algorithm to be a large-scale graph learning algorithm.

Table 1 Comparison of our algorithm (denoted OUR) to the GDS algorithm in terms of average run-time (in seconds) with respect to node size p and sample size n

n	$p = 20$		$p = 50$		$p = 80$
	OUR	GDS	OUR	GDS	OUR
100	0.63	233.21	5.07	2617.53	17.01
200	0.68	268.20	5.74	3504.60	20.30
300	0.72	302.58	6.71	4284.35	24.76
400	0.75	325.94	7.24	4832.54	27.07
500	0.83	355.60	8.39	5734.61	32.18
600	0.84	370.94	8.61	6109.63	33.61
700	0.90	396.83	9.97	7047.25	39.48
800	0.94	412.48	10.16	7517.26	40.36
900	1.01	436.60	11.57	8234.65	46.70
1000	1.01	448.28	11.62	8695.12	46.87

**Fig. 5** Correlation and partial correlation plots for examination marks

5 Real multivariate data: mathematics marks

We now apply our algorithm and state-of-the-art PC, GES, and GDS algorithms to a real multivariate Gaussian data involving mathematics marks. More precisely, the variables are examination marks for 88 students on five different subjects: mechanics, vectors, algebra, analysis, and statistics. All are measured on the same scale from 0 to 100. This dataset is provided in bnlearn R package.

As we can see in Fig. 5, left, the correlation plot shows that all 5 variables are positively correlated. This makes sense because students that do well on one subject are more likely to do well on the others. To see the conditional independence relationships, we provide the partial correlation plot in Fig. 5, right. As we can see, some components are very close to 0 between (mechanics, analysis), (mechanics, statistics) and (vectors, statistics). It also makes sense because not all other marks are necessary to explain the mark for a subject. Lastly, we performed multivariate normality test based on kurtosis. From the test result of p value 0.798, there is no evidence to conclude that the data does not come from a multivariate normal distribution.

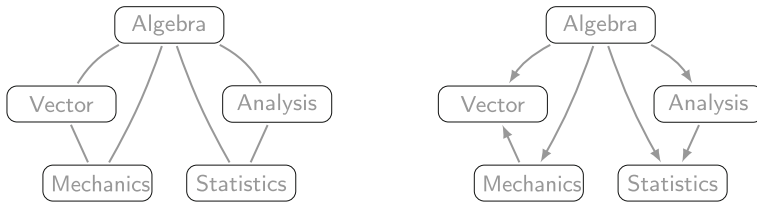


Fig. 6 Examination marks undirected graph (left) and directed acyclic graph estimated by our algorithm (right)

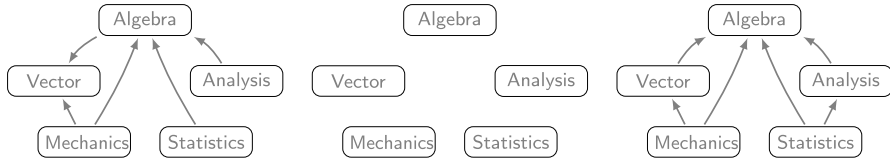


Fig. 7 Examination marks directed acyclic graphs estimated by the PC (left), GES (middle), and GDS (right) algorithms

The mathematics marks data is originally modeled using an Gaussian undirected graphical model in Edwards (2012). The estimated undirected graph is provided in Fig. 6, left. Edwards (2012) claims that the Gaussian undirected graphical model successfully captures the conditional independence relationships shown in Fig. 5, right. The marks for analysis and statistics are conditionally independent of mechanics and vectors, given algebra. Hence, the graph shows that for prediction of the statistics marks, the marks for algebra and analysis are sufficient, and for prediction of the analysis marks, the marks for algebra and statistics are sufficient. In addition for prediction of the marks for algebra, all marks for other subjects are required.

We believe that there exist directional relationships between subjects, because a course is essential for another. For example, algebra is an evidently central subject for all other subjects. In addition, analysis and vectors are prerequisites for statistics and mechanics, respectively. Clearly, the undirected graph cannot uncover these directional relationships. Hence, in order to recover these directional relationships, we applied our algorithm with the significance level $\alpha = 5\%$, and the estimated directed graph is provided in Fig. 6, right. Figure 6 shows that the estimated directed and undirected graphs have the same skeleton, which implies that our algorithm recovers all important links. Moreover, the estimated directed graph shows the most of directional relationships between the subjects.

We acknowledge that our algorithm returns an reversed edge between vector and mechanics due to the lack of samples or restrictive assumption that are not completely satisfied by the real data. However, the advantages of our algorithm can be seen when compared to other DAG learning algorithms. Figure 7 shows the estimated directed graphs via PC, GES, and GDS algorithms. Figure 7, left shows that the PC algorithm misses the important edge between analysis and statistics, and cannot recover the legitimate directions of other edges. Figure 7, middle shows that the GES algorithm cannot recover any directed edges. It is not a surprising result since it is for recovering a MEC instead of a DAG. More precisely, the GES algorithm cannot recover any

directed edges without v-structures, and the true directed graph has no v-structures. Lastly, Fig. 7, right shows that the GDS algorithm successfully recovers the important links while cannot capture their directions. Therefore, we believe that our method more reliably recovers the directional/causal relationships between the marks of 5-courses.

6 Discussion

We proved the identifiability of Gaussian SEMs with both identical and non-identical errors only from joint distribution in a surprisingly simple way. Our approach requires commonly assumed causal sufficiency, the non-zero edge weights assumption, and the new identifiability assumption in Theorem 2. We assume neither causal minimality nor faithfulness that can be very restrictive. Based on our identifiability assumption, we propose a statistically consistent and computationally feasible algorithm. Our algorithm can be implemented with any combination of conditional variance estimation methods and independence tests. In addition, it can be applied to high-dimensional data using ℓ_1 -regularized regression if a graph is sparse. Moreover, our theoretical findings can be combined with an existing MEC learning algorithm for recovering the causal graph, because our method can estimate the ordering independent of directed edges or skeleton.

Although we relax the previous identifiability condition for Gaussian SEMs, we acknowledge that like most other DAG-learning approaches, our assumption might be very strong. However, we believe that all the biological data sets considered in Peters and Bühlmann (2014), Ghoshal and Honorio (2017) can be also applied where they assume the error variances are same. Since our method is the first identifiability result for the Gaussian linear SEM with unknown homogeneous and heterogeneous error variances to the best of our knowledge, our method can more reliably capture the directional/causal relationships between variables.

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A Appendix

A.1 Proof for Theorem 2

Proof Without loss of generality, we assume that the true ordering $\pi = (\pi_1, \dots, \pi_p)$ is unique. For simplicity, we define $X_{1:j} = (X_{\pi_1}, X_{\pi_2}, \dots, X_{\pi_j})$ and $X_{1:0} = \emptyset$. We restate the identifiability assumption of Gaussian SEMs.

Assumption 5 (Identifiability) For any node $m \in V$, let $j = \pi_m$ and $k \in V \setminus \text{Nd}(j)$. The conditional variance of X_j given its parents is smaller than the conditional variance of X_k given the variables before j in ordering π :

$$\sigma_j^2 < \sigma_k^2 + \mathbb{E}(\text{Var}(\mathbb{E}(X_k \mid X_{\text{Pa}(k)}) \mid X_{1:(j-1)})).$$

Now, we prove identifiability of Gaussian SEMs using mathematical induction.

Step (1) By Assumption 5, for any node $k \in V \setminus \{\pi_1\}$, we have

$$\text{Var}(X_{\pi_1}) = \sigma_{\pi_1}^2 < \sigma_k^2 + \text{Var}(\mathbb{E}(X_k \mid X_{\text{Pa}(k)})) = \text{Var}(X_k).$$

Therefore, π_1 can be correctly identified.

Step (m–1) For the $(m - 1)$ th element of the ordering, assume that the first $m - 1$ elements of the ordering and their parents are correctly estimated.

Step (m) Now, we consider the m th element of the causal ordering and its parents. By Assumption 5, for $k \in \{\pi_{m+1}, \dots, \pi_p\}$,

$$\begin{aligned} \mathbb{E}(\text{Var}(X_{\pi_m} \mid X_{1:(m-1)})) &= \sigma_{\pi_m}^2 < \sigma_k^2 + \mathbb{E}(\text{Var}(\mathbb{E}(X_k \mid X_{\text{Pa}(k)}) \mid X_{1:(m-1)})) \\ &= \mathbb{E}(\text{Var}(X_k \mid X_{1:(m-1)})). \end{aligned}$$

Hence, we can choose the true m^{th} element of the ordering π_m .

In terms of the parents search, it is clear that conditional independence relations naturally encoded by the factorization (1) and imply causal minimality (see details in Pearl 2014; Peters and Bühlmann 2014). In our settings, causal minimality states that for any node $j \in V$ and one of its parents $k \in \text{Pa}(j)$,

$$X_j \not\perp\!\!\!\perp X_k \mid X_S, \quad \forall \text{Pa}(j) \setminus \{k\} \subset S \subset \text{Nd}(j) \setminus \{k\}.$$

Therefore, we can choose the correct parents of π_m . By mathematical induction, this completes the proof. \square

A.2 Identifiability for three-node chain graph

Consider a Gaussian SEM, $X_1 \rightarrow X_2 \rightarrow X_3$, where $X_1 = \epsilon_1$, $X_2 = \beta_1 X_1 + \epsilon_2$, and $X_3 = \beta_2 X_2 + \epsilon_3$ with $\epsilon_j \sim N(0, \sigma_j^2)$ for all $j \in \{1, 2, 3\}$. Then the first element of the ordering can be determined by comparing the variances of nodes:

$$\begin{aligned} \text{Var}(X_2) &= \mathbb{E}(\text{Var}(X_2 \mid X_1)) + \text{Var}(\mathbb{E}(X_2 \mid X_1)) = \sigma_2^2 + \beta_1^2 \sigma_1^2 > \sigma_1^2 = \text{Var}(X_1) \\ \text{Var}(X_3) &= \mathbb{E}(\text{Var}(X_3 \mid X_2)) + \text{Var}(\mathbb{E}(X_3 \mid X_2)) \\ &= \sigma_3^2 + \beta_2^2 \sigma_2^2 + \beta_2^2 \beta_1^2 \sigma_1^2 > \sigma_1^2 = \text{Var}(X_1). \end{aligned}$$

as long as $\sigma_2^2/\sigma_1^2 > (1 - \beta_1^2)$ and $\sigma_3^2/\sigma_1^2 > (1 - \beta_2^2)$.

The second element of the ordering can also be recovered by comparing the expectation of the conditional variance of the remaining variables given the estimated first element of the ordering:

$$\begin{aligned} \mathbb{E}(\text{Var}(X_3 \mid X_1)) &= \mathbb{E}(\mathbb{E}(\text{Var}(X_3 \mid X_2) \mid X_1)) + \mathbb{E}(\text{Var}(\mathbb{E}(X_3 \mid X_2) \mid X_1)) \\ &= \sigma_3^2 + \beta_2^2 \sigma_2^2 > \sigma_2^2 = \mathbb{E}(\text{Var}(X_2 \mid X_1)). \end{aligned}$$

as long as $\sigma_3^2/\sigma_2^2 > (1 - \beta_2^2)$.

Under the minimality and the Markov condition, we also have the following (conditional) dependence relations: $X_1 \not\perp\!\!\!\perp X_2$, $X_1 \perp\!\!\!\perp X_3$, $X_2 \not\perp\!\!\!\perp X_3$. Therefore, the true graph can be recovered.

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