EFFICIENT AND TRUSTWORTHY CAUSAL DISCOVERY WITH LATENT VARIABLES AND COMPLEX RELATIONS

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ABSTRACT

Most traditional causal discovery methods assume that all task-relevant variables are observed, an assumption often violated in practice. Although some recent works allow the presence of latent variables, they typically assume the absence of certain special causal relations to ensure a degree of simplicity, which might also be invalid in real-world scenarios. This paper tackles a challenging and important setting where latent and observed variables are interconnected through complex causal relations. Under an assumption ensuring that latent variables leave adequate footprints in observed variables, we develop a series of novel theoretical results, leading to an efficient causal discovery algorithm which is the first one capable of handling the setting with both latent variables and complex relations within polynomial time. Our algorithm first sequentially identifies latent variables from leaves to roots and then sequentially infers causal relations from roots to leaves. Moreover, we prove trustworthiness of our algorithm, meaning that when the assumption is invalid, it can raise an error rather than draw an incorrect causal conclusion, thus preventing potential damage to downstream tasks. We demonstrate the efficacy of our algorithm through experiments. Our work significantly enhances efficiency and reliability of causal discovery in complex systems.

1 INTRODUCTION

Causality is a fundamental notion in natural and social sciences, which plays a crucial role in explanation, prediction, decision making and control (Zhang et al., 2018). Uncovering causality through analysis of observational data, commonly known as causal discovery, has garnered significant attention. Most traditional causal discovery methods (Spirtes & Glymour, 1991; Chickering, 2002; Shimizu et al., 2006) assume that all task-relevant variables are observed. However, we often fail to collect and measure all of them in practice, making latent variables ubiquitous. Although some previous works such as FCI (Spirtes et al., 1995) allows the presence of latent variables, their results are not informative of the number of latent variables and their causal relations. By utilizing linear models, some recent works can represent latent variables and their causal relations explicitly in their results. However, they often assume the absence of certain special causal relations to ensure a degree of simplicity, including the *purity assumption* (Cai et al., 2019; Xie et al., 2020) positing the absence of edges between observed variables, the *measurement assumption* (Silva et al., 2006; Kummerfeld & Ramsey, 2016) positing the absence of edges from observed variables to latent ones, and the *no-triangle assumption* (Huang et al., 2022; Dong et al., 2024) positing the absence of triangles formed by three mutually adjacent variables. Unfortunately, these assumptions are invalid in many real-world scenarios. Consider the causal structure shown as Fig. 1 where L and O respectively denote latent and observed variables. Clearly, $O_2 \to O_3$ violates the purity assumption, $O_1 \to L$ violates the measurement assumption, and the triangle composed of L, O_2, O_3 violates the no-triangle assumption. This structure can be found in business contexts, where O_1, L, O_2, O_3 refer to advertisement spending, consumer interest, product views, and product sales respectively. In this paper, given observational data generated by a linear non-Gaussian acyclic model (LiNGAM) with latent variables, we aim to correctly identify the underlying complete causal structure, which is a directed acyclic graph (DAG) that explicitly represents both observed and latent variables along with their causal relations, in an important and

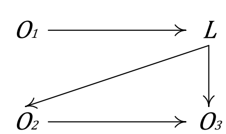


Figure 1: A causal structure violating all of the purity, measurement, and no-triangle assumptions.

challenging setting where latent and observed variables are interconnected through complex causal relations, where "complex" means that none of the above three assumptions is employed.

Adams et al. (2021) first investigate the setting with both latent variables and complex relations. They develop a causal discovery algorithm under the assumption which is exactly sufficient and necessary for identifiability of LiNGAM with latent variables, but it requires the number of latent variables as prior knowledge and lacks robustness, hence is not advisable in practice. Subsequently, Jin et al. (2024) introduce a stronger assumption that latent variables have pure children, ensuring latent variables leave adequate footprints in observed variables. Under this assumption, they propose the first practical algorithm capable of handling this challenging and important setting, which recovers the causal graph in a bottom-up manner, progressing from leaves to roots. Unfortunately, its has exponential time complexity with respect to the number of variables, substantially limiting its applicability. In this paper, under a similar assumption also involving pure children, we propose an efficient algorithm with only cubic time complexity. Our algorithm follows a bottom-up then top-down pattern. In stage 1, it sequentially identifies latent variables through their pure children, progressing from leaves to roots. In stage 2, for variables not recognized as others' pure children in stage 1, it sequentially infers their causal relations, progressing from roots to leaves.

As mentioned above, both Jin et al. (2024) and we both make assumptions involving pure children to enable a practical causal discovery algorithm. In fact, the pure children assumption is also used in many previous works allowing the presence of latent variables but not complex relations (Silva et al., 2006; Kummerfeld & Ramsey, 2016; Cai et al., 2019; Xie et al., 2020; Huang et al., 2022; Dong et al., 2024). However, no existing study can reliably verify the validity of this assumption, leaving no guarantee that their recovered causal graph is correct, which could be potentially harmful in practical applications. For instance, in financial markets, a plausible but incorrect causal conclusion might mislead investors to make poor investment choices and cause significant financial losses. To overcome this limitation, we additionally prove trustworthiness of our algorithm, meaning that it can raise an error rather than return an incorrect causal structure when the pure children assumption is invalid. Specifically, if the assumption is violated, we prove at the end of stage 1, there exists an unidentified latent variable or an identified latent variable whose recognized pure children are not actually its pure children. In stage 2, this hidden risk will be triggered, prompting the error signal.

The major innovations of our work are summarized as follows.

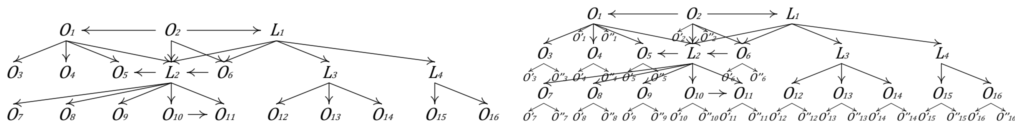
- We investigate an understudied setting in causal discovery where latent and observed variables are interconnected through complex causal relations, which is important and challenging.
- Under a pure children assumption, we develop a series of novel theoretical results, leading to an efficient causal discovery algorithm. This is the first one capable of handling the setting with latent variables and complex relations within polynomial time.
- We prove trustworthiness of our algorithm, meaning that when the pure children assumption is invalid, it can raise an error rather than return an incorrect result, thus preventing potential damage to downstream tasks. To the best of our knowledge, there is a lack of similar results in the literature of causal discovery with latent variables.

In summary, our work significantly enhances efficiency and reliability of causal discovery in complex systems. It may both inspire further research in causal discovery and benefit research in natural and social sciences. Due to space limit, we defer detailed discussion on related works to App. A.

2 PRELIMINARY

We focus on the linear non-Gaussian acyclic model (LiNGAM) with latent variables whose graph structure $\mathcal{G}_0$ is a DAG. Its vertex set is $\mathbf{V}_0 = \mathbf{L} \cup \mathbf{O}_0$ where $\mathbf{L}$ and $\mathbf{O}_0$ respectively denote the set of latent and observed variables. We augment $\mathcal{G}_0$ to $\mathcal{G}$ by creating two children for every $O \in \mathbf{O}_0$, each of which is O plus an independent non-Gaussian noise. We denote the set of such created variables by $\mathbf{O}_1$[1] and let $\mathbf{O} = \mathbf{O}_0 \cup \mathbf{O}_1$, $\mathbf{V} = \mathbf{L} \cup \mathbf{O}$. Trivially, identifying $\mathcal{G}_0$ is equivalent to identifying $\mathcal{G}$.

[1] While the values of observed variables are directly accessible for causal discovery, the causal relations of latent variables can only be inferred indirectly, e.g., through their pure children (Def. 1). By introducing $\mathbf{O}_1$ to create pure children for each observed variable, we can uniformly handle both types of variables through analyzing their pure children, thereby eliminating the need to repeatedly distinguish between treatments of latent and observed variables and keeping our core methodology clear.



(a) $\mathcal{G}_0$: $\mathbf{L} = \{L_1, ..., L_4\}, \mathbf{O}_0 = \{O_1, ..., O_{16}\}$. (b) $\mathcal{G}$: $\mathbf{O}_1 = \{O'_1, ..., O'_{16}, O''_1, ..., O''_{16}\}$.

Figure 2: An illustrative example of augmenting (a) $\mathcal{G}_0$ to (b) $\mathcal{G}$.

An example is shown as Fig. 2. Because of the linearity, each variable $V_i \in \mathbf{V}$ follows

$$V_i = \sum_{V_j \in \mathbf{V}} a_{ij} V_j + \epsilon_{V_i}, \tag{1}$$

where ϵ_{V_i} refers to an exogenous noise. All exogenous noises have non-Gaussian distributions and are independent of each other. $a_{ij} \neq 0$ iff V_j is a parent of V_i. Eq. (1) can also be written as

$$V_i = \sum_{V_j \in \mathbf{V}} m_{ij} \epsilon_{V_j}. \tag{2}$$

where $M = (I - A)^{-1}$ with M and A being matrices composed of m_{ij} and a_{ij} respectively. By convention, we assume the distribution over $\mathbf{V}$ is both Markov and rank-faithful (see Asmp. 3 in App. C) to $\mathcal{G}$. Given $V \in \mathbf{V}$, we denote its parents, children, neighbors, ancestors, and descendants by $\mathrm{Pa}(V), \mathrm{Ch}(V), \mathrm{Ne}(V), \mathrm{An}(V)$, and $\mathrm{De}(V)$. Particularly, a variable's ancestors/descendants do not include itself. We call a variable's ancestors/descendants plus itself its generalized ancestors/descendants, denoted by $\mathrm{GAn}(V)$ and $\mathrm{GDe}(V)$. We abbreviate $\bigcup_{V \in \mathbf{V}'} \mathrm{Pa}(V)$ to $\bigcup \mathrm{Pa}(\mathbf{V}')$.

3 Efficient Causal Discovery

In this section, we develop a series of novel theoretical results under Asmp. 1, leading to an efficient causal discovery algorithm with only cubic time complexity.

Definition 1. *(Pure child) We say V_2 is a pure child of V_1, denoted by $V_2 \in \mathrm{PCh}(V_1)$, if (i) $\mathrm{Pa}(V_2) = \{V_1\}$ and (ii) $\forall V \in \mathrm{De}(V_2), |\mathrm{Pa}(V)| = 1$.*

Example. In Fig. 2(a), $\mathrm{PCh}^{\mathcal{G}_0}(L_2) = \{O_7, O_8, O_9\}$. $O_{11} \notin \mathrm{PCh}^{\mathcal{G}_0}(L_2)$ as $\mathrm{Pa}^{\mathcal{G}_0}(O_{11}) = \{L_2, O_{10}\} \neq \{L_2\}$. $O_{10} \notin \mathrm{PCh}^{\mathcal{G}_0}(L_2)$ as $O_{11} \in \mathrm{De}^{\mathcal{G}_0}(O_{10})$ but $|\mathrm{Pa}^{\mathcal{G}_0}(O_{11})| = 2$.

Remark. This concept has been widely used in related works, but there is no consensus on its exact definition. For instance, a pure child in Silva et al. (2006); Kummerfeld & Ramsey (2016); Xie et al. (2020); Li et al. (2024) must be an observed variable with no child, which is more restrictive than ours. In Jin et al. (2024), a variable's pure child can have a descendant with multiple parents provided that these parents do not include the variable itself, which is less restrictive than ours.

Assumption 1. $\forall L \in \mathbf{L}$, $|\mathrm{PCh}^{\mathcal{G}_0}(L)| \geq 2$ *and* $|\mathrm{Ne}^{\mathcal{G}_0}(L)| \geq 3$.

Example. The graph in Fig. 2(a) satisfies this assumption, where $\mathrm{PCh}^{\mathcal{G}_0}(L_1) = \{L_3, L_4\}$ and $\mathrm{Ne}^{\mathcal{G}_0}(L_1) = \{L_2, L_3, L_4, O_2, O_6\}$.

Remark. This assumption allows each latent variable to leave footprints in observed variables adequate for identification. It naturally holds in the scenarios with many directly measured variables such as topic model (Arora et al., 2013). Similar assumptions involving pure children were also made in many previous works (Silva et al., 2006; Kummerfeld & Ramsey, 2016; Cai et al., 2019; Xie et al., 2020; Zeng et al., 2021; Chen et al., 2022; Xie et al., 2022; Huang et al., 2022; Chen et al., 2023; Dong et al., 2024; Jin et al., 2024; Xie et al., 2024).

3.1 Stage 1: Identifying Latent Variables

§ High-level Overview. In stage 1, we identify latent variables through their pure children. Concretely, we initialize an active set as $\mathbf{O}_0$. First, we locate some variables that are pure children of others from the active set (Thms. 1 and 2). Second, we identify these pure children's parents (Thm. 3). Third, we update the active set by replacing these pure children with their parents. Repeating this process until the active set cannot be updated, all latent variables can be identified finally (Thm. 4). Clearly, we follow a bottom-up pattern in stage 1, progressing from leaves to roots.

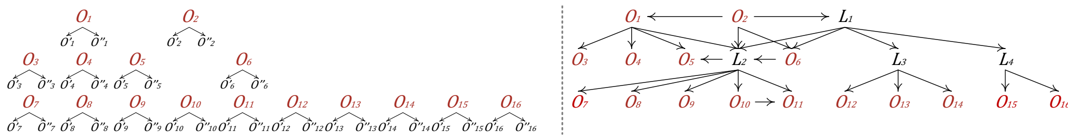


Figure 3: Left: Initial $\mathcal{H}_1$, where $\mathbf{V}_c$ and $\mathbf{V}_p$ are marked in red and black respectively; Right: Initial $\mathcal{H}_2$, which is exactly $\mathcal{G}_0$, where $\mathbf{V}_c$ and $\mathbf{V}_f$ are marked in red and black respectively.

§ Initialization. During stage 1, we maintain two sets of variables $\mathbf{V}_c, \mathbf{V}_p$ and a graph $\mathcal{H}_1$ over $\mathbf{V}_c \cup \mathbf{V}_p$. Initially, we let $\mathbf{V}_c, \mathbf{V}_p$ be $\mathbf{O}_0, \mathbf{O}_1$ respectively and let $V_i \in \mathrm{Pa}^{\mathcal{H}_1}(V_j)$ iff $V_i \in \mathbf{O}_0, V_j \in \mathbf{O}_1$, and $V_i \in \mathrm{Pa}^{\mathcal{G}}(V_j)$. For $\mathcal{G}$ shown as Fig. 2(b), the initial $\mathcal{H}_1$ is displayed on the left of Fig. 3. Subsequently, $\mathbf{V}_c, \mathbf{V}_p$, and $\mathcal{H}_1$ will be updated following the rules described later in § Update. Intuitively, $\mathbf{V}_c$ consists of identified variables whose causal relations (i.e., both incoming and outgoing edges of the variable in the underlying causal graph) are not fully identified, $\mathbf{V}_p$ consists of identified variables whose causal relations are fully identified, and $\mathcal{H}_1$ consists of all identified causal relations. Considering the initial case, such intuitions become particularly apparent. Clearly, Cond. 1 holds initially, and we will show later Cond. 1 always holds throughout stage 1.

Condition 1. *(1)* $\forall V \in \mathbf{V}_p$, $|\mathrm{Pa}^{\mathcal{H}_1}(V)| = 1$ *and* $\mathrm{Ch}^{\mathcal{H}_1}(V) = \mathrm{PCh}^{\mathcal{G}}(V)$*; (2)* $\forall V \in \mathbf{V}_c$, $\mathrm{Pa}^{\mathcal{H}_1}(V) = \emptyset$, $|\mathrm{Ch}^{\mathcal{H}_1}(V)| \geq 2$, *and* $\mathrm{Ch}^{\mathcal{H}_1}(V) \subset \mathrm{PCh}^{\mathcal{G}}(V)$.

For ease of exposition, we denote $\mathbf{V} \backslash (\mathbf{V}_c \cup \mathbf{V}_p)$ by $\mathbf{V}_f$ and the induced subgraph of $\mathcal{G}$ over $\mathbf{V}_c \cup \mathbf{V}_f$ by $\mathcal{H}_2$. For $\mathcal{G}$ shown as Fig. 2(b), the initial $\mathbf{V}_f$ is exactly $\mathbf{L}$ and the initial $\mathcal{H}_2$ is displayed on the right of Fig. 3, which is exactly $\mathcal{G}_0$. Intuitively, while $\mathbf{V}_c \cup \mathbf{V}_p$ consists of all identified variables, $\mathbf{V}_f$ consists of all unidentified variables. While $\mathcal{H}_1$ consists of all identified causal relations, $\mathcal{H}_2$ consists of all unidentified causal relations. Considering the initial case, such intuitions become apparent.

§ Locating Pure Children. Ideally, we want to locate pure children in a single step, but this is impossible because of the existence of complex causal relations. Instead, we first locate identifiable pairs (Def. 2) from $\mathbf{V}_c$ (Thm. 1) and then locate pure children from these identifiable pairs (Thm. 2).

Definition 2. *(Identifiable pair, IP) We say* $\{V_1, V_2\} \subset \mathbf{V}_c$ *is an IP, denoted by* $\{V_1, V_2\} \in \mathbb{S}$, *if*

(1) $\mathrm{Pa}^{\mathcal{H}_2}(V_2) = \{V_1\}$, $\mathrm{Ch}^{\mathcal{H}_2}(V_2) = \emptyset$, *and* $\mathrm{Ne}^{\mathcal{H}_2}(V_1) \backslash \{V_2\} \neq \emptyset$. *We denote this by* $\{V_1, V_2\} \in \mathbb{S}_1$*; or*

(2) $\exists V_0 \in \mathbf{V}_c \cup \mathbf{V}_f \backslash \{V_1, V_2\}$ *s.t.* $\mathrm{Pa}^{\mathcal{H}_2}(V_1) = \mathrm{Pa}^{\mathcal{H}_2}(V_2) = \{V_0\}$, $\mathrm{Ch}^{\mathcal{H}_2}(V_1) = \mathrm{Ch}^{\mathcal{H}_2}(V_2) = \emptyset$, *and* $V_0 \in \mathbf{V}_c$ *or* $\mathrm{Ne}^{\mathcal{H}_2}(V_0) \backslash \{V_1, V_2\} \neq \emptyset$. *We denote this by* $\{V_1, V_2\} \in \mathbb{S}_2$*; or*

(3) $\exists V_0 \in \mathbf{V}_c \cup \mathbf{V}_f \backslash \{V_1, V_2\}$ *s.t.* $\mathrm{Pa}^{\mathcal{H}_2}(V_1) = \{V_0\}$, $\mathrm{Ch}^{\mathcal{H}_2}(V_1) = \{V_2\}$, $\mathrm{Pa}^{\mathcal{H}_2}(V_2) = \{V_0, V_1\}$, *and* $\mathrm{Ch}^{\mathcal{H}_2}(V_2) = \emptyset$. *We denote this by* $\{V_1, V_2\} \in \mathbb{S}_3$.

Example. In the right sub-figure of Fig. 3, $\mathbb{S}_1 = \{\{O_1, O_3\}, \{O_1, O_4\}\}$, $\mathbb{S}_2 = \{\{O_3, O_4\}, \{O_7, O_8\}, \{O_7, O_9\}, \{O_8, O_9\}\{O_{12}, O_{13}\}, \{O_{12}, O_{14}\}, \{O_{13}, O_{14}\}, \{O_{15}, O_{16}\}\}$, $\mathbb{S}_3 = \{\{O_{10}, O_{11}\}\}$.

Intuition. Although $\mathcal{H}_2$ is unknown, we will show later that identifiable pairs can still be located from $\mathbf{V}_c$ via statistical analysis (Thm. 1), this is what "identifiable" means.

The connection between identifiable pairs and pure children are as follows:

(1) If $\{V_1, V_2\} \in \mathbb{S}_1$, V_2 is V_1's pure child or V_1 is V_2's pure child.
(2) If $\{V_1, V_2\} \in \mathbb{S}_2$, V_1 and V_2 are both pure children of V_0.
(3) If $\{V_1, V_2\} \in \mathbb{S}_3$, neither V_1 nor V_2 is a pure child of any other variable.

Definition 3. *(Pseudo-residual (Cai et al., 2019)) Given three variables* V_1, V_2, V_3 *s.t.* $\mathrm{Cov}(V_2, V_3) \neq 0$*, the pseudo-residual of* V_1, V_2 *relative to* V_3 *is defined as*

$$\mathrm{R}(V_1, V_2|V_3) = V_1 - \frac{\mathrm{Cov}(V_1, V_3)}{\mathrm{Cov}(V_2, V_3)} V_2. \tag{3}$$

Intuition. Pseudo-residual is a simple variant of the conventional residual. The former reduces to the latter when $V_2 = V_3$. Before Cai et al. (2019), similar concepts have already been used by earlier works (Drton & Richardson, 2004; Chen et al., 2017).

Theorem 1. $\forall \{V_i, V_j\} \subset \mathbf{V}_c$, $\{V_i, V_j\} \in \mathbb{S}$ *iff there exists* $V_k \in \mathbf{V}_c \backslash \{V_i, V_j\}$ *s.t.* $\mathrm{Cov}(V_i, V_j)\mathrm{Cov}(V_i, V_k)\mathrm{Cov}(V_j, V_k) \neq 0$ *and for each such* V_k, $\mathrm{R}(V_i, V_j|V_k) \perp\!\!\!\perp \mathbf{V}_c \backslash \{V_i, V_j\}$.

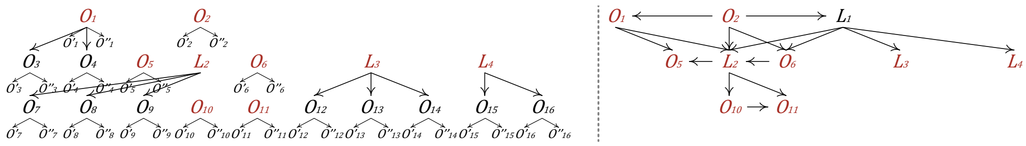


Figure 4: Left: $\mathcal{H}_1$ after the first iteration, where $\mathbf{V}_c$ and $\mathbf{V}_p$ are marked in red and black respectively; Right: $\mathcal{H}_2$ after the first iteration, where $\mathbf{V}_c$ and $\mathbf{V}_f$ are marked in red and black respectively.

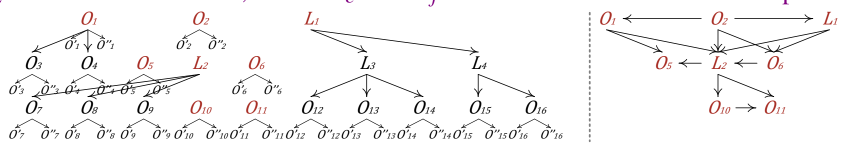


Figure 5: Left: $\mathcal{H}_1$ at the end of stage 1, where $\mathbf{V}_c$ and $\mathbf{V}_p$ are marked in red and black respectively; Right: $\mathcal{H}_2$ at the end of stage 1, where $\mathbf{V}_c$ and $\mathbf{V}_f$ are marked in red and black respectively.

Remark. This theorem provides a method for locating identifiable pairs from $\mathbf{V}_c$ via statistical analysis. In principle, we need to do independence test for each V_k. But in fact, it is sufficient to only consider any single V_k (see Prop. 1 in App. C.2.1), reducing the time complexity.

By the way, this theorem significantly differs from Thm. 2 in Cai et al. (2019) although they both involve pseudo-residuals. Specifically, with the measurement assumption, the purity assumption, and an implicit assumption that each observe variable has only one parent, the latter implies that observed pure children can be located by independence involving pseudo-residuals readily. In contrast, without these assumptions, the former indicates that with both correlations and independence involving pseudo-residuals, we can only locate identifiable pairs.

Definition 4. *(Quintuple constraint) We say* $(V_1, V_2, V_3, V_4, V_5)$ *satisfies the quintuple constraint if there exist* α, β *s.t.* $V_1 + \alpha V_3 + \beta V_4 \perp\!\!\!\perp V_2$ *and* $\mathrm{Cov}(V_1 + \alpha V_3 + \beta V_4, V_5) = 0$.

Theorem 2. $\forall \{V_i, V_j\} \in \mathbb{S}$, *let* $\{V_{i_1}, V_{i_2}\} \subset \mathrm{Ch}^{\mathcal{H}_1}(V_i)$.

(1) $\mathrm{R}(V_{i_1}, V_j | V_{i_2}) \perp\!\!\!\perp V_{i_2}$ *iff* $\{V_i, V_j\} \in \mathbb{S}_1$ *and* $V_i \in \mathrm{Pa}^{\mathcal{G}}(V_j)$.

(2) Suppose $\{V_i, V_j\} \notin \mathbb{S}_1$, $\exists \{V'_i, V'_j\} \in \mathbb{S} \backslash \{\{V_i, V_j\}\}$ *s.t.* $\{V'_i, V'_j\} \cap \{V_i, V_j\} \neq \emptyset$ *only if (but not if)* $\{V_i, V_j\} \in \mathbb{S}_2$.

(3) Suppose $\{V_i, V_j\} \notin \mathbb{S}_1$, $\exists \{V_k, V_l\} \subset \bigcup \mathrm{Ch}^{\mathcal{H}_1}(\mathbf{V}_c \backslash \{V_i, V_j\})$ *s.t.* $(V_{i_1}, V_{i_2}, V_j, V_k, V_l)$ *satisfies the quintuple constraint iff* $\{V_i, V_j\} \in \mathbb{S}_3$ *and* $V_i \in \mathrm{Pa}^{\mathcal{G}}(V_j)$.

Remark. This theorem provides a method to divide $\mathbb{S}$ into $\mathbb{S}_1, \mathbb{S}_2, \mathbb{S}_3$ via statistical analysis, that is, we can locate pure children from identifiable pairs. Given $\{V_i, V_j\} \in \mathbb{S}$, we first check whether $\{V_i, V_j\} \in \mathbb{S}_1$ based on (1). If it is and $V_i \in \mathrm{Pa}^{\mathcal{G}}(V_j)$, then V_j is V_i's pure child. Otherwise, we further check whether $\{V_i, V_j\} \in \mathbb{S}_2$ based on (2,3). If it is, then both V_i and V_j are pure children of another unknown variable; otherwise, they are not.

§ Identifying Pure Children's Parents. As mentioned in Rem. of Thm. 2, for any pair in $\mathbb{S}_2$, its parent is unknown. To avoid duplicate identification of latent variables, we need to check whether its parent is in $\mathbf{V}_c$ or $\mathbf{V}_f$ (Thm. 3(1)) and whether it shares the parent with other pairs in $\mathbb{S}_2$ (Thm. 3(2)).

Theorem 3. *(1)* $\forall \{V_i, V_j\} \in \mathbb{S}_2$, $\bigcap \mathrm{Pa}^{\mathcal{G}}(\{V_i, V_j\}) \subset \mathbf{V}_c$ *iff* $\exists \{V'_i, V'_j\} \in \mathbb{S}_1$ *s.t.* $\{V_i, V_j\} \cap \{V'_i, V'_j\} \neq \emptyset$. *(2)* $\forall \{\{V_i, V_j\}, \{V'_i, V'_j\}\} \subset \mathbb{S}_2$, $\bigcap \mathrm{Pa}^{\mathcal{G}}(\{V_i, V_j\}) = \bigcap \mathrm{Pa}^{\mathcal{G}}(\{V'_i, V'_j\})$ *iff* $\exists \{V''_i, V''_j\} \in \mathbb{S}_2$ *s.t.* $\{V_i, V_j\} \cap \{V''_i, V''_j\} \neq \emptyset$ *and* $\{V'_i, V'_j\} \cap \{V''_i, V''_j\} \neq \emptyset$.

Example. In Fig. 3, an example of (1) is that $\{V_i, V_j\} = \{O_3, O_4\}$ and $\{V'_i, V'_j\} = \{O_1, O_3\}$; an example of (2) is that $\{V_i, V_j\} = \{O_7, O_8\}$ and $\{V'_i, V'_j\} = \{V''_i, V''_j\} = \{O_7, O_9\}$.

§ Update. For pairs in $\mathbb{S}_1$, we move the children from $\mathbf{V}_c$ to $\mathbf{V}_p$ and add edges from parents to children into $\mathcal{H}_1$. For pairs in $\mathbb{S}_2$ whose parents are in $\mathbf{V}_f$ rather than $\mathbf{V}_c$, we merge multiple pairs that share a common parent into a single set, move each set from $\mathbf{V}_c$ to $\mathbf{V}_p$, create and add a new latent variable into $\mathbf{V}_c$ as the set's parent, and add edges from parents to children into $\mathcal{H}_1$. For initialization shown as Fig. 3, the updated result is shown as Fig. 4.

Algorithm 1: Stage 1: Identifying latent variables (overview)

Input: Observed variables $\mathbf{O}_0$ and $\mathbf{O}_1$
Output: $\mathbf{V}_c$, $\mathbf{V}_p$, and $\mathcal{H}_1$

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Initializing V_c, V_p, and H_1 following § Initialization in Sec. 3.1.
while the current V_c is not identical to the previous V_c do
    Locating identifiable pairs S from V_c based on Thm. 1.
    Locating pure children from identifiable pairs based on Thm. 2. // Dividing S into S_1, S_2, S_3.
    Identifying pure children's parents based on Thm. 3. // For each pair in S_2, chech whether
        its parents is in V_c or V_f and whether it shares the parent with other pairs in V_f.
    Updating V_c, V_p, and H_1 following § Update in Sec. 3.1.
end
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§ Repeating This Process. After update, Cond. 1 is still valid (see Prop. 2 in App. C.2.1). By induction, all the above theorems still hold, so we can repeat the above process until $\mathbf{V}_c$ cannot be updated. Here, an additional question emerges: how to test independence/correlation involving latent variables. For any $L \in \mathbf{V}_c \cup \mathbf{V}_p$, let O be its any observed descendant in $\mathcal{H}_1$. With the fact implied by Cond. 1 that O can be expressed as scaled L plus a noise independent of all variables except L's descendants in $\mathcal{H}_1$ (this can also be implied by Cond. 3 in Sec. 4.1), any independence/correlation in our theoretical results involving L holds iff it holds when L is replaced with O. Therefore, we can replace latent variables with their any observed descendant in $\mathcal{H}_1$. Finally, all latent variables can be identified (Thm. 4). For $\mathcal{G}$ shown as Fig. 2(b), the result of stage 1 is shown as Fig. 5. An overview of our algorithm in stage 1 is shown as Alg. 1 while a detailed version is deferred to Alg. 3 in App. E. It has $O(R|\mathbf{O}_0|^3)$ complexity where R is the number of iterations.

Theorem 4. *If $\mathbb{S}_1 \cup \mathbb{S}_2 = \emptyset$, $\mathbf{V}_f = \emptyset$.*

Remark. If both $\mathbb{S}_1$ and $\mathbb{S}_2$ are empty, then $\mathbf{V}_c$ cannot be updated, that is, stage 1 comes to an end. At this moment, $\mathbf{V}_f = \emptyset$, which means that all latent variables are identified.

3.2 Stage 2: Inferring Causal Relations

§ High-level Overview. The aim of stage 2 is to infer causal relations between variables not recognized as others' pure children in stage 1, i.e., to recover $\mathcal{H}_2$ at the end of stage 1, when $\mathbf{V}_f = \emptyset$ based on Thm. 4. We initialize an active set as $\mathbf{V}_c$ at the end of stage 1. First, we identify a root variable in the active set (Thm. 5). Second, we estimate the root variable's effects on others (Thm. 6). Third, we remove the root variable from the active set and also removes its effects on others. Repeating this process until there is no variable in the active set, we can estimate all causal effects and then recover $\mathcal{H}_2$. Finally, we can obtain $\mathcal{G}$ by combining $\mathcal{H}_1$ with $\mathcal{H}_2$. Clearly, we follow a top-down pattern in stage 2, progressing from roots to leaves.

§ Initialization. We denote the active set by $\mathbf{U}_c$ and initialize it as $\mathbf{V}_c$ at the end of stage 1. For the sake of uniform processing, we view observed variables in $\mathbf{U}_c$ as latent variables, and assign each $V_i \in \mathbf{U}_c$ with two observed surrogates X_{2i-1} and X_{2i}, which can be any variable in $\mathrm{GDe}^{\mathcal{H}_1}(V_{i_1}) \cap \mathbf{O}_1$ and $\mathrm{GDe}^{\mathcal{H}_1}(V_{i_2}) \cap \mathbf{O}_1$ where $\{V_{i_1}, V_{i_2}\} \subset \mathrm{Ch}^{\mathcal{H}_1}(V_i)$. Taking $\mathcal{H}_1$ shown on the left of Fig. 5 as an example, L_1's two observed surrogates O'_{12} and O'_{15}. Clearly, Cond. 2 holds initially ($e'_{X_j} = 0$ for any j). we will show later Cond. 2 always holds throughout stage 2. Without loss of generality, we assume in Eq. (4), each c_{i_1} is positive and each ϵ_{V_j} has variance 1.

Condition 2. *(1) $\forall V \in \mathbf{U}_c, \mathrm{De}^{\mathcal{H}_2}(V) \subset \mathbf{U}_c$. (2) $\forall V_i \in \mathbf{U}_c$, X_{2i-1}, X_{2i} can be written as*

$$X_{2i-1} = c_{i_1} \sum_{V_j \in \mathbf{U}_c} m_{ij}\epsilon_{V_j} + e_{X_{2i-1}} + e'_{X_{2i-1}}, \quad X_{2i} = c_{i_2} \sum_{V_j \in \mathbf{U}_c} m_{ij}\epsilon_{V_j} + e_{X_{2i}} + e'_{X_{2i}}, \tag{4}$$

where $\forall j, k, l$, (i) $\epsilon_{V_j} \perp\!\!\!\perp e_{X_k} \perp\!\!\!\perp e'_{X_l}$, (ii) $e_{X_j} \perp\!\!\!\perp e_{X_k}$ if $j \neq k$, and (iii) $e'_{X_{2j-1}} \perp\!\!\!\perp e'_{X_{2k}}$.

§ Identifying a Root Variable. Thm. 5 provides a method via independence tests.

Theorem 5. *$\forall V_i \in \mathbf{U}_c$, $\mathrm{An}^{\mathcal{H}_2}(V_i) \cap \mathbf{U}_c = \emptyset$ iff $\forall V_j \in \mathbf{U}_c \backslash \{V_i\}$, $\mathrm{R}(X_{2j-1}, X_{2i-1}|X_{2i}) \perp\!\!\!\perp X_{2i}$.*

§ Estimating the Root Variable's Effects. This can be accomplished based on Thm. 6.

Algorithm 2: Stage 2: Inferring causal relations (overview)

Input: $\mathbf{V}_c$, $\mathbf{V}_p$, and $\mathcal{H}_1$ output by Alg. 1
Output: a complete causal structure $\mathcal{G}$

```
1  Initialize U_c following § Initialization in Sec. 3.2.
2  while U_c ≠ ∅ do
3      if no variable in U_c satisfies the independence condition in Thm. 5 then
4          raise error // This will not happen if Asmp. 1 is valid.
5      end
6      Identifying a root variable V_i ∈ U_c based on Thm. 5.
7      Estimating V_i's effects on other variables in U_c based on Thm. 6.
8      Removing V_i from U_c and updating X_{2j−1}, X_{2j} for each V_j ∈ U_c following Eq. (6).
9  end
10 G := H_1 ∪ H_2 where H_2 is recovered from the estimated effects.
```

Theorem 6. *If $V_i \in \mathbf{U}_c$ and $\mathrm{An}^{\mathcal{H}_2}(V_i) \cap \mathbf{U}_c = \emptyset$, then $\mathrm{Cov}(X_{2i-1}, X_{2i}) = c_{i_1}c_{i_2}$ and $\forall V_j \in \mathbf{U}_c \backslash \{V_i\}$,*

$$\mathrm{sgn}(m_{ji}) = \mathrm{sgn}(\frac{\mathrm{Cov}(X_{2i-1}, X_{2j})}{\mathrm{Cov}(X_{2j-1}, X_{2j})}), \quad \mathrm{Cov}(X_{2i-1}, X_{2j})\mathrm{Cov}(X_{2i}, X_{2j-1}) = c_{i_1}c_{i_2}c_{j_1}c_{j_2}m_{ji}^2. \tag{5}$$

Remark. Within the current iteration, m_{ji} cannot be determined since $c_{j_1}c_{j_2}$ is still unknown. At some later iteration when V_j becomes the root variable, $c_{j_1}c_{j_2}$ is known and m_{ji} can be determined.

§ Removal. We remove the identified root variable V_i from $\mathbf{U}_c$ and eliminate its effects on X_{2j-1}, X_{2j} following Eq. (6) for each $V_j \in \mathbf{U}_c$.

$$X_{2j-1} := \mathrm{R}(X_{2j-1}, X_{2i-1}|X_{2i}), \quad X_{2j} := X_{2j}. \tag{6}$$

§ Repeating This Process. After removal, Cond. 2 is still valid (see Prop. 3 in App. C.2.2). By the principal of induction, all the above theorems still hold, so we can repeat the above process until there is no variable in $\mathbf{U}_c$. Finally, all causal effects can be estimated, from which $\mathcal{H}_2$ can be recovered following Eqs. (1) and (2). Combining $\mathcal{H}_1$ with $\mathcal{H}_2$, we can obtain $\mathcal{G}$. An overview of our algorithm in stage 2 is shown as Alg. 2 while a detailed version is deferred to Alg. 4 in App. E. It has $O(|\mathbf{V}_c|^3)$ time complexity.

3.3 Summary

Theorem 7. *Suppose the observed variables are generated by a LiNGAM with latent variables satisfying the rank-faithfulness assumption and Asmp. 1, in the limit of infinite data, our algorithm correctly identifies the underlying complete causal structure.*

4 Trustworthy Causal Discovery

In this section, we prove that our algorithm is trustworthy in the sense that it can raise an error rather than return an incorrect result if Asmp. 1 is invalid. This is quite challenging since we need to precisely characterize the behavior of our algorithm when Asmp. 1 is violated, that is, we have to carefully examine, modify, and re-prove all theoretical results in Sec. 3 in the case without Asmp. 1.

Definition 5. *(Paired pseudo-pure children) We say $\{V_2, V_3\}$ is a pair of pseudo-pure children of V_1, denoted by $\{V_2, V_3\} \in \mathrm{P}^3\mathrm{Ch}(V_1)$, if (i) $\bigcap \mathrm{Pa}(\{V_2, V_3\}) = \{V_1\}$, (ii) $\bigcup \mathrm{Pa}(\{V_2, V_3\}) \backslash \{V_1, V_2, V_3\} = \emptyset$, (iii) $V_2 \in \mathrm{Ne}(V_3)$, and (iv) $\forall V \in \bigcup \mathrm{De}(\{V_2, V_3\}) \backslash \{V_2, V_3\}$, $|\mathrm{Pa}(V)| = 1$.*

Example. In Fig. 2(a), $\mathrm{P}^3\mathrm{Ch}(L_2) = \{\{O_{10}, O_{11}\}\}$. In Fig. 6(a), $\{L, V_2\} \notin \mathrm{P}^3\mathrm{Ch}(V_1)$ since $V_4 \in \bigcup \mathrm{De}(\{L, V_2\}) \backslash \{L, V_2\}$ but $|\mathrm{Pa}(V_4)| = 2$.

Intuition. With the edge between V_2 and V_3 removed, they both become pure children of V_1.

Definition 6. *(Pathological variable, PV) Given a latent variable L, we say a L is a type-I PV (I-PV) if $\mathrm{Pa}(L) = \{V_1\}$ and $\mathrm{Ch}(L) = \{V_2, V_3, V_4\}$ where $\mathrm{Pa}(V_2) = \{V_1, L\}$, $|\mathrm{Pa}(V)| = 1$ for each $V \in \mathrm{De}(V_2)$, and $\mathrm{P}^3\mathrm{Ch}(L) = \{\{V_3, V_4\}\}$. We say L is a type-II PV (II-PV) if $\mathrm{Pa}(L) = \emptyset$, $\mathrm{Ch}(L) = \{V_1, V_2, V_3, V_4\}$, and $\mathrm{P}^3\mathrm{Ch}(L) = \{\{V_1, V_2\}, \{V_3, V_4\}\}$. L is a PV if it is either a I-PV or a II-PV.*

Remark. If a I-PV shown as Fig. 6(a) exists in $\mathcal{G}_0$, running our algorithm, there might be $V_1 \in \mathbf{V}_c$ and $\mathrm{Ch}^{\mathcal{H}_1}(V_1) = \{L, V_2\}$ sometime; if a II-PV shown as Fig. 6(b) exists in $\mathcal{G}_0$, running our algorithm, there might be $L \in \mathbf{V}_c$ and $\mathrm{Ch}^{\mathcal{H}_1}(L) = \{V_1, V_2\}$ sometime. In both cases, there exists $V \in \mathbf{V}_c$ s.t. neither $\mathrm{Ch}^{\mathcal{H}_1}(V) \subset \mathrm{PCh}^{\mathcal{G}}(V)$ nor $\{\mathrm{Ch}^{\mathcal{H}_1}(V)\} = \mathrm{P}^3\mathrm{Ch}^{\mathcal{G}}(V)$.

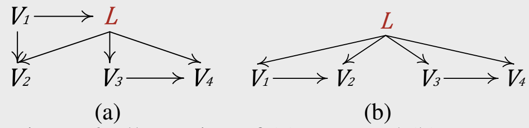

Figure 6: Illustration of (a) I-PV and (b) II-PV.

A pathological variable must satisfy many restrictive conditions, including but not limited to (1) it is a latent variable; (2) it has just the right number of parents and children; (3) its each descendant has the right number of parents.

Assumption 2. *(1) $\forall L \in \mathbf{L}, V \in \mathbf{V}_0 \backslash \{L\}$, $\mathrm{Ch}^{\mathcal{G}_0}(L) \not\subset \mathrm{Ch}^{\mathcal{G}_0}(V) \cup \{V\}$. (2) $\forall V \in \mathbf{V}_0$, $\mathrm{Ch}^{\mathcal{G}_0}(V)$ is the unique minimal bottleneck (see Def. 8 in App. C.3) from $\mathrm{Ch}^{\mathcal{G}_0}(V)$ to $\mathbf{O}_0$. (3) $\forall L \in \mathbf{L}$, L is not a PV.*

Remark. Adams et al. (2021) have proven that (1) and (2) are both necessary for identifiability, implying that it might be unreasonable to expect trustworthiness without them. For instance, suppose $\mathcal{G}_0$ is shown as Fig. 7(a). It violates (1) so it is unidentifiable, that is, its observational distribution (i.e. $p(O_1, O_2, O_3)$) can be explained by another causal graph, such as Fig. 7(b) satisfying Asmp. 1, so Fig. 7(b) will be returned as the result. (3) is a technical assumption not strictly necessary but significantly eases the readability and accessibility of the proof as it ensures that for every $V \in \mathbf{V}_c$, either $\mathrm{Ch}^{\mathcal{H}_1}(V) \subset \mathrm{PCh}^{\mathcal{G}}(V)$ or $\{\mathrm{Ch}^{\mathcal{H}_1}(V)\} = \mathrm{P}^3\mathrm{Ch}^{\mathcal{G}}(V)$. Considering that (3) is rather weak since a PV must satisfy many restrictive conditions, it does not damage the generalizability of our results substantially.

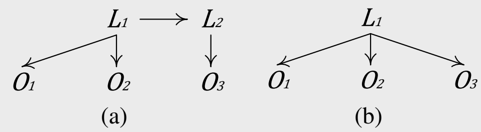

Figure 7: The observational distribution generated by (a) which violates Asmp. 2(1) can also be explained by (b) which satisfies Asmp. 1.

4.1 Stage 1: Identifying Latent Variables

§ High-level Overview. We provide a variant for each theoretical result in Sec. 3.1. At the end of Sec. 3.1, all latent variables are identified and each variable's children in the reconstructed graph are all its actual pure children. But at the end of this section, there is an unidentified latent variable or an identified latent variable whose recognized pure children are not actually its pure children. This potential risk will be triggered in stage 2 such that an error can be raised.

Condition 3. *(1) $\forall V \in \mathbf{V}_p$, $|\mathrm{Pa}^{\mathcal{H}_1}(V)| = 1$ and $\mathrm{Ch}^{\mathcal{H}_1}(V) = \mathrm{PCh}^{\mathcal{G}}(V)$; (2) $\forall V \in \mathbf{V}_c$, $\mathrm{Pa}^{\mathcal{H}_1}(V) = \emptyset$ and $|\mathrm{Ch}^{\mathcal{H}_1}(V)| \geq 2$. If $\mathrm{Ch}^{\mathcal{H}_1}(V) \not\subset \mathrm{PCh}^{\mathcal{G}}(V)$, then $\{\mathrm{Ch}^{\mathcal{H}_1}(V)\} = \mathrm{P}^3\mathrm{Ch}^{\mathcal{G}}(V)$ and V satisfies some other conditions (more details are deferred to App. C.3.1).*

Remark. (1) is identical to Cond. 1(1) and (2) is different from Cond. 1(2).

Theorem 8. *$\forall \{V_i, V_j\} \subset \mathbf{V}_c$, $\{V_i, V_j\} \in \mathbb{S}$ iff there exists $V_k \in \mathbf{V}_c \backslash \{V_i, V_j\}$ s.t. $\mathrm{Cov}(V_i, V_j)\mathrm{Cov}(V_i, V_k)\mathrm{Cov}(V_j, V_k) \neq 0$ and for each such V_k, $\mathrm{R}(V_i, V_j | V_k) \perp\!\!\!\perp \mathbf{V}_c \backslash \{V_i, V_j\}$.*

Remark. It is identical to Thm. 1, so the identifiable pairs will still be located from observed variables correctly and exhaustively.

Theorem 9. *$\forall \{V_i, V_j\} \in \mathbb{S}$, let $\{V_{i_1}, V_{i_2}\} \subset \mathrm{Ch}^{\mathcal{H}_1}(V_i)$.*

(1) $\mathrm{R}(V_{i_1}, V_j | V_{i_2}) \perp\!\!\!\perp V_{i_2}$ iff $\{V_i, V_j\} \in \mathbb{S}_1$ and $V_i \in \mathrm{Pa}^{\mathcal{G}}(V_j)$.

(2) Suppose $\{V_i, V_j\} \notin \mathbb{S}_1$, $\exists \{V_i', V_j'\} \in \mathbb{S} \backslash \{\{V_i, V_j\}\}$ s.t. $\{V_i', V_j'\} \cap \{V_i, V_j\} \neq \emptyset$ only if (but not if) $\{V_i, V_j\} \in \mathbb{S}_2$.

(3) Suppose $\{V_i, V_j\} \notin \mathbb{S}_1$, $\exists \{V_k, V_l\} \subset \bigcup \mathrm{Ch}^{\mathcal{H}_1}(\mathbf{V}_c \backslash \{V_i, V_j\})$ s.t. $(V_{i_1}, V_{i_2}, V_j, V_k, V_l)$ satisfies the quintuple constraint only if (but not if) $\{V_i, V_j\} \in \mathbb{S}_3$ and $V_i \in \mathrm{Pa}^{\mathcal{G}}(V_j)$.

Remark. (1,2) here are identical to (1,2) in Thm. 2 while (3) here is different from (3) in Thm. 2. Denote the result of our algorithm at this step by $\tilde{\mathbb{S}}_1, \tilde{\mathbb{S}}_2, \tilde{\mathbb{S}}_3$, this means that all pairs in $\mathbb{S}_1$ will be incorporated into $\tilde{\mathbb{S}}_1$, all pairs in $\mathbb{S}_2$ will be incorporated into $\tilde{\mathbb{S}}_2$, but some pairs in $\mathbb{S}_3$ will be incorporated into $\tilde{\mathbb{S}}_2$ rather than $\tilde{\mathbb{S}}_3$. Formally, there is $\tilde{\mathbb{S}}_1 = \mathbb{S}_1$, $\tilde{\mathbb{S}}_2 \supset \mathbb{S}_2$, and $\tilde{\mathbb{S}}_3 \subset \mathbb{S}_3$.

Theorem 10. *(1) $\forall \{V_i, V_j\} \in \tilde{\mathbb{S}}_2$, $\bigcap \mathrm{Pa}^{\mathcal{G}}(\{V_i, V_j\}) \subset \mathbf{V}_c$ iff $\exists \{V'_i, V'_j\} \in \tilde{\mathbb{S}}_1$ s.t. $\{V_i, V_j\} \cap \{V'_i, V'_j\} \neq \emptyset$. (2) $\forall \{\{V_i, V_j\}, \{V'_i, V'_j\}\} \subset \tilde{\mathbb{S}}_2$, $\bigcap \mathrm{Pa}^{\mathcal{G}}(\{V_i, V_j\}) = \bigcap \mathrm{Pa}^{\mathcal{G}}(\{V'_i, V'_j\})$ iff $\exists \{V''_i, V''_j\} \in \tilde{\mathbb{S}}_2$ s.t. $\{V_i, V_j\} \cap \{V''_i, V''_j\} \neq \emptyset$ and $\{V'_i, V'_j\} \cap \{V''_i, V''_j\} \neq \emptyset$.*

Remark. Similar to Thm. 3, it also guarantees no duplicate identification of latent variables.

Theorem 11. *If Asmp. 1 is invalid, when $\tilde{\mathbb{S}}_1 \cup \tilde{\mathbb{S}}_2 = \emptyset$, there is $\mathbf{V}_f \neq \emptyset$ or exists $L \in \mathbf{V}_c$ s.t. $\mathrm{Ch}^{\mathcal{H}_1}(L) \not\subset \mathrm{PCh}^{\mathcal{G}}(L)$.*

Remark. It is a variant of Thm. 4, which means that at the end of this section, there is an unidentified latent variable (e.g., Fig. 8(b)) or an identified latent variable whose recognized pure children (i.e., children in $\mathcal{H}_1$) are not actually its pure children (e.g., Fig. 8(d)).

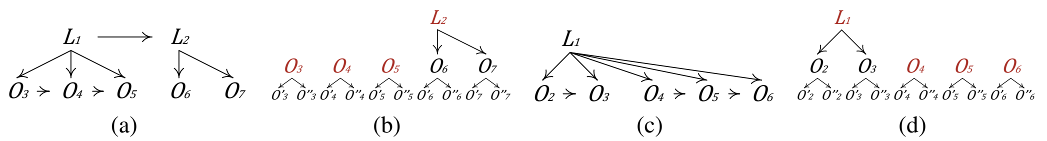

Figure 8: Suppose $\mathcal{G}_0$ is shown as (a), $\mathcal{H}_1$ at the end of stage 1 is shown as (b), where $\mathbf{V}_f = \{L_1\} \neq \emptyset$. Suppose $\mathcal{G}_0$ is shown as (c), $\mathcal{H}_1$ at the end of stage 1 is shown as (d), where $L_1 \in \mathbf{V}_c, \mathrm{Ch}^{\mathcal{H}_1}(L_1) = \{O_2, O_3\} \not\subset \mathrm{PCh}^{\mathcal{G}}(L_1)$.

4.2 Stage 2: Inferring Causal Relations

§ High-level Overview. We provide a variant of Thm. 5 as Thm. 12. In Sec. 3.2, there always exists a variable satisfying Thm. 5 at each iteration. But in this section, there exists no variable satisfying Thm. 12 at some iteration, when an error can be raised.

Condition 4. *(1) $\forall V \in \mathbf{V}_c \backslash \mathbf{U}_c, \mathrm{Ch}^{\mathcal{H}_1}(V_i) \subset \mathrm{PCh}^{\mathcal{G}}(V_i)$. (2) $\forall V \in \mathbf{U}_c \cup \mathbf{V}_f, \mathrm{De}^{\mathcal{H}_2}(V) \subset \mathbf{U}_c \cup \mathbf{V}_f$. (3) $\forall V_i \in \mathbf{U}_c$, X_{2i-1}, X_{2i} can be written as*

$$X_{2i-1} = c_{i_1} \sum_{V_j \in \mathbf{U}_c \cup \mathbf{V}_f} m_{ij} \epsilon_{V_j} + e_{X_{2i-1}} + e'_{X_{2i-1}}, \quad X_{2i} = c_{i_2} \sum_{V_j \in \mathbf{U}_c \cup \mathbf{V}_f} m_{ij} \epsilon_{V_j} + e_{X_{2i}} + e'_{X_{2i}}, \tag{7}$$

where $\forall j, k, l$, (i) $\epsilon_{V_j} \perp\!\!\!\perp e_{X_k} \perp\!\!\!\perp e'_{X_l}$, (ii) $\{e_{X_{2j-1}}, e_{X_{2j}}\} \perp\!\!\!\perp \{e_{X_{2k-1}}, e_{X_{2k}}\}$ if $j \neq k$, (iii) $e_{X_{2j-1}} \perp\!\!\!\perp e_{X_{2j}}$ iff $\mathrm{Ch}^{\mathcal{H}_1}(V_j) \subset \mathrm{PCh}^{\mathcal{G}}(V_j)$, and (iv) $e'_{X_{2j-1}} \perp\!\!\!\perp e'_{X_{2k}}$.

Remark. It is a variant of Cond. 3.

Theorem 12. *$\forall V_i \in \mathbf{U}_c$, $\mathrm{An}^{\mathcal{H}_2}(V_i) \cap (\mathbf{U}_c \cup \mathbf{V}_f) = \emptyset$ and $\mathrm{Ch}^{\mathcal{H}_1}(V_i) \subset \mathrm{PCh}^{\mathcal{G}}(V_i)$ iff $\forall V_j \in \mathbf{U}_c \backslash \{V_i\}$, $\mathrm{R}(X_{2j-1}, X_{2i-1} | X_{2i}) \perp\!\!\!\perp X_{2i}$.*

Remark. It is a variant of Thm. 5, which implies that if at some iteration, there exists no $V_i \in \mathbf{U}_c$ s.t. $\mathrm{An}^{\mathcal{H}_2}(V_i) \cap (\mathbf{U}_c \cup \mathbf{V}_f) = \emptyset$ and $\mathrm{Ch}^{\mathcal{H}_1}(V_i) \subset \mathrm{PCh}^{\mathcal{G}}(V_i)$, we cannot find a $V_i \in \mathbf{U}_c$ satisfying the independence condition, when an error can be raised. Combining Thm. 11 and Cor. 6 in App. C.3.2, we can conclude that this must happen before $\mathbf{U}_c$ becomes an empty set. More details are provided in the proof Thm. 13.

4.3 Summary

Theorem 13. *Suppose the observed variables are generated by a LiNGAM with latent variables satisfying the rank-faithfulness assumption and Asmp. 2, if Asmp. 1 is invalid, in the limit of infinite data, our algorithm raises an error.*

5 Experiment

We first use four causal graphs shown as Fig. 9 to generate synthetic data. For each graph, we draw 10 sample sets of size 2k, 5k, 10k respectively. Each causal strength is sampled from a uniform

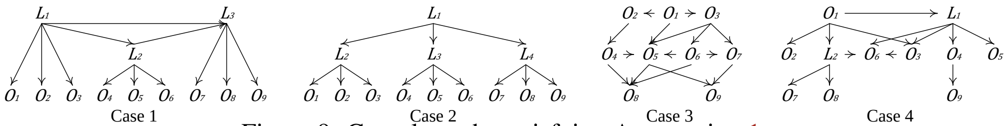

Figure 9: Causal graphs satisfying Assumption 1.

Table 1: Comparison on synthetic data. ↑ means higher is better while ↓ means lower is better.

		Error in Latent Variables ↓			Correct-Ordering Rate ↑			F1-Score ↑			Running Time(s) ↓		
		2k	5k	10k	2k	5k	10k	2k	5k	10k	2k	5k	10k
Case 1	GIN	**0.0±0.0**	**0.0±0.0**	**0.0±0.0**	**1.00±0.00**	**1.00±0.00**	**1.00±0.00**	**1.00±0.00**	**1.00±0.00**	**1.00±0.00**	**1.21±0.18**	**1.39±0.13**	**1.63±0.16**
	LaHME	0.3±0.5	0.1±0.3	0.2±0.4	0.83±0.26	0.94±0.17	0.89±0.23	0.93±0.11	0.98±0.08	0.95±0.10	1.39±0.15	1.61±0.11	1.87±0.14
	Po-LiNGAM	0.2±0.4	0.1±0.3	**0.0±0.0**	0.92±0.16	0.98±0.07	**1.00±0.00**	0.70±0.19	0.93±0.17	0.99±0.04	61.69±21.19	65.24±20.98	67.68±13.64
	Ours	**0.0±0.0**	0.1±0.3	**0.0±0.0**	0.92±0.13	0.91±0.18	**1.00±0.00**	0.98±0.03	0.97±0.07	**1.00±0.00**	1.80±0.19	2.18±0.23	2.49±0.11
Case 2	GIN	1.0±0.0	1.0±0.0	1.0±0.0	0.43±0.00	0.43±0.02	0.43±0.00	0.75±0.00	0.74±0.02	0.75±0.00	**1.29±0.11**	**1.58±0.15**	**1.71±0.18**
	LaHME	**0.0±0.0**	**0.0±0.0**	**0.0±0.0**	**1.00±0.00**	**1.00±0.00**	**1.00±0.00**	**1.00±0.00**	**1.00±0.00**	**1.00±0.00**	1.38±0.13	1.63±0.24	1.81±0.18
	PO-LiNGAM	0.6±0.5	0.4±0.5	0.1±0.3	0.73±0.26	0.77±0.28	0.94±0.17	0.77±0.16	0.90±0.10	0.98±0.06	36.54±11.98	38.89±10.87	37.56±9.16
	Ours	**0.0±0.0**	**0.0±0.0**	**0.0±0.0**	**1.00±0.00**	**1.00±0.00**	**1.00±0.00**	**1.00±0.00**	**1.00±0.00**	**1.00±0.00**	1.56±0.03	1.81±0.05	2.26±0.17
Case 3	GIN	**0.0±0.0**	**0.0±0.0**	**0.0±0.0**	0.00±0.00	0.00±0.00	0.00±0.00	0.00±0.00	0.00±0.00	0.00±0.00	**0.54±0.07**	**0.58±0.06**	**0.68±0.06**
	LaHME	1.0±0.0	0.9±0.3	1.0±0.0	0.00±0.00	0.00±0.00	0.00±0.00	0.00±0.00	0.00±0.00	0.00±0.00	7.83±0.79	8.71±0.52	10.38±0.49
	PO-LiNGAM	**0.0±0.0**	**0.0±0.0**	**0.0±0.0**	0.75±0.22	0.79±0.27	0.91±0.21	0.50±0.15	0.63±0.18	0.89±0.19	56.88±15.50	75.78±12.07	89.10±8.05
	Ours	**0.0±0.0**	**0.0±0.0**	**0.0±0.0**	**0.98±0.04**	**1.00±0.00**	**1.00±0.00**	**0.92±0.10**	**0.98±0.03**	**0.99±0.01**	3.64±0.10	4.20±0.13	5.02±0.14
Case 4	GIN	0.9±0.3	0.9±0.3	0.9±0.3	0.19±0.03	0.20±0.00	0.19±0.03	0.28±0.02	0.29±0.01	0.27±0.05	**0.91±0.10**	**0.94±0.10**	**1.11±0.11**
	LaHME	1.8±0.6	2.0±0.0	2.0±0.0	0.22±0.02	0.20±0.00	0.20±0.00	0.34±0.03	0.32±0.00	0.32±0.01	2.27±0.34	2.61±0.37	3.22±0.79
	PO-LiNGAM	0.9±0.5	0.4±0.5	**0.0±0.0**	0.63±0.31	0.71±0.35	**1.00±0.00**	0.53±0.24	0.73±0.29	**1.00±0.00**	36.76±2.13	44.31±9.78	45.65±4.39
	Ours	**0.3±0.5**	**0.0±0.0**	**0.0±0.0**	**0.91±0.15**	**1.00±0.00**	**1.00±0.00**	**0.87±0.19**	**1.00±0.01**	**1.00±0.00**	4.30±0.25	4.90±0.13	5.94±0.12

distribution over $[-2.0, -0.5] \cup [0.5, 2.0]$ and each noise is generated from the seventh power of uniform distribution. We compare our methods with GIN (Xie et al., 2020), LaHME (Xie et al., 2022), and PO-LiNGAM (Jin et al., 2024). We use 3 metrics to evaluate the performance, including (i) *Error in Latent Variables*, the absolute difference between the estimated number of latent variables and the ground-truth one; (ii) *Correct-Ordering Rate*, the number of correctly estimated causal ordering divided by the number of causal ordering in the ground-truth graph; (iii) *F1-Score* of causal edges. The results are summarized in Tab. 1, where we also report the running time. In particular, we set the size of the largest atomic unit in GIN and PO-LiNGAM to 1 for a fair comparison.

With sufficient samples, all methods can handle case 1 properly. GIN does not perform well in case 2 where some latent variable has no observed pure child. Both GIN and LaHME are not suitable for case 3 and case 4 where the purity or measurement assumption is invalid. While PO-LiNGAM and our algorithm can both handle all cases properly, ours is far more efficient. As mentioned in Introduction, PO-LiNGAM alternates between inferring causal relations and inferring causal relations from leaves to roots, whereas ours first identifying latent variables from leaves to roots and then infers causal relations from roots to leaves. The efficiency gap arises from distinct approaches for inferring causal relations. Take case 3 as an example, PO-LiNGAM first identifies O_9 as a leaf node by finding a subset $\mathbf{P} \subset \mathbf{O}_0 \backslash \{O_9\}$ s.t. a particular linear combination of $\mathbf{P} \cup \{O_9\}$ is independent of $\mathbf{O}_0 \backslash \{O_9\}$, where $\mathbf{P}$ is exactly O_9's parents $\{O_5, O_7\}$. In contrast, our algorithm first identifies O_1 as a root node because for any $O_i \in \mathbf{O}_0 \backslash \{O_1\}$, $\mathrm{R}(X_{2i-1}, X_1|X_2) \perp\!\!\!\perp X_2$. Clearly, PO-LiNGAM needs to traverse the power set of $\mathbf{O}_0 \backslash \{O_9\}$ while the ours only needs to traverse $\mathbf{O}_0 \backslash \{O_1\}$ itself.

In addition, we also do experiments on data generated by the graphs shown in Fig. 10, where Asmp. 1 is invalid. On 10 sample sets sized 10k for each case, while other algorithms all yield incorrect results, ours raises an error 8 times in case 5 and 7 times in case 6.

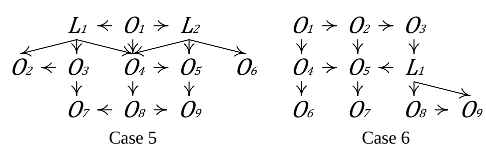

Figure 10: Causal graphs violating Asmp. 1.

We also apply our proposed algorithm to real-world data, more details are deferred to App. D.

6 Conclusion

In this paper, we focus on the setting where latent variables and observed variables are interconnected through complex causal relations. Under a pure children assumption, we propose an efficient algorithm, which is the first one capable of handling the setting with both latent variables and complex relations within polynomial time. Also, we prove trustworthiness of our algorithm. To the best of our knowledge, there is no similar result in the literature of causal discovery with latent variables.

Limitations. First, although Asmp. 1 allows the presence of complex causal relations, it is still somewhat restrictive, we will attempt to relax it without compromising efficiency significantly in our future work. Second, this work does not accommodate non-stationary (Liu & Kuang, 2023) and cyclic (Sethuraman et al., 2023) causal relations, on which we defer the research to our future work.

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A RELATED WORKS

Traditional causal discovery methods mostly assume that all task-relevant variables are observed (Spirtes & Glymour, 1991; Colombo & Maathuis, 2014; Chickering, 2002; Shimizu et al., 2006; 2011; Hoyer et al., 2009; Peters et al., 2014; Mooij et al., 2016). Unfortunately, latent variables are pervasive in practice, in which case these methods usually introduce spurious causal relations. This limitation has inspired extensive works on causal discovery with latent variables. While some of these works cannot uncover the number of latent variables and their causal relations (Spirtes et al., 1995; Claassen et al., 2013; Claassen & Bucur, 2022) or explicitly assume that latent variables are independent of each other (Hoyer et al., 2008; Tashiro et al., 2014; Maeda & Shimizu, 2020; Salehkaleybar et al., 2020; Yang et al., 2022; Cai et al., 2023), others allow the presence of causally-related latent variables and can also infer their causal relations by utilizing linear models (Silva et al., 2006; Anandkumar et al., 2013; Kummerfeld & Ramsey, 2016; Cai et al., 2019; Xie et al., 2020; Zeng et al., 2021; Adams et al., 2021; Chen et al., 2022; Xie et al., 2022; Huang et al., 2022; Chen et al., 2023; Dong et al., 2024; Jin et al., 2024; Li et al., 2024; Xie et al., 2024). Among the latter line of works, the *measurement assumption* is employed by all except Adams et al. (2021); Dong et al. (2024); Jin et al. (2024) and the *purity assumption* is used by all except Silva et al. (2006); Kummerfeld & Ramsey (2016); Adams et al. (2021); Dong et al. (2024); Jin et al. (2024); Li et al. (2024); Xie et al. (2024). In addition, Huang et al. (2022) employ the *non-triangle assumption* that any three variables are not mutually adjacent while Dong et al. (2024) weaken this assumption slightly by allowing three mutually adjacent variables only if they are all observed variables. That is, only Adams et al. (2021) and Jin et al. (2024) can handle setting where latent variables and observed variables are interconnected through complex causal relations, which are of particular relevance to our work.

Adams et al. (2021) are the first one investigating the important and challenging setting with both latent variables and complex relations, they present the sufficient and necessary condition for identifiability of LiNGAMs with latent variables, which is a really profound theoretical contribution. Also, using this condition as the assumption, they develop a causal discovery method, which is unfortunately inadvisable in practice as acknowledged by themselves. First, because it is based on overcomplete independent component analysis (OICA) which needs to know the number of source signals (Podosinnikova et al., 2019; Ding et al., 2019), it requires the number of latent variables as prior knowledge and is computationally intractable. Given the mixing matrix returned by OICA, it still needs to test which submatrices' singular values are exact zeros, which is rather sensitive to noise. Subsequently, Jin et al. (2024) strike a delicate balance between theoretical identifiability and practical feasibility. Specifically, under a stronger assumption involving pure children similar to many previous works (Cai et al., 2019; Xie et al., 2020; 2022; Huang et al., 2022; Dong et al., 2024), they propose the first practical algorithm capable of handling the setting with both latent variables and complex relations. But this algorithm has exponential time complexity with respect to the number of variables, seriously limiting its applicability. To overcome this limitation, under a similar assumption also involving pure children that is moderately more restrictive than Jin et al. (2024)'s[2], we propose an efficient algorithm which is the first one capable of handling the challenging setting within only polynomial time. Our algorithm differs significantly from theirs. Specifically, their algorithm follows a bottom-up pattern, which alternates between inferring causal relations and identifying latent variables, progressing from leaves to roots. Instead, ours follows a bottom-up then top-down pattern, which first sequentially identifies all latent variables, progressing from leaves to roots, and then sequentially infers causal relations, progressing from roots to leaves. Also, we prove trustworthiness of our algorithm, which means that it can raise an error rather than return an incorrect result when the pure children assumption is invalid. To the best of our knowledge, there is a complete lack of similar results in the literature of causal discovery with latent variables.

While the works discussed above all focus on the linear case, there are also some studies investigating nonlinear problems, but most assume access to counterfactual data (Brehmer et al., 2022; Ahuja et al., 2022) or interventional data (Ahuja et al., 2023; Jiang & Aragam, 2023; Buchholz et al., 2023; Zhang et al., 2023). Notably, without structural restrictions such as the pure children assumption,

[2]On the one hand, our definition of pure child is more restrictive than Jin et al. (2024)'s as stated in Rem. of Def. 1, so our assumption is also more restrictive than theirs. On the other hand, the gap between these two assumptions is narrower than that between Adams et al. (2021)'s and Jin et al. (2024)'s because Adams et al. (2021) have absolutely no need for pure children, so we say our assumption is "moderately" more restrictive than Jin et al. (2024)'s.

even linear causal models satisfying the measurement assumption are unidentifiable without comprehensive interventional data obtained by intervening on each latent variable individually (Squires et al., 2023). To the best of our knowledge, in the presence of latent variables, only Kivva et al. (2021) and Kong et al. (2023) can handle non-linear problems through only observational data, but they both make rather strong assumptions. Specifically, Kivva et al. (2021) require that all latent variables are discrete. Kong et al. (2023) require that the mapping from all exogenous noises to observed variables is invertible. We leave further research on nonlinear problems to our future work.

B NOTATIONS

We summarize notations in Tab. 2

Table 2: Summary of notations.

Notation	Description	First appeared
$\mathcal{G}_0$	Original ground-truth causal graph	Sec. 2
$\mathbf{L}$	Latent variables	Sec. 2
$\mathbf{O}_0$	Original observed variables	Sec. 2
$\mathbf{V}_0$	$\mathbf{L} \cup \mathbf{O}_0$	Sec. 2
$\mathcal{G}$	Augmented ground-truth causal graph	Sec. 2
$\mathbf{O}_1$	Created observed variables	Sec. 2
$\mathbf{O}$	$\mathbf{O}_0 \cup \mathbf{O}_1$	Sec. 2
$\mathbf{V}$	$\mathbf{V}_0 \cup \mathbf{O}_1$	Sec. 2
$\mathrm{Pa}(V)$	Parents of V	Sec. 2
$\mathrm{Ch}(V)$	Children of V	Sec. 2
$\mathrm{Ne}(V)$	Neighbors of V	Sec. 2
$\mathrm{An}(V)$	Ancestors of V	Sec. 2
$\mathrm{De}(V)$	Descendants of V	Sec. 2
$\mathrm{GAn}(V)$	Generalized ancestors of V, that is, $\mathrm{An}(V) \cup \{V\}$	Sec. 2
$\mathrm{GDe}(V)$	Generalized descendants of V, that is, $\mathrm{De}(V) \cup \{V\}$	Sec. 2
$\mathrm{PCh}(V)$	Pure children of V	Def. 1 in Sec. 3
$\mathrm{P^3Ch}(V)$	Paired pseudo-pure children of V	Def. 5 in Sec. 4
$\mathrm{PDe}(V)$	Pure descendants of V	Def. 7 in App. C.2.1
$\mathrm{P^2De}(V)$	Pseudo-pure descendants of V	Def. 9 in App. C.3.1
$\mathbf{V}_c$	A set of variables maintained during stage 1 with specific initialization and update rules	Sec. 3.1
$\mathbf{V}_p$	A set of variables maintained during stage 1 with specific initialization and update rules	Sec. 3.1
$\mathbf{V}_f$	$\mathbf{V} \backslash (\mathbf{V}_p \cup \mathbf{V}_c)$	Sec. 3.1
$\mathcal{H}_1$	A graph over $\mathbf{V}_c \cup \mathbf{V}_p$ maintained during stage 1 with specific initialization and update rules	Sec. 3.1
$\mathcal{H}_2$	Induced subgraph of $\mathcal{G}$ over $\mathbf{V}_f \cup \mathbf{V}_c$	Sec. 3.1
$\mathbb{S}$	Identifiable pairs in $\mathbf{V}_c$	Def. 2 in Sec. 3.1
$\mathbb{S}_1, \mathbb{S}_2, \mathbb{S}_3$	Subsets of $\mathbb{S}$	Def. 2 in Sec. 3.1
$\tilde{\mathbb{S}}_1, \tilde{\mathbb{S}}_2, \tilde{\mathbb{S}}_3$	Subsets of $\mathbb{S}$ return by our algorithm when Asmp. 1 is invalid	Rem. of Thm. 9 in Sec. 4.1
$\mathrm{R}(V_1, V_2 \vert V_3)$	Pseudo-residual of V_1, V_2 relative to V_3	Def. 3 in Sec. 3.1
$\mathbf{U}_c$	Active set in stage 2	Sec. 3.2

C PROOF

Assumption 3. *(Rank faithfulness) Given a probability distribution p and a DAG $\mathcal{G}$, p is rank faithful to $\mathcal{G}$ if every rank constraint on a sub-covariance matrix that holds in p is entailed by every linear structural model with respect to $\mathcal{G}$.*

Intuition. This assumption implies that

(1) $m_{ij} \neq 0$ iff $V_j \in \mathrm{GAn}(V_i)$.

(2) Suppose $m_{ik}m_{jk}m_{il}m_{jl} \neq 0$, $m_{ik}/m_{jk} \neq m_{il}/m_{jl}$ iff there exists two non-intersecting paths from $\{V_k, V_l\}$ to $\{V_i, V_j\}$.

For ease of exposition, given $V \in \mathbf{V}$ and $\mathbf{V}' \subset \mathbf{V}$, we abbreviate $\mathrm{Pa}(V) \cap \mathbf{V}'$ as $\mathrm{Pa}_{\mathbf{V}'}(V)$ in the following.

C.1 Important Lemmas

In this section, we summarize several important properties of the pseudo-residual (Lem. 1) and the quintuple constraint (Lem. 2), which serve as the cornerstones of the proofs of many following theoretical results.

Darmois-Skitovitch (D-S) Theorem. (Kagan et al., 1973) Suppose two random variables V_1 and V_2 are both linear combinations of independent random variables $\{n_i\}_i$:

$$V_1 = \sum_i \alpha_i n_i, \quad V_2 = \sum_i \beta_i n_i. \tag{8}$$

Then, if $V_1 \perp\!\!\!\perp V_2$, each n_i for which $\alpha_i\beta_i \neq 0$ follows Gaussian distribution. That is, if there exists a non-Gaussian n_j s.t. $\alpha_j\beta_j \neq 0$, $V_1 \not\perp\!\!\!\perp V_2$.

Lemma 1. *Given V_1, V_2, V_3, V_4, V_5 where $\mathrm{Cov}(V_1, V_2)\mathrm{Cov}(V_1, V_3)\mathrm{Cov}(V_2, V_3) \neq 0$ (it is possible that $V_3 = V_4 = V_5$),*

(1) If $V_1 = \lambda_1 e + e'_1$ and $V_2 = \lambda_2 e + e'_2$ where $\{e'_1, e'_2\} \perp\!\!\!\perp \{e, V_3, V_4\}$, $\mathrm{Cov}(e, V_3) \neq 0$, $\mathrm{Var}(e) \neq 0$, and $\lambda_1\lambda_2 \neq 0$, then $\mathrm{R}(V_1, V_2|V_3) \perp\!\!\!\perp V_4$.

(2) If there exists V_i s.t. only one of m_{1i} and m_{2i} is non-zero and $m_{4i} \neq 0$, then $\mathrm{R}(V_1, V_2|V_3) \not\perp\!\!\!\perp V_4$.

(3) If there exists V_i, V_j s.t. $m_{1i}m_{1j}m_{2i}m_{2j}m_{4i}m_{5j} \neq 0$ and $m_{1i}/m_{1j} \neq m_{2i}/m_{2j}$, then $\mathrm{R}(V_1, V_2|V_3) \not\perp\!\!\!\perp V_4$ or $\mathrm{R}(V_1, V_2|V_3) \not\perp\!\!\!\perp V_5$.

Remark. (1) provides a sufficient condition for independence involving the pseudo-residual to hold while (2, 3) provides two sufficient conditions for independence involving the pseudo-residual to not hold.

Proof. The proofs of are as follows.

(1) $\mathrm{R}(V_1, V_2|V_3) = (\lambda_1 e + e'_1) - \frac{\mathrm{Cov}(\lambda_1 e + e'_1, V_3)}{\mathrm{Cov}(\lambda_2 e + e'_2, V_3)}(\lambda_2 e + e'_2) = (\lambda_1 e + e'_1) - \frac{\lambda_1}{\lambda_2}(\lambda_2 e + e'_2) = e'_1 - \frac{\lambda_1}{\lambda_2} e'_2 \perp\!\!\!\perp V_4$.

(2) As only one of m_{1i} and m_{2i} is non-zero, $\mathrm{R}(V_1, V_2|V_3)$ contains ϵ_{V_i}. Since $m_{4i} \neq 0$, based on D-S Theorem, $\mathrm{R}(V_1, V_2|V_3) \not\perp\!\!\!\perp V_4$.

(3) As $m_{1i}m_{1j}m_{2i}m_{2j} \neq 0$ and $m_{1i}/m_{1j} \neq m_{2i}/m_{2j}$, $\mathrm{R}(V_1, V_2|V_3)$ contains ϵ_{V_i} or ϵ_{V_j}. Since $m_{4i}m_{5j} \neq 0$, based on D-S Theorem, $\mathrm{R}(V_1, V_2|V_3) \not\perp\!\!\!\perp V_4$ or $\mathrm{R}(V_1, V_2|V_3) \not\perp\!\!\!\perp V_5$.

□

Lemma 2. *Given V_1, V_2, V_3, V_4, V_5,*

(1) If there exists V_i s.t. $m_{1i}m_{2i} \neq 0$ and $m_{3i} = m_{4i} = 0$, then $(V_1, V_2, V_3, V_4, V_5)$ does not satisfy the quintuple constraint.

(2) Suppose $e_i, e_j, e'_1, e'_2, e'_3, e'_4$ are mutually independent and V_1, V_2, V_3, V_4 can be written as

$$V_1 = \lambda_1 e_i + \gamma_1 e_j + e'_1, \quad V_2 = \lambda_2 e_i + \gamma_2 e_j + e'_2, \quad V_3 = \lambda_3 e_i + \gamma_3 e_j + e'_3, \quad V_4 = \lambda_4 e_i + e'_4, \tag{9}$$

where $\mathrm{Var}(e_i)\mathrm{Var}(e_j) \neq 0$, $\lambda_1\lambda_2\lambda_3\lambda_4 \neq 0$, and $\gamma_1\gamma_2\gamma_3 \neq 0$. (2.a) If $V_5 \perp\!\!\!\perp \{e_j, e'_1, e'_2, e'_3, e'_4\}$ and $\mathrm{Cov}(V_5, e_i) \neq 0$, then $(V_1, V_2, V_3, V_4, V_5)$ satisfies the quintuple constraint; (2.b) If $V_5 \perp\!\!\!\perp \{e_j, e'_1, e'_2, e'_3\}$, $\mathrm{Cov}(V_5, e_i)\mathrm{Cov}(V_5, e'_4) \neq 0$, and $\lambda_1/\lambda_3 \neq \gamma_1/\gamma_3$, then $(V_1, V_2, V_3, V_4, V_5)$ does not satisfy the quintuple constraint.

Remark. (2.a) provides a sufficient condition for the quintuple constraint to hold while (1, 2.b) provides two sufficient conditions for the quintuple constraint to not hold.

Proof. The proofs are as follows.

(1) As $m_{1i} \neq 0$ and $m_{3i} = m_{4i} = 0$, $V_1 + \alpha V_3 + \beta V_4$ contains ϵ_{V_i}. Since $m_{2i} \neq 0$, based on D-S Theorem, for any α, β, $V_1 + \alpha V_3 + \beta V_4 \not\perp\!\!\!\perp V_2$.

(2) If $V_5 \perp\!\!\!\perp \{e_j, e'_1, e'_2, e'_3, e'_4\}$ and $\mathrm{Cov}(V_5, e_i) \neq 0$, let $\mathrm{Cov}(V_1 + \alpha V_3 + \beta V_4, V_2) = 0$ and $\mathrm{Cov}(V_1 + \alpha V_3 + \beta V_4, V_5) = 0$, we have

$$\lambda_1 + \alpha\lambda_3 + \beta\lambda_4 = 0, \quad \gamma_1 + \alpha\gamma_3 = 0,$$

then

$$V_1 + \alpha V_3 + \beta V_4 = (\lambda_1 + \alpha\lambda_3 + \beta\lambda_4)e_i + (\gamma_1 + \alpha\gamma_3)e_j + e'_1 + \alpha e'_3 + \beta e'_4 = e'_1 + \alpha e'_3 + \beta e'_4 \perp\!\!\!\perp V_5.$$

If $V_5 \perp\!\!\!\perp \{e_j, e'_1, e'_2, e'_3\}$, $\mathrm{Cov}(V_5, e_i)\mathrm{Cov}(V_5, e'_4) \neq 0$, and $\lambda_1/\lambda_3 \neq \gamma_1/\gamma_3$, let $\mathrm{Cov}(V_1 + \alpha V_3 + \beta V_4, V_2) = 0$ and $\mathrm{Cov}(V_1 + \alpha V_3 + \beta V_4, V_5) = 0$, we have

$$\lambda_1 + \alpha\lambda_3 + \beta\lambda_4 \neq 0, \quad \gamma_1 + \alpha\gamma_3 \neq 0,$$

then

$$V_1 + \alpha V_3 + \beta V_4 = (\lambda_1 + \alpha\lambda_3 + \beta\lambda_4)e_i + (\gamma_1 + \alpha\gamma_3)e_j + e'_1 + \alpha e'_3 + \beta e'_4 \tag{10}$$

contains e_i and e_j, so $V_1 + \alpha V_3 + \beta V_4 \not\perp\!\!\!\perp V_2$.

□

C.2 Proof of theoretical results in Sec. 3

Assumption 1. $\forall L \in \mathbf{L}$, $|\mathrm{PCh}^{\mathcal{G}_0}(L)| \geq 2$ and $|\mathrm{Ne}^{\mathcal{G}_0}(L)| \geq 3$.

Trivially, if Asmp. 1 holds, then $\forall L \in \mathbf{L}$, $|\mathrm{PCh}^{\mathcal{G}}(L)| \geq 2$ and $|\mathrm{Ne}^{\mathcal{G}}(L)| \geq 3$.

C.2.1 Proof of theoretical results in Sec. 3.1

Condition 1. (1) $\forall V \in \mathbf{V}_p$, $|\mathrm{Pa}^{\mathcal{H}_1}(V)| = 1$ and $\mathrm{Ch}^{\mathcal{H}_1}(V) = \mathrm{PCh}^{\mathcal{G}}(V)$; (2) $\forall V \in \mathbf{V}_c$, $\mathrm{Pa}^{\mathcal{H}_1}(V) = \emptyset$, $|\mathrm{Ch}^{\mathcal{H}_1}(V)| \geq 2$, and $\mathrm{Ch}^{\mathcal{H}_1}(V) \subset \mathrm{PCh}^{\mathcal{G}}(V)$.

Before proving theoretical results in the main text one by one, we first introduce two corollaries (Cors. 1 and 2) readily derived from Cond. 1.

Corollary 1. *(1) $\forall V \in \mathbf{V}_p, \mathrm{Ch}^{\mathcal{G}}(V) = \mathrm{Ch}^{\mathcal{H}_1}(V)$ and $\mathrm{Pa}^{\mathcal{G}}(V) = \mathrm{Pa}^{\mathcal{H}_1}(V)$; (2) $\forall V \in \mathbf{V}_f, \mathrm{Ch}^{\mathcal{G}}(V) = \mathrm{Ch}^{\mathcal{H}_2}(V)$ and $\mathrm{Pa}^{\mathcal{G}}(V) = \mathrm{Pa}^{\mathcal{H}_2}(V)$.*

Remark. This corollary reveals the properties of variables in $\mathbf{V}_p$ and those in $\mathbf{V}_f$. (1) means that for each variable in $\mathbf{V}_p$, its parents and children in the underlying causal graph $\mathcal{G}$ are exactly its parents and children in $\mathcal{H}_1$. (2) means that for each variable in $\mathbf{V}_f$, its parents and children in the underlying causal graph $\mathcal{G}$ are exactly its parents and children in $\mathcal{H}_2$. This corollary is widely used in the following proofs. To maintain fluency, we will use it without further citation.

Proof. First, if $V_i \in \mathbf{V}_p$, then there exists $V_j \in \mathbf{V}_c \cup \mathbf{V}_p$ s.t. $V_i \in \mathrm{Ch}^{\mathcal{H}_1}(V_j)$ because $\mathrm{Pa}^{\mathcal{H}_1}(V_i) \neq \emptyset$ based on Cond. 1(1). Moreover, since $\mathrm{Ch}^{\mathcal{H}_1}(V_j) = \mathrm{PCh}^{\mathcal{G}}(V_j)$ if $V_j \in \mathbf{V}_p$ and $\mathrm{Ch}^{\mathcal{H}_1}(V_j) \subset \mathrm{PCh}^{\mathcal{G}}(V_j)$ if $V_j \in \mathbf{V}_c$ based on Cond. 1(1,2), there is always $V_i \in \mathrm{PCh}^{\mathcal{G}}(V_j)$. According to the definition of pure children, we can conclude that $\mathrm{Pa}^{\mathcal{G}}(V_i) = \{V_j\} = \mathrm{Pa}^{\mathcal{H}_1}(V_i)$ and $\mathrm{Ch}^{\mathcal{G}}(V_i) = \mathrm{PCh}^{\mathcal{G}}(V_i) = \mathrm{Ch}^{\mathcal{H}_1}(V_i)$, this completes the proof of (1).

Second, if $V_i \in \mathbf{V}_f$, based on (1), then $\mathrm{Ch}^{\mathcal{G}}(V_i) \subset \mathbf{V}_c \cup \mathbf{V}_f$ and $\mathrm{Pa}^{\mathcal{G}}(V_i) \subset \mathbf{V}_c \cup \mathbf{V}_f$, which is equivalent to $\mathrm{Ch}^{\mathcal{G}}(V_i) = \mathrm{Ch}^{\mathcal{H}_2}(V_i)$ and $\mathrm{Pa}^{\mathcal{G}}(V_i) = \mathrm{Pa}^{\mathcal{H}_2}(V_i)$, this completes the proof of (2). □

Definition 7. *(Pure descendant) We say V_2 is a pure descendant of V_1, denoted by $V_2 \in \mathrm{PDe}(V_1)$, if $V_2 \in \bigcup \mathrm{GDe}(\mathrm{PCh}(V_1))$*

Example. In Fig. 2(a), $\mathrm{PDe}(L_1) = \{L_3, L_4, O_{12}, O_{13}, O_{14}, O_{15}, O_{16}\}$.

Corollary 2. $\forall V \in \mathbf{V}_f$, $|\mathrm{PDe}^{\mathcal{G}}_{\mathbf{V}_c}(V)| \geq 2$. *If* $|\mathrm{De}^{\mathcal{G}}_{\mathbf{V}_c}(V)| = 2$, *then* $\mathrm{De}^{\mathcal{G}}_{\mathbf{V}_c}(V) = \mathrm{PCh}^{\mathcal{G}}(V)$.

Remark. This corollary means that each variable in $\mathbf{V}_f$ has at least two pure descendants in $\mathbf{V}_c$, and if it has exactly two descendants in $\mathbf{V}_c$, these two descendants are exactly its all pure children. Intuitively, this enables us to identify variables in $\mathbf{V}_f$ through analyzing variables in $\mathbf{V}_c$.

Proof. As $\mathbf{V}_f \subset \mathbf{L}$, $\forall V \in \mathbf{V}_f$, $|\mathrm{PCh}^{\mathcal{G}}(V)| \geq 2$. Besides, $\mathrm{PCh}^{\mathcal{G}}(V) \subset \mathbf{V}_c \cup \mathbf{V}_f$ because $\mathrm{PCh}^{\mathcal{G}}(V) \subset \mathrm{Ch}^{\mathcal{G}}(V) = \mathrm{Ch}^{\mathcal{H}_2}(V) \subset \mathbf{V}_c \cup \mathbf{V}_f$. If $|\mathrm{PCh}^{\mathcal{G}}_{\mathbf{V}_c}(V)| \geq 2$, we have $|\mathrm{PDe}^{\mathcal{G}}_{\mathbf{V}_c}(V)| \geq 2$ naturally. Otherwise, $\mathrm{PDe}^{\mathcal{G}}_{\mathbf{V}_f}(V) \supset \mathrm{PCh}^{\mathcal{G}}_{\mathbf{V}_f}(V) \neq \emptyset$. Let $V_i \in \mathrm{PDe}^{\mathcal{G}}_{\mathbf{V}_f}(V)$ s.t. $\mathrm{Ch}^{\mathcal{H}_2}(V_i) \subset \mathbf{V}_c$. Since $\mathrm{Ch}^{\mathcal{H}_2}(V_i) = \mathrm{Ch}^{\mathcal{G}}(V_i)$, $|\mathrm{PDe}^{\mathcal{G}}_{\mathbf{V}_c}(V)| \geq |\mathrm{PCh}^{\mathcal{G}}_{\mathbf{V}_c}(V_i)| \geq 2$.

Therefore, we have

$$|\mathrm{De}^{\mathcal{G}}_{\mathbf{V}_c}(V)| \geq 2|\mathrm{PCh}^{\mathcal{G}}_{\mathbf{V}_f}(V)| + |\mathrm{PCh}^{\mathcal{G}}_{\mathbf{V}_c}(V)|. \tag{11}$$

Note that

$$|\mathrm{PCh}^{\mathcal{G}}(V)| = |\mathrm{PCh}^{\mathcal{G}}_{\mathbf{V}_f}(V)| + |\mathrm{PCh}^{\mathcal{G}}_{\mathbf{V}_c}(V)| \geq 2, \tag{12}$$

if $|\mathrm{De}^{\mathcal{G}}_{\mathbf{V}_c}(V)| = 2$, then $\mathrm{PCh}^{\mathcal{G}}_{\mathbf{V}_f}(V) = \emptyset$ and $\mathrm{De}^{\mathcal{G}}_{\mathbf{V}_c}(V) = \mathrm{PCh}^{\mathcal{G}}_{\mathbf{V}_c}(V)$, that is, $\mathrm{De}^{\mathcal{G}}_{\mathbf{V}_c}(V) = \mathrm{PCh}^{\mathcal{G}}(V)$. □

Theorem 1. $\forall \{V_i, V_j\} \subset \mathbf{V}_c$, $\{V_i, V_j\} \in \mathbb{S}$ iff there exists $V_k \in \mathbf{V}_c \backslash \{V_i, V_j\}$ s.t. $\mathrm{Cov}(V_i, V_j)\mathrm{Cov}(V_i, V_k)\mathrm{Cov}(V_j, V_k) \neq 0$ and for each such V_k, $\mathrm{R}(V_i, V_j | V_k) \perp\!\!\!\perp \mathbf{V}_c \backslash \{V_i, V_j\}$.

Proof Sketch. If $\{V_i, V_j\} \in \mathbb{S}$, we can prove correlation and independence based on Lem. 1(1). Otherwise, for each possible case, we can prove either non-correlation or dependence based on Lem. 1(2,3).

Proof. "Only if".

(1) Suppose $\{V_i, V_j\} \in \mathbb{S}_1$. Let $V_i \in \mathrm{Pa}^{\mathcal{H}_2}(V_j)$ without loss of generality and $V_k \in \mathrm{Ne}^{\mathcal{H}_2}(V_i) \backslash \{V_j\}$, we have $\mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k) \backslash \{V_i, V_j\} \neq \emptyset$[3] and let $V_l \in \mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k) \backslash \{V_i, V_j\}$. Clearly, $V_i = V_i + 0, V_j = a_{ji} V_i + \epsilon_{V_j}$ where $\{0, \epsilon_{V_j}\} \perp\!\!\!\perp \{V_i\} \cup (\mathbf{V}_c \backslash \{V_i, V_j\})$ and $\mathrm{Cov}(V_i, V_l) \neq 0$, so $\mathrm{R}(V_i, V_j | V_l) \perp\!\!\!\perp \mathbf{V}_c \backslash \{V_i, V_j\}$ based on Lem. 1(1). Combined with Prop. 1, we reach the conclusion.

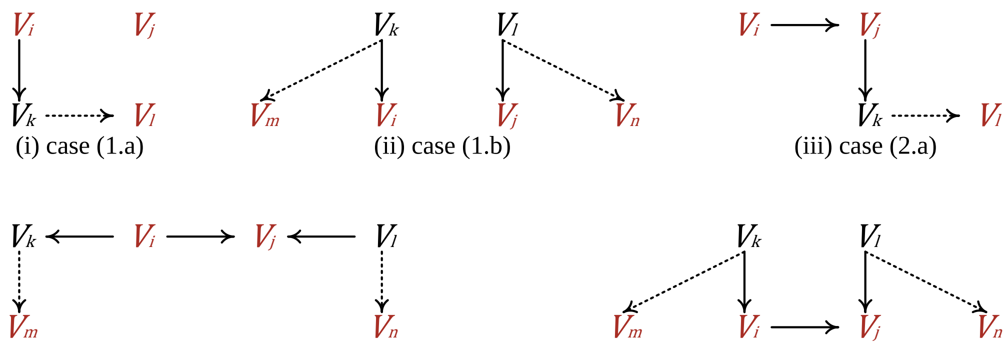
(2) Suppose $\{V_i, V_j\} \in \mathbb{S}_2$. Let $\mathrm{Pa}^{\mathcal{H}_2}(V_i) = \mathrm{Pa}^{\mathcal{H}_2}(V_j) = \{V_k\}$. If $V_k \in \mathbf{V}_c$, we let $V_m = V_k$. Otherwise, let $V_l \in \mathrm{Ne}^{\mathcal{H}_2}(V_k) \backslash \{V_i, V_j\}$. Similarly to fn. 3, we have $\mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_l) \backslash \{V_i, V_j\} \neq \emptyset$ and let $V_m \in \mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_l) \backslash \{V_i, V_j\}$. Clearly, $V_i = a_{ik} V_k + \epsilon_{V_i}, V_j = a_{jk} V_k + \epsilon_{V_j}$, $\{\epsilon_{V_i}, \epsilon_{V_j}\} \perp\!\!\!\perp \{V_k\} \cup (\mathbf{V}_c \backslash \{V_i, V_j\})$ and $\mathrm{Cov}(V_k, V_m) \neq 0$, so $\mathrm{R}(V_i, V_j | V_m) \perp\!\!\!\perp \mathbf{V}_c \backslash \{V_i, V_j\}$ based on Lem. 1(1). Combined with Prop. 1, we reach the conclusion.

(3) Suppose $\{V_i, V_j\} \in \mathbb{S}_3$. Let $V_i \in \mathrm{Pa}^{\mathcal{H}_2}(V_j)$ without loss of generality and $\mathrm{Pa}^{\mathcal{H}_2}(V_i) = \{V_k\}$. Similarly to fn. 3, we also have $\mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k) \backslash \{V_i, V_j\} \neq \emptyset$ and let $V_l \in \mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k) \backslash \{V_i, V_j\}$. Clearly, $V_i = a_{ik} V_k + \epsilon_{V_i}, V_j = (a_{ik} a_{ji} + a_{jk}) V_k + (a_{ji} \epsilon_{V_i} + \epsilon_{V_j})$ where $\{\epsilon_{V_i}, a_{ji} \epsilon_{V_i} + \epsilon_{V_j}\} \perp\!\!\!\perp \{V_k\} \cup (\mathbf{V}_c \backslash \{V_i, V_j\})$ and $\mathrm{Cov}(V_k, V_l) \neq 0$, so $\mathrm{R}(V_i, V_j | V_l) \perp\!\!\!\perp \mathbf{V}_c \backslash \{V_i, V_j\}$ based on Lem. 1(1). Combined with Prop. 1, we reach the conclusion.

"If". We prove this part by contradiction. Suppose $\{V_i, V_j\} \notin \mathbb{S}$.

(1) Suppose $V_i \notin \mathrm{Ne}^{\mathcal{H}_2}(V_j)$, all possible cases are as follows.

[3] There are three possible cases. (1) If $V_k \in \mathbf{V}_c$, we have $V_k \in \mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k) \backslash \{V_i, V_j\} \neq \emptyset$. (2) If $V_k \in \mathbf{V}_f$ and $\{V_i, V_j\} \not\subset \mathrm{PDe}^{\mathcal{G}}(V_k)$, based on Cor. 2, we have $\mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k) \backslash \{V_i, V_j\} \neq \emptyset$. (3) If $V_k \in \mathbf{V}_f$ and $\{V_i, V_j\} \subset \mathrm{PDe}^{\mathcal{G}}(V_k)$, since $V_j \notin \mathrm{PCh}^{\mathcal{G}}(V_k)$, based on Cor. 2, we have $\mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k) \backslash \{V_i, V_j\} \neq \emptyset$.



(i) case (1.a) (ii) case (1.b) (iii) case (2.a)

(iv) case (2.c) (v) case (2.d)

Figure 11: Illustration of "if" part in proof of Thm. 1. A dotted arrow from V_1 to V_2 means that $V_2 \in \mathrm{GDe}^{\mathcal{H}_2}(V_1)$. V is marked in red if $V \in \mathbf{V}_c$.

(a) Suppose $\mathrm{Ch}^{\mathcal{H}_2}(V_i) \neq \emptyset$ or $\mathrm{Ch}^{\mathcal{H}_2}(V_j) \neq \emptyset$, we take the former as an example without loss of generality. Let $V_k \in \mathrm{Ch}^{\mathcal{H}_2}(V_i)$. Similarly to fn. 3, we have $\mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k)\backslash\{V_i, V_j\} \neq \emptyset$ and let $V_l \in \mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k)\backslash\{V_i, V_j\}$. An illustrative example is shown as Fig. 11(i). If $V_j \notin \mathrm{De}^{\mathcal{H}_2}(V_i)$, $m_{ii}m_{li} \neq 0$ and $m_{ji} = 0$, so for any $V \in \mathbf{V}_c\backslash\{V_i, V_j\}$ s.t. V, V_i, V_j are correlated to each other, $\mathrm{R}(V_i, V_j|V) \not\perp V_l$ based on Lem. 1(2), which leads to contradiction. Otherwise, if $V_j \in \mathrm{De}^{\mathcal{H}_2}(V_i)$, without loss of generality, we assume $V_j \in \mathrm{De}^{\mathcal{H}_2}(V_k)$, in which case $m_{jk}m_{lk} \neq 0$ and $m_{ik} = 0$, so for any $V \in \mathbf{V}_c\backslash\{V_i, V_j\}$ s.t. V, V_i, V_j are correlated to each other, $\mathrm{R}(V_i, V_j|V) \not\perp V_l$ based on Lem. 1(2), which leads to contradiction.

(b) Suppose $\mathrm{Ch}^{\mathcal{H}_2}(V_i) = \mathrm{Ch}^{\mathcal{H}_2}(V_j) = \emptyset$, $\mathrm{Pa}^{\mathcal{H}_2}(V_i) \neq \emptyset$, and $\mathrm{Pa}^{\mathcal{H}_2}(V_j) \neq \emptyset$. Since $\{V_i, V_j\} \notin \mathbb{S}_2$, there exist $\{V_k, V_l\} \subset \mathbf{V}_c \cup \mathbf{V}_f\backslash\{V_i, V_j\}$ s.t. $V_k \in \mathrm{Pa}^{\mathcal{H}_2}(V_i)$ and $V_l \in \mathrm{Pa}^{\mathcal{H}_2}(V_j)$. Similarly to fn. 3, we have $\mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k)\backslash\{V_i, V_j\} \neq \emptyset$, $\mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_l)\backslash\{V_i, V_j\} \neq \emptyset$ and let $V_m \in \mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k)\backslash\{V_i, V_j\}$, $V_n \in \mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_l)\backslash\{V_i, V_j\}$ (It is possible that $V_m = V_n$). An illustrative example is shown as Fig. 11(ii). If $V_i \notin \mathrm{De}^{\mathcal{H}_2}(V_l)$ or $V_j \notin \mathrm{De}^{\mathcal{H}_2}(V_k)$, we take the former as an example without loss of generality, then $m_{jl}m_{nl} \neq 0$ and $m_{il} = 0$, so for any $V \in \mathbf{V}_c\backslash\{V_i, V_j\}$ s.t. V, V_i, V_j are correlated to each other, $\mathrm{R}(V_i, V_j|V) \not\perp V_m$ based on Lem. 1(2), which leads to contradiction. Otherwise, $m_{ik}m_{jk}m_{il}m_{jl} \neq 0$. Since there exist two non-intersecting directed paths from $\{V_k, V_l\}$ to $\{V_i, V_j\}$ (e.g., $V_k \to V_i$ and $V_l \to V_j$), $m_{ik}/m_{il} \neq m_{jk}/m_{jl}$. Also, $m_{mk}m_{nl} \neq 0$. So for any $V \in \mathbf{V}_c\backslash\{V_i, V_j\}$ s.t. V, V_i, V_j are correlated to each other, $\mathrm{R}(V_i, V_j|V) \not\perp V_m$ or $\mathrm{R}(V_i, V_j|V) \not\perp V_n$ based on Lem. 1(3), which leads to contradiction.

(c) Suppose $\mathrm{Ne}^{\mathcal{H}_2}(V_i) = \emptyset$ or $\mathrm{Ne}^{\mathcal{H}_2}(V_j) = \emptyset$, we take the former as an example without loss of generality. Clearly, $\mathrm{Cov}(V_i, V_j) = 0$, which leads to contradiction.

(2) Assume $V_i \in \mathrm{Pa}^{\mathcal{H}_2}(V_j)$ or $V_j \in \mathrm{Pa}^{\mathcal{H}_2}(V_i)$, we take the former as an example without loss of generality, all possible cases are as follows.

(a) Suppose $\mathrm{Ch}^{\mathcal{H}_2}(V_j) \neq \emptyset$. Let $V_k \in \mathrm{Ch}^{\mathcal{H}_2}(V_j)$. Similarly to fn. 3, we have $\mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k)\backslash\{V_i, V_j\} \neq \emptyset$ and let $V_l \in \mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k)\backslash\{V_i, V_j\}$. An illustrative example is shown as Fig. 11(iii). Clearly, $m_{jj}m_{lj} \neq 0$ and $m_{ij} = 0$, so for any $V \in \mathbf{V}_c\backslash\{V_i, V_j\}$ s.t. V, V_i, V_j are correlated to each other, $\mathrm{R}(V_i, V_j|V) \not\perp V_l$ based on Lem. 1(2), which leads to contradiction.

(b) Suppose $\mathrm{Pa}^{\mathcal{H}_2}(V_j)\backslash\{V_i\} = \emptyset$ and $\mathrm{Ch}^{\mathcal{H}_2}(V_j) = \emptyset$. Since $\{V_i, V_j\} \notin \mathbb{S}_1$, we have $\mathrm{Ne}^{\mathcal{H}_2}(V_i)\backslash\{V_j\} = \emptyset$. Clearly, for any $V \in \mathbf{V}_c\backslash\{V_i, V_j\}$, $\mathrm{Cov}(V, V_i) = 0$ which leads to contradiction.

(c) Suppose $\mathrm{Ch}^{\mathcal{H}_2}(V_i)\backslash\{V_j\} \neq \emptyset$, $\mathrm{Pa}^{\mathcal{H}_2}(V_j)\backslash\{V_i\} \neq \emptyset$, and $\mathrm{Ch}^{\mathcal{H}_2}(V_j) = \emptyset$. Let $V_k \in \mathrm{Ch}^{\mathcal{H}_2}(V_i)\backslash\{V_j\}$ and $V_l \in \mathrm{Pa}^{\mathcal{H}_2}(V_j)\backslash\{V_i\}$ (It is possible that $V_k = V_l$). Similarly to fn. 3, we have $\mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k)\backslash\{V_i, V_j\} \neq \emptyset$, $\mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_l)\backslash\{V_i, V_j\} \neq \emptyset$ and let $V_m \in$

$\text{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k)\backslash\{V_i, V_j\}$, $V_n \in \text{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_l)\backslash\{V_i, V_j\}$ (It is possible that $V_m = V_n$). An illustrative example is shown as Fig. 11(iv). If $V_i \notin \text{De}^{\mathcal{H}_2}(V_l)$, $m_{jl}m_{nl} \neq 0$ and $m_{il} = 0$, so for any $V \in \mathbf{V}_c\backslash\{V_i, V_j\}$ s.t. V, V_i, V_j are correlated to each other, $\text{R}(V_i, V_j|V) \not\perp\!\!\!\perp V_n$ based on Lem. 1(2), which leads to contradiction. Otherwise, $m_{ii}m_{il}m_{ji}m_{jl} \neq 0$, since there exist two non-intersecting directed paths from $\{V_i, V_l\}$ to $\{V_i, V_j\}$ (e.g., V_i and $V_l \rightarrow V_j$), $m_{ii}/m_{il} \neq m_{ji}/m_{jl}$. Also, $m_{mi}m_{nl} \neq 0$, so for any $V \in \mathbf{V}_c\backslash\{V_i, V_j\}$ s.t. V, V_i, V_j are correlated to each other, $\text{R}(V_i, V_j|V) \not\perp\!\!\!\perp V_m$ or $\text{R}(V_i, V_j|V) \not\perp\!\!\!\perp V_n$ based on Lem. 1(3), which leads to contradiction.

(d) Suppose $\text{Pa}^{\mathcal{H}_2}(V_i) \neq \emptyset$, $\text{Ch}^{\mathcal{H}_2}(V_i)\backslash\{V_j\} = \emptyset$, $\text{Pa}^{\mathcal{H}_2}(V_j)\backslash\{V_i\} \neq \emptyset$, and $\text{Ch}^{\mathcal{H}_2}(V_j) = \emptyset$. Since $\{V_i, V_j\} \notin \mathbb{S}_3$, there exist $\{V_k, V_l\} \subset \mathbf{V}_c \cup \mathbf{V}_f\backslash\{V_i, V_j\}$ s.t. $V_k \in \text{Pa}^{\mathcal{H}_2}(V_i)$ and $V_l \in \text{Pa}^{\mathcal{H}_2}(V_j)$. Similarly to fn. 3, we have $\text{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k)\backslash\{V_i, V_j\} \neq \emptyset$, $\text{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_l)\backslash\{V_i, V_j\} \neq \emptyset$ and let $V_m \in \text{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k)\backslash\{V_i, V_j\}$, $V_n \in \text{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_l)\backslash\{V_i, V_j\}$ (It is possible that $V_m = V_n$). An illustrative example is shown as Fig. 11(v). Then the proof is similar to case (1.b).

(e) Suppose $\text{Pa}^{\mathcal{H}_2}(V_i) = \emptyset$, $\text{Ch}^{\mathcal{H}_2}(V_i)\backslash\{V_j\} = \emptyset$, $\text{Pa}^{\mathcal{H}_2}(V_j)\backslash\{V_i\} \neq \emptyset$, and $\text{Ch}^{\mathcal{H}_2}(V_j) = \emptyset$. Clearly, for any $V \in \mathbf{V}_c\backslash\{V_i, V_j\}$, $\text{Cov}(V, V_i) = 0$, which leads to contradiction.

□

Proposition 1. *$\forall\{V_i, V_j, V_k, V_l\} \subset \mathbf{V}_c$ where $\text{Cov}(V_i, V_j)\text{Cov}(V_i, V_k)\text{Cov}(V_j, V_k) \neq 0$ and $\text{Cov}(V_i, V_j)\text{Cov}(V_i, V_l)\text{Cov}(V_j, V_l) \neq 0$, $\text{R}(V_i, V_j|V_k) \perp\!\!\!\perp \mathbf{V}_c\backslash\{V_i, V_j\}$ iff $\text{R}(V_i, V_j|V_l) \perp\!\!\!\perp \mathbf{V}_c\backslash\{V_i, V_j\}$.*

Remark. Given $\{V_i, V_j\} \subset \mathbf{V}_c$, denote $\{V \in \mathbf{V}_c\backslash\{V_i, V_j\}|\text{Cov}(V_i, V_j)\text{Cov}(V, V_i)\text{Cov}(V, V_j) \neq 0\}$ by $\mathbf{V}_{ij}$, this proposition means that there exists no $\{V_k, V_l\} \subset \mathbf{V}_{ij}$ s.t. $\text{R}(V_i, V_j|V_k) \perp\!\!\!\perp \mathbf{V}_c\backslash\{V_i, V_j\}$ and $\text{R}(V_i, V_j|V_l) \not\perp\!\!\!\perp \mathbf{V}_c\backslash\{V_i, V_j\}$. Therefore, if we want to know whether for each $V \in \mathbf{V}_{ij}$, $\text{R}(V_i, V_j|V) \perp\!\!\!\perp \mathbf{V}_c\backslash\{V_i, V_j\}$, we only need to consider any single $V_k \in \mathbf{V}_{ij}$.

Proof. If $\text{R}(V_i, V_j|V_k) \perp\!\!\!\perp \mathbf{V}_c\backslash\{V_i, V_j\}$, then $\text{R}(V_i, V_j|V_k) \perp\!\!\!\perp V_l$, which means that $\text{Cov}(\text{R}(V_i, V_j|V_k), V_l) = 0$, that is, $\frac{\text{Cov}(V_i, V_k)}{\text{Cov}(V_j, V_k)} = \frac{\text{Cov}(V_i, V_l)}{\text{Cov}(V_j, V_l)}$, so $\text{R}(V_i, V_j|V_l) = \text{R}(V_i, V_j|V_k) \perp\!\!\!\perp \mathbf{V}_c\backslash\{V_i, V_j\}$. Similarly, if $\text{R}(V_i, V_j|V_l) \perp\!\!\!\perp \mathbf{V}_c\backslash\{V_i, V_j\}$, there is also $\text{R}(V_i, V_j|V_k) \perp\!\!\!\perp \mathbf{V}_c\backslash\{V_i, V_j\}$. □

Theorem 2. $\forall\{V_i, V_j\} \in \mathbb{S}$, let $\{V_{i_1}, V_{i_2}\} \subset \text{Ch}^{\mathcal{H}_1}(V_i)$.

(1) $\text{R}(V_{i_1}, V_j|V_{i_2}) \perp\!\!\!\perp V_{i_2}$ iff $\{V_i, V_j\} \in \mathbb{S}_1$ and $V_i \in \text{Pa}^{\mathcal{G}}(V_j)$.

(2) Suppose $\{V_i, V_j\} \notin \mathbb{S}_1$, $\exists\{V'_i, V'_j\} \in \mathbb{S}\backslash\{\{V_i, V_j\}\}$ s.t. $\{V'_i, V'_j\} \cap \{V_i, V_j\} \neq \emptyset$ only if (but not if) $\{V_i, V_j\} \in \mathbb{S}_2$.

(3) Suppose $\{V_i, V_j\} \notin \mathbb{S}_1$, $\exists\{V_k, V_l\} \subset \bigcup \text{Ch}^{\mathcal{H}_1}(\mathbf{V}_c\backslash\{V_i, V_j\})$ s.t. $(V_{i_1}, V_{i_2}, V_j, V_k, V_l)$ satisfies the quintuple constraint iff $\{V_i, V_j\} \in \mathbb{S}_3$ and $V_i \in \text{Pa}^{\mathcal{G}}(V_j)$.

Proof Sketch. For (1), if $\{V_i, V_j\} \in \mathbb{S}_1$ and $V_i \in \text{Pa}^{\mathcal{G}}(V_j)$, we can prove independence based on Lem. 1(1); otherwise, for each possible case, we can prove dependence based on Lem. 1(2,3). For (2), "only if" can be readily derived from the definitions of $\mathbb{S}_2$ and $\mathbb{S}_3$ while "not if" can be proven by an example, which is $\{O_7, O_8\}$ in Fig. 3. For (3), if $\{V_i, V_j\} \in \mathbb{S}_3$ and $V_i \in \text{Pa}^{\mathcal{G}}(V_j)$, letting V be the common parent of V_i, V_j and V_k, V_l be respective generalized descendants of V's any two pure children, we can prove the quintuple constraint is satisfied based on Lem. 2(2.a); otherwise, for each possible case, we can prove it is not satisfied based on Lem. 2(1).

Proof. Cond. 1 indicates that $\forall V \in \mathbf{V}_c, \text{Ch}^{\mathcal{H}_1}(V) \subset \text{PCh}^{\mathcal{G}}(V)$.

- "If" of (1): Clearly, $V_{i_1} = a_{i_1 i}V_i + \epsilon_{V_{i_1}}, V_j = a_{ji}V_i + \epsilon_{V_j}$ where $\{\epsilon_{V_{i_1}}, \epsilon_{V_j}\} \perp\!\!\!\perp \{V_i, V_{i_2}\}$, and $\text{Cov}(V_i, V_{i_2}) \neq 0$, so we can reach the conclusion based on Lem. 1(1).
- "Only if" of (1): We prove this part by contradiction.

- Suppose (i) $\{V_i, V_j\} \in \mathbb{S}_1$ and $V_j \in \mathrm{Pa}^{\mathcal{G}}(V_i)$, or (ii) $\{V_i, V_j\} \in \mathbb{S}_2$, or (iii) $\{V_i, V_j\} \in \mathbb{S}_3$ and $V_j \in \mathrm{Pa}^{\mathcal{G}}(V_i)$. Since $m_{i_1 i} m_{i_2 i} \neq 0$ and $m_{ji} = 0$, $\mathrm{R}(V_{i_1}, V_j | V_{i_2}) \not\perp\!\!\!\perp V_{i_2}$ based on Lem. 1(2), which leads to contradiction.
- Suppose $\{V_i, V_j\} \in \mathbb{S}_3$ and $V_i \in \mathrm{Pa}^{\mathcal{G}}(V_j)$. Let $\mathrm{Pa}^{\mathcal{H}_2}(V_i) = \{V_k\}$. Clearly, $m_{i_1 i} m_{i_1 k} m_{ji} m_{jk} \neq 0$. Since there exist two non-intersecting directed paths from $\{V_i, V_k\}$ to $\{V_{i_1}, V_j\}$ (e.g., $V_i \to V_{i_1}$ and $V_k \to V_j$), $m_{i_1 i}/m_{i_1 k} \neq m_{ji}/m_{jk}$. Also, $m_{i_2 i} m_{i_2 k} \neq 0$, so $\mathrm{R}(V_{i_1}, V_j | V_{i_2}) \not\perp\!\!\!\perp V_{i_2}$ based on Lem. 1(3), which leads to contradiction.

- "If" of (2): This follows the definition of $\mathbb{S}_2$.
- "Not only if" of (2): An example is $\{O_7, O_8\}$ in Fig. 3.
- "If" of (3): Let $\mathrm{Pa}^{\mathcal{H}_2}(V_i) = \{V_h\}$. If $V_h \in \mathbf{V}_c$, let $\{V_k, V_l\} \subset \mathrm{Ch}^{\mathcal{H}_1}(V_h)$. Otherwise, $V_h \in \mathbf{V}_f \subset \mathbf{L}$, let $\{V_{h_1}, V_{h_2}\} \subset \mathrm{PCh}^{\mathcal{G}}(V_h)$. Similarly to fn. 3, we can obtain $\mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_{h_1}) \backslash \{V_i, V_j\} \neq \emptyset$ and $\mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_{h_2}) \backslash \{V_i, V_j\} \neq \emptyset$, let $V_k \in \bigcup \mathrm{Ch}^{\mathcal{H}_1}(\mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_{h_1}))$ and $V_l \in \bigcup \mathrm{Ch}^{\mathcal{H}_1}(\mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_{h_2}))$. In both cases, $V_{i_1}, V_{i_2}, V_j, V_k$ can be expressed as
$$V_{i_1} = a_{ih} a_{i_1 i} V_h + a_{i_1 i} \epsilon_{V_i} + \epsilon_{V_{i_1}} \tag{13}$$
$$V_{i_2} = a_{ih} a_{i_2 i} V_h + a_{i_2 i} \epsilon_{V_i} + \epsilon_{V_{i_2}} \tag{14}$$
$$V_j = (a_{ih} a_{ji} + a_{jh}) V_h + a_{ji} \epsilon_{V_i} + \epsilon_{V_j}, \tag{15}$$
$$V_k = \lambda_k V_h + e_{V_k}, \tag{16}$$
where $V_h, \epsilon_{V_i}, \epsilon_{V_{i_1}}, \epsilon_{V_{i_2}}, \epsilon_{V_j}, e_{V_k}$ are independent of each other, $V_l \perp\!\!\!\perp \{\epsilon_{V_i}, \epsilon_{V_{i_1}}, \epsilon_{V_{i_2}}, \epsilon_{V_j}, e_{V_k}\}$ and $\mathrm{Cov}(V_l, V_h) \neq 0$, so $(V_{i_1}, V_{i_2}, V_j, V_k, V_l)$ satisfies the quintuple constraint based on Lem. 2(2.a).
- "Only if" of (3): We prove this part by contradiction. Suppose $\{V_i, V_j\} \in \mathbb{S}_3$ and $V_j \in \mathrm{Pa}^{\mathcal{H}_2}(V_i)$ or $\{V_i, V_j\} \in \mathbb{S}_2$. Clearly, $m_{i_1 i} m_{i_2 i} \neq 0$, $m_{ji} = 0$, and for any V_k, $m_{ki} = 0$, so $(V_{i_1}, V_{i_2}, V_j, V_k, V_l)$ does not satisfy the quintuple constraint based on Lem. 2(1), which leads to contradiction.

□

Theorem 3. (1) $\forall \{V_i, V_j\} \in \mathbb{S}_2$, $\bigcap \mathrm{Pa}^{\mathcal{G}}(\{V_i, V_j\}) \subset \mathbf{V}_c$ iff $\exists \{V_i', V_j'\} \in \mathbb{S}_1$ s.t. $\{V_i, V_j\} \cap \{V_i', V_j'\} \neq \emptyset$. (2) $\forall \{\{V_i, V_j\}, \{V_i', V_j'\}\} \subset \mathbb{S}_2$, $\bigcap \mathrm{Pa}^{\mathcal{G}}(\{V_i, V_j\}) = \bigcap \mathrm{Pa}^{\mathcal{G}}(\{V_i', V_j'\})$ iff $\exists \{V_i'', V_j''\} \in \mathbb{S}_2$ s.t. $\{V_i, V_j\} \cap \{V_i'', V_j''\} \neq \emptyset$ and $\{V_i', V_j'\} \cap \{V_i'', V_j''\} \neq \emptyset$.

Proof. This can be readily derived from the definitions of $\mathbb{S}_1$ and $\mathbb{S}_2$. □

Proposition 2. *Cond. 1 is still valid after update.*

Proof. We denote $\mathbf{V}_p, \mathbf{V}_c, \mathbf{V}_f, \mathcal{H}_1, \mathcal{H}_2$ after update by $\mathbf{V}_p', \mathbf{V}_c', \mathbf{V}_f', \mathcal{H}_1', \mathcal{H}_2'$ respectively. While Cond. 1 is valid for $\mathbf{V}_p' \cap \mathbf{V}_p$ and $\mathbf{V}_c' \cap \mathbf{V}_c$ trivially, we focus on $\mathbf{V}_p' \backslash \mathbf{V}_p$ and $\mathbf{V}_c' \backslash \mathbf{V}_c$.

- If $V_j \in \mathbf{V}_p' \backslash \mathbf{V}_p$, then $V_j \in \mathbf{V}_c$ and there exists $V_i \in \mathbf{V}_c$ s.t. (1) $\{V_i, V_j\} \in \mathbb{S}_1$ and $V_i \in \mathrm{Pa}^{\mathcal{H}_2}(V_j)$ or (2) $\{V_i, V_j\} \in \mathbb{S}_2$. In both cases, $|\mathrm{Pa}^{\mathcal{H}_1'}(V_j)| = 1$ because $\mathrm{Pa}^{\mathcal{H}_1'}(V_j) = \{V_i\}$ in case (1) and $\mathrm{Pa}^{\mathcal{H}_1'}(V_j) = \bigcap \mathrm{Pa}^{\mathcal{H}_2}(\{V_i, V_j\})$ in case (2). Also, $\mathrm{PCh}^{\mathcal{H}_2}(V_j) = \emptyset$, so $\mathrm{Ch}^{\mathcal{H}_1}(V_j) \subset \mathrm{PCh}^{\mathcal{G}}(V_j)$ reduces to $\mathrm{Ch}^{\mathcal{H}_1}(V_j) = \mathrm{PCh}^{\mathcal{G}}(V_j)$, then $\mathrm{Ch}^{\mathcal{H}_1'}(V_j) = \mathrm{Ch}^{\mathcal{H}_1}(V_j) = \mathrm{PCh}^{\mathcal{G}}(V_j)$.
- If $V_j \in \mathbf{V}_c' \backslash \mathbf{V}_c$, then $V_j \in \mathbf{V}_f$, $|\mathrm{Ch}^{\mathcal{H}_1'}(V_j)| \geq 2$, and $\forall \{V_k, V_l\} \subset \mathrm{Ch}^{\mathcal{H}_1'}(V_j)$, $\{V_k, V_l\} \in \mathbb{S}_2$ and $\bigcup \mathrm{Pa}^{\mathcal{H}_2}(\{V_k, V_l\}) = \{V_j\}$, so $\mathrm{Ch}^{\mathcal{H}_1'}(V_j) \subset \mathrm{PCh}^{\mathcal{G}}(V_j)$. Besides, it is trivial that $\mathrm{Pa}^{\mathcal{H}_1'}(V_j) = \emptyset$.

□

Theorem 4. If $\mathbb{S}_1 \cup \mathbb{S}_2 = \emptyset$, $\mathbf{V}_f = \emptyset$.

Proof. We prove this by contradiction. Suppose $\mathbf{V}_f \neq \emptyset$ and $V_i \in \mathbf{V}_f \subset \mathbf{L}$.

- If $\bigcup \mathrm{Ch}^{\mathcal{H}_2}(\mathrm{PCh}^{\mathcal{G}}(V_i)) = \emptyset$, then $\mathrm{PCh}^{\mathcal{G}}(V_i) \subset \mathbf{V}_c$. Conversely, if $\mathrm{PCh}^{\mathcal{G}}(V_i) \not\subset \mathbf{V}_c$, there exists $V \in \mathrm{PCh}^{\mathcal{G}}_{\mathbf{V}_f}(V_i) \subset \mathbf{L}$ and $\mathrm{Ch}^{\mathcal{G}}(V) = \mathrm{Ch}^{\mathcal{H}_2}(V) = \emptyset$, contradicting Asmp. 1. For each $\{V_j, V_k\} \subset \mathrm{PCh}^{\mathcal{G}}(V_i)$, $\{V_j, V_k\} \in \mathbb{S}_2$, which leads to contradiction.

- If $\bigcup \mathrm{Ch}^{\mathcal{H}_2}(\mathrm{PCh}^{\mathcal{G}}(V_i)) \neq \emptyset$, let $\mathbf{V}' = \{V | V \in \mathrm{PDe}^{\mathcal{G}}(V_i), \mathrm{Ch}^{\mathcal{H}_2}(V) \neq \emptyset\}$ and $V_j \in \mathbf{V}'$ s.t. $\bigcup \mathrm{Ch}^{\mathcal{H}_2}(\mathrm{Ch}^{\mathcal{H}_2}(V_j)) = \emptyset$, then $\mathrm{Ch}^{\mathcal{H}_2}(V_j) \subset \mathbf{V}_c$. If $V_j \in \mathbf{V}_c$, then for any $V_k \in \mathrm{Ch}^{\mathcal{H}_2}(V_j)$, $\{V_j, V_k\} \in \mathbb{S}_1$. Otherwise, $V_j \in \mathbf{V}_f \subset \mathbf{L}$, for each $\{V_k, V_l\} \subset \mathrm{Ch}^{\mathcal{H}_2}(V_j)$, $\{V_k, V_l\} \in \mathbb{S}_2$.

□

C.2.2 Proof of theoretical results in Sec. 3.2

Condition 2. (1) $\forall V \in \mathbf{U}_c, \mathrm{De}^{\mathcal{H}_2}(V) \subset \mathbf{U}_c$. (2) $\forall V_i \in \mathbf{U}_c$, X_{2i-1}, X_{2i} can be written as

$$X_{2i-1} = c_{i_1} \sum_{V_j \in \mathbf{U}_c} m_{ij} \epsilon_{V_j} + e_{X_{2i-1}} + e'_{X_{2i-1}}, \quad X_{2i} = c_{i_2} \sum_{V_j \in \mathbf{U}_c} m_{ij} \epsilon_{V_j} + e_{X_{2i}} + e'_{X_{2i}}, \tag{17}$$

where $\forall j,k,l$, (i) $\epsilon_{V_j} \perp\!\!\!\perp e_{X_k} \perp\!\!\!\perp e'_{X_l}$, (ii) $e_{X_j} \perp\!\!\!\perp e_{X_k}$ if $j \neq k$, and (iii) $e'_{X_{2j-1}} \perp\!\!\!\perp e'_{X_{2k}}$.

Theorem 5. $\forall V_i \in \mathbf{U}_c$, $\mathrm{An}^{\mathcal{H}_2}(V_i) \cap \mathbf{U}_c = \emptyset$ iff $\forall V_j \in \mathbf{U}_c \backslash \{V_i\}$, $\mathrm{R}(X_{2j-1}, X_{2i-1}|X_{2i}) \perp\!\!\!\perp X_{2i}$.

Proof. When $|\mathbf{U}_c| = 1$, the proof is trivial, we focus on the case $|\mathbf{U}_c| > 1$.

"Only if": As $\forall V_i \in \mathbf{U}_c$, $\mathrm{An}^{\mathcal{H}_2}(V_i) \cap \mathbf{U}_c = \emptyset$, X_{2i-1} and X_{2i} can be written as

$$X_{2i-1} = c_{i_1} \epsilon_{V_i} + e_{X_{2i-1}} + e'_{X_{2i-1}}, \quad X_{2i} = c_{i_2} \epsilon_{V_i} + e_{X_{2i}} + e'_{X_{2i}}. \tag{18}$$

- If $\mathrm{Cov}(X_{2j-1}, X_{2i}) = 0$, then $m_{ji} = 0$, so $\mathrm{R}(X_{2j-1}, X_{2i-1}|X_{2i}) = X_{2j-1} \perp\!\!\!\perp X_{2i}$.
- If $\mathrm{Cov}(X_{2j-1}, X_{2i}) \neq 0$, then $m_{ji} \neq 0$. X_{2j-1} can be written as

$$X_{2j-1} = c_{j_1} m_{ji} \epsilon_{V_i} + c_{j_1} \sum_{V_k \in \mathbf{U}_c \backslash \{V_i\}} m_{jk} \epsilon_{V_k} + e_{X_{2j-1}} + e'_{X_{2j-1}}, \tag{19}$$

  where $\{c_{j_1} \sum_{V_k \in \mathbf{U}_c \backslash \{V_i\}} m_{jk} \epsilon_{V_k} + e_{X_{2j-1}} + e'_{X_{2j-1}}, e_{X_{2i-1}} + e'_{X_{2i-1}}\} \perp\!\!\!\perp \{\epsilon_{V_i}, X_{2i}\}$ and $\mathrm{Cov}(\epsilon_{V_i}, X_{2i}) \neq 0$, so $\mathrm{R}(X_{2j-1}, X_{2i-1}|X_{2i}) \perp\!\!\!\perp X_{2i}$ based on Lem. 1(1).

"If": We prove this part by contradiction. Let $V_j \in \mathrm{An}^{\mathcal{H}_2}_{\mathbf{U}_c}(V_i) \neq \emptyset$. Since X_{2i-1} and X_{2i} both contain ϵ_{V_i} while X_{2j-1} does not contain ϵ_{V_i}, so $\mathrm{R}(X_{2j-1}, X_{2i-1}|X_{2i}) \not\!\perp\!\!\!\perp X_{2i}$ based on Lem. 1(2), which leads to contradiction. □

Theorem 6. If $V_i \in \mathbf{U}_c$ and $\mathrm{An}^{\mathcal{H}_2}(V_i) \cap \mathbf{U}_c = \emptyset$, then $\mathrm{Cov}(X_{2i-1}, X_{2i}) = c_{i_1} c_{i_2}$ and $\forall V_j \in \mathbf{U}_c \backslash \{V_i\}$,

$$\mathrm{sgn}(m_{ji}) = \mathrm{sgn}(\frac{\mathrm{Cov}(X_{2i-1}, X_{2j})}{\mathrm{Cov}(X_{2j-1}, X_{2j})}), \quad \mathrm{Cov}(X_{2i-1}, X_{2j})\mathrm{Cov}(X_{2i}, X_{2j-1}) = c_{i_1} c_{i_2} c_{j_1} c_{j_2} m_{ji}^2. \tag{20}$$

Proof. Since we assume each ϵ_{V_i} has variance 1 and each c_{i_1} is positive without loss of generality,

$$\frac{\mathrm{Cov}(X_{2i-1}, X_{2j})}{\mathrm{Cov}(X_{2j-1}, X_{2j})} = \frac{c_{i_1} m_{ji}}{c_{j_1} \mathrm{Var}(\sum_{V_k \in \mathbf{U}_c} m_{jk} \epsilon_{V_k})}, \tag{21}$$

so $\mathrm{sgn}(m_{ji}) = \mathrm{sgn}(\frac{\mathrm{Cov}(X_{2i-1}, X_{2j})}{\mathrm{Cov}(X_{2j-1}, X_{2j})})$. Besides, it is trivial that

$$\mathrm{Cov}(X_{2i-1}, X_{2j})\mathrm{Cov}(X_{2i}, X_{2j-1}) = c_{i_1} c_{i_2} c_{j_1} c_{j_2} m_{ji}^2, \quad \mathrm{Cov}(X_{2i-1}, X_{2i}) = c_{i_1} c_{i_2}. \tag{22}$$

□

Proposition 3. *Cond. 2 is still valid after removal.*

Proof. Based on Thm. 5, Cond. 2(1) holds trivially. Besides,

$$\mathrm{R}(X_{2j-1}, X_{2i-1}|X_{2i}) = c_{j_1} \sum_{V_k \in \mathbf{U}_c \backslash \{V_i\}} m_{jk}\epsilon_{V_k} + e_{X_{2j-1}} + \underbrace{e'_{X_{2j-1}} - \frac{m_{ji}c_{j_1}}{c_{i_1}}(e_{X_{2i-1}} + e'_{X_{2i-1}})}_{\text{updated } e'_{X_{2j-1}}}, \quad (23)$$

$$X_{2j} = c_{j_2} \sum_{V_k \in \mathbf{U}_c} m_{jk}\epsilon_{V_k} + e_{X_{2j}} + e'_{X_{2j}} = c_{j_2} \sum_{V_k \in \mathbf{U}_c \backslash \{V_i\}} m_{jk}\epsilon_{V_k} + e_{X_{2j}} + \underbrace{e'_{X_{2j}} + c_{j_2}m_{ji}\epsilon_{V_i}}_{\text{updated } e'_{X_{2j}}}, \quad (24)$$

so Cond. 2(2) is still valid. □

C.2.3 Proof of theoretical results in Sec. 3.3

Theorem 7. Suppose the observed variables are generated by a LiNGAM with latent variables satisfying the rank-faithfulness assumption and Asmp. 1, in the limit of infinite data, our algorithm correctly identifies the underlying complete causal structure.

Proof. In Stage 1, our algorithm sequentially identifies latent variables and their pure children. During this process, $\mathcal{H}_1$ records all identified causal relations. According to the theoretical results in Sec. 3.1, causal relations in $\mathcal{H}_1$ are correct. In Stage 2, with $\mathcal{H}_1$ fixed, our algorithm recovers $\mathcal{H}_2$. According to the theoretical results in Sec. 3.2, causal relations in $\mathcal{H}_2$ are correct. Combining $\mathcal{H}_1$ and $\mathcal{H}_2$, our algorithm correctly identifies the underlying complete causal structure. □

C.3 Proof of theoretical results in Sec. 4

Definition 8. *(Unique minimal bottleneck) We say* $\mathbf{B}$ *is a bottleneck from* $\mathbf{J}$ *to* $\mathbf{K}$ *(*$\mathbf{J}, \mathbf{K}, \mathbf{B}$ *need not be mutually disjoint) if* $\forall J \in \mathbf{J}$ *and* $K \in \mathbf{K}$*, each directed path from* J *to* K *includes some* $B \in \mathbf{B}$*. Given a bottleneck* $\mathbf{B}_1$ *from* $\mathbf{J}$ *to* $\mathbf{K}$*, if any other bottleneck* $\mathbf{B} \neq \mathbf{B}_1$ *satisfying* $|\mathbf{B}| \geq |\mathbf{B}_1|$*, we say* $\mathbf{B}_1$ *is a minimal bottleneck. Furthermore, if* $|\mathbf{B}| > |\mathbf{B}_1|$*, we say* $\mathbf{B}_1$ *is the unique minimal bottleneck.*

Assumption 2. (1) $\forall L \in \mathbf{L}, V \in \mathbf{V}_0 \backslash \{L\}$, $\mathrm{Ch}^{\mathcal{G}_0}(L) \not\subset \mathrm{Ch}^{\mathcal{G}_0}(V) \cup \{V\}$. (2) $\forall V \in \mathbf{V}_0$, $\mathrm{Ch}^{\mathcal{G}_0}(V)$ is the unique minimal bottleneck from $\mathrm{Ch}^{\mathcal{G}_0}(V)$ to $\mathbf{O}_0$. (3) $\forall L \in \mathbf{L}$, L is not a PV.

Trivially, if Asmp. 2 holds, then (1) $\forall L \in \mathbf{L}, V \in \mathbf{V} \backslash \{L\}$, $\mathrm{Ch}^{\mathcal{G}}(L) \not\subset \mathrm{Ch}^{\mathcal{G}}(V) \cup \{V\}$. (2) $\forall V \in \mathbf{V}$, $\mathrm{Ch}^{\mathcal{G}}(V)$ is the unique minimal bottleneck from $\mathrm{Ch}^{\mathcal{G}}(V)$ to $\mathbf{O}$. (3) $\forall L \in \mathbf{L}$, L is not a PV.

C.3.1 Proof of theoretical results in Sec. 4.1

Definition 9. *(Pseudo-pure descendant) We say* V_2 *is a pseudo-pure descendant of* V_1*, denoted by* $V_2 \in \mathrm{P}^2\mathrm{De}(V_1)$*, if* $V_2 \in \mathrm{De}(V_1)$ *and there exists no common cause between* V_1 *and* V_2*.*

Example. In Fig. 2(a), $\mathrm{P}^2\mathrm{De}(O_2) = \{L_1, ..., L_4, O_1, O_3, ..., O_{16}\}$.

Condition 3. (1) $\forall V \in \mathbf{V}_p$, $|\mathrm{Pa}^{\mathcal{H}_1}(V)| = 1$ and $\mathrm{Ch}^{\mathcal{H}_1}(V) = \mathrm{PCh}^{\mathcal{G}}(V)$; (2) $\forall V \in \mathbf{V}_c$, $\mathrm{Pa}^{\mathcal{H}_1}(V) = \emptyset$ and $|\mathrm{Ch}^{\mathcal{H}_1}(V)| \geq 2$. If $\mathrm{Ch}^{\mathcal{H}_1}(V) \not\subset \mathrm{PCh}^{\mathcal{G}}(V)$, then $\{\mathrm{Ch}^{\mathcal{H}_1}(V)\} = \mathrm{P}^3\mathrm{Ch}^{\mathcal{G}}(V)$ and $\nexists\{V_i, V_j\} \subset \mathbf{V}_c \backslash \{V\}$ s.t. $V_i \in \mathrm{P}^2\mathrm{De}^{\mathcal{G}}(V)$, $V_j \not\perp V$, and $V_i \perp\!\!\!\perp V_j | V$.

Before proving theoretical results in the main text one by one, we first introduce two corollaries (Cors. 3 and 4) readily derived from Cond. 3.

Corollary 3. *(1)* $\forall V \in \mathbf{V}_p, \mathrm{Ch}^{\mathcal{G}}(V) = \mathrm{Ch}^{\mathcal{H}_1}(V)$ *or* $\exists V' \in \mathbf{V}_p \backslash \{V\}$ *s.t.* $\mathrm{Ch}^{\mathcal{G}}(V) = \mathrm{Ch}^{\mathcal{H}_1}(V) \cup \{V'\}$*, and* $\mathrm{Pa}^{\mathcal{G}}(V) = \mathrm{Pa}^{\mathcal{H}_1}(V)$ *or* $\exists V' \in \mathbf{V}_p \backslash \{V\}$ *s.t.* $\mathrm{Pa}^{\mathcal{G}}(V) = \mathrm{Pa}^{\mathcal{H}_1}(V) \cup \{V'\}$*; (2)* $\forall V \in \mathbf{V}_f, \mathrm{Ch}^{\mathcal{G}}(V) = \mathrm{Ch}^{\mathcal{H}_2}(V)$ *and* $\mathrm{Pa}^{\mathcal{G}}(V) = \mathrm{Pa}^{\mathcal{H}_2}(V)$.

Remark. This is a variant of Cor. 1 in App. C.2.1. While (2) here is identical to (2) in Cor. 1, (1) here is slightly different from (1) in Cor. 1 in the sense that for each $V \in \mathbf{V}_p$, $\mathrm{Ch}^{\mathcal{G}}(V)$ and $\mathrm{Pa}^{\mathcal{G}}(V)$

contain at most one more variable in $\mathbf{V}_p$ than $\mathrm{Ch}^{\mathcal{H}_1}(V)$ and $\mathrm{Pa}^{\mathcal{H}_2}(V)$ here. This corollary is widely used in the following proofs. To maintain fluency, we will use it without further citation.

Proof. First, if $V_i \in \mathbf{V}_p$, then there exists $V_j \in \mathbf{V}_c \cup \mathbf{V}_p$ s.t. $V_i \in \mathrm{Ch}^{\mathcal{H}_1}(V_j)$ because $\mathrm{Pa}^{\mathcal{H}_1}(V_i) \neq \emptyset$ based on Cond. 3(1). Moreover, since $\mathrm{Ch}^{\mathcal{H}_1}(V_j) = \mathrm{PCh}^{\mathcal{G}}(V_j)$ if $V_j \in \mathbf{V}_p$ and $\mathrm{Ch}^{\mathcal{H}_1}(V_j) \subset \mathrm{PCh}^{\mathcal{G}}(V_j)$ or $\{\mathrm{Ch}^{\mathcal{H}_1}(V_j)\} = \mathrm{P}^3\mathrm{Ch}^{\mathcal{G}}(V_j)$ if $V_j \in \mathbf{V}_c$ based on Cond. 1(1,2), there is $V_i \in \mathrm{PCh}^{\mathcal{G}}(V_j)$ or there exists $V_i' \in \mathbf{V}_p \backslash \{V_i\}$ s.t. $\mathrm{P}^3\mathrm{Ch}^{\mathcal{G}}(V_j) = \{\{V_i, V_i'\}\}$. According to the definition of pure children and paired pseudo-pure children, we can conclude that $\mathrm{Pa}^{\mathcal{G}}(V_i) = \{V_j\} = \mathrm{Pa}^{\mathcal{H}_1}(V_i)$ or $\mathrm{Pa}^{\mathcal{G}}(V_i) = \{V_j, V_i'\} = \mathrm{Pa}^{\mathcal{H}_1}(V_i) \cup \{V_i'\}$ and $\mathrm{Ch}^{\mathcal{G}}(V_i) = \mathrm{PCh}^{\mathcal{G}}(V_i) = \mathrm{Pa}^{\mathcal{H}_1}(V_i)$ or $\mathrm{Ch}^{\mathcal{G}}(V_i) = \{V_j, V_i'\} = \mathrm{Ch}^{\mathcal{H}_1}(V_i) \cup \{V_i'\}$, this completes the proof of (1).

Second, if $V_i \in \mathbf{V}_f$, based on (1), then $\mathrm{Ch}^{\mathcal{G}}(V_i) \subset \mathbf{V}_c \cup \mathbf{V}_f$ and $\mathrm{Pa}^{\mathcal{G}}(V_i) \subset \mathbf{V}_c \cup \mathbf{V}_f$, which is equivalent to $\mathrm{Ch}^{\mathcal{G}}(V_i) = \mathrm{Ch}^{\mathcal{H}_2}(V_i)$ and $\mathrm{Pa}^{\mathcal{G}}(V_i) = \mathrm{Pa}^{\mathcal{H}_2}(V_i)$, this completes the proof of (2). □

Corollary 4. *$\forall V \in \mathbf{V}_f$, $|\mathrm{De}^{\mathcal{H}_2}_{\mathbf{V}_c}(V)| \geq 2$. If $|\mathrm{De}^{\mathcal{H}_2}_{\mathbf{V}_c}(V)| = 2$, $\mathrm{De}^{\mathcal{H}_2}_{\mathbf{V}_c}(V) = \mathrm{Ch}^{\mathcal{G}}(V)$.*

Remark. This is a variant of Cor. 2 in App. C.2.1, where "pure descendants" and "pure children" in Cor. 2 degenerate to "descendants" and "children" here. Although this is not sufficient to identify variables in $\mathbf{V}_f$, we can still infer some of their properties through analyzing variables in $\mathbf{V}_c$.

Proof. For any $V \in \mathbf{V}_f \cup \mathbf{V}_c$ and $\mathrm{Ch}^{\mathcal{H}_2}(V) = \emptyset$, $V \in \mathbf{V}_c$. Conversely, if $V \notin \mathbf{V}_c$, there is $V \in \mathbf{V}_f \subset \mathbf{L}$ and $\mathrm{Ch}^{\mathcal{G}}(V) = \mathrm{Ch}^{\mathcal{H}_2}(V) = \emptyset$, contradicting Asmp. 2(1). That is, $\mathbf{V}_c$ is a bottleneck from $\mathbf{V}_c \cup \mathbf{V}_f$ to $\mathbf{V}_c \cup \mathbf{V}_p$, so for any $\mathbf{V}' \subset \mathbf{V}_c \cup \mathbf{V}_f$, $\bigcup \mathrm{GDe}^{\mathcal{G}}_{\mathbf{V}_c}(\mathbf{V}')$ is a bottleneck from $\mathbf{V}'$ to $\mathbf{O}$ given that $\mathbf{O} \subset \mathbf{V}_c \cup \mathbf{V}_p$. For any $V \in \mathbf{V}_f$, $\mathrm{Ch}^{\mathcal{G}}(V) = \mathrm{Ch}^{\mathcal{H}_2}(V) \subset \mathbf{V}_c \cup \mathbf{V}_f$, so $\mathrm{De}^{\mathcal{H}_2}_{\mathbf{V}_c}(V) = \bigcup \mathrm{GDe}^{\mathcal{G}}_{\mathbf{V}_c}(\mathrm{Ch}^{\mathcal{G}}(V))$ is a bottleneck from $\mathrm{Ch}^{\mathcal{G}}(V)$ to $\mathbf{O}$. Based on Asmp. 2(1,2), we have $|\mathrm{De}^{\mathcal{H}_2}_{\mathbf{V}_c}(V)| \geq |\mathrm{Ch}^{\mathcal{G}}(V)| \geq 2$. Furthermore, the first "$\geq$" becomes "$=$" iff $\mathrm{De}^{\mathcal{H}_2}_{\mathbf{V}_c}(V) = \mathrm{Ch}^{\mathcal{G}}(V)$ because of Asmp. 2(2). □

Theorem 8. $\forall \{V_i, V_j\} \subset \mathbf{V}_c$, $\{V_i, V_j\} \in \mathbb{S}$ iff there exists $V_k \in \mathbf{V}_c \backslash \{V_i, V_j\}$ s.t. $\mathrm{Cov}(V_i, V_j)\mathrm{Cov}(V_i, V_k)\mathrm{Cov}(V_j, V_k) \neq 0$ and for each such V_k, $\mathrm{R}(V_i, V_j | V_k) \perp\!\!\!\perp \mathbf{V}_c \backslash \{V_i, V_j\}$.

Proof. "Only if"

(1) Suppose $\{V_i, V_j\} \in \mathbb{S}_1$. The proof is similar to case (1) of "only if" part in proof of Thm. 1, except that we obtain $\mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k) \backslash \{V_i, V_j\} \neq \emptyset$ in a different way[4].

(2) Suppose $\{V_i, V_j\} \in \mathbb{S}_2$. The proof is similar to case (2) of "only if" part in proof of Thm. 1, except that we obtain $\mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_l) \backslash \{V_i, V_j\} \neq \emptyset$ similarly to fn. 4.

(3) Suppose $\{V_i, V_j\} \in \mathbb{S}_3$. The proof is similar to case (3) of "only if" part in proof of Thm. 1, except that we obtain $\mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k) \backslash \{V_i, V_j\} \neq \emptyset$ in a different way[5].

"If". We prove this part by contradiction. Suppose $\{V_i, V_j\} \notin \mathbb{S}$.

(1) Suppose $V_i \notin \mathrm{Ne}^{\mathcal{H}_2}(V_j)$. All possible cases are as follows.

[4]There are three possible cases. (1) If $V_k \in \mathbf{V}_c$, we have $V_k \in \mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k) \backslash \{V_i, V_j\} \neq \emptyset$. (2) If $V_k \in \mathbf{V}_f$ and $\{V_i, V_j\} \not\subset \mathrm{De}^{\mathcal{H}_2}(V_k)$, based on Cor. 4, we have $\mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k) \backslash \{V_i, V_j\} \neq \emptyset$. (3) If $V_k \in \mathbf{V}_f$ and $\{V_i, V_j\} \subset \mathrm{De}^{\mathcal{H}_2}(V_k)$, since $V_j \notin \mathrm{Ch}^{\mathcal{G}}(V_k)$, based on Cor. 4, we have $\mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k) \backslash \{V_i, V_j\} \neq \emptyset$.

[5]If $V_k \in \mathbf{V}_c$, then $V_k \in \mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k) \backslash \{V_i, V_j\} \neq \emptyset$. If $V_k \in \mathbf{V}_f \subset \mathbf{L}$, suppose $\mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k) \backslash \{V_i, V_j\} = \emptyset$, base on Cor. 4, $\mathrm{Ch}^{\mathcal{G}}(V_k) = \{V_i, V_j\}$, which leads to $\mathrm{Ch}^{\mathcal{G}}(V_k) \subset \mathrm{Ch}^{\mathcal{G}}(V_i) \cup \{V_i\}$, contradicting Asmp. 2(1).

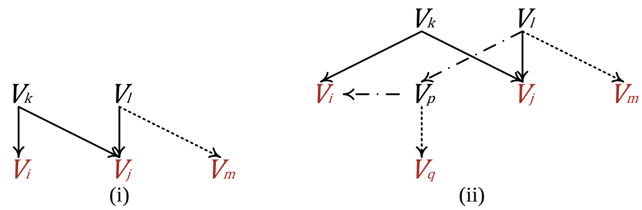


Figure 12: Illustration of case (1.b.ii) of "if" part in proof of Thm. 8. A dotted arrow from V_1 to V_2 means that $V_2 \in \mathrm{GDe}^{\mathcal{H}_2}(V_1)$. A dot-dash arrow from V_1 to V_2 means that $V_2 \in \mathrm{De}^{\mathcal{H}_2}(V_1)$. V is marked in red if $V \in \mathbf{V}_c$.

(a) Suppose $\mathrm{Ch}^{\mathcal{H}_2}(V_i) \neq \emptyset$ or $\mathrm{Ch}^{\mathcal{H}_2}(V_j) \neq \emptyset$. The proof is similar to case (1.a) of "if" part in proof of Thm. 1, except that we obtain $\mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k)\backslash\{V_i, V_j\} \neq \emptyset$ similarly to fn. 4.

(b) Suppose $\mathrm{Ch}^{\mathcal{H}_2}(V_i) = \mathrm{Ch}^{\mathcal{H}_2}(V_j) = \emptyset$, $\mathrm{Pa}^{\mathcal{H}_2}(V_i) \neq \emptyset$ and $\mathrm{Pa}^{\mathcal{H}_2}(V_j) \neq \emptyset$. Since $\{V_i, V_j\} \notin \mathbb{S}_2$, there are two possible cases. This is different from case (1.b) of "if" part in proof of Thm. 1 because without Asmp. 1, there may exist L s.t. $|\mathrm{Ne}^{\mathcal{G}}(L)| < 3$.

  (i) Suppose $\mathrm{Pa}^{\mathcal{H}_2}(V_i) = \mathrm{Pa}^{\mathcal{H}_2}(V_j) = \{V_k\}$ where $V_k \in \mathbf{V}_f$ and $\mathrm{Ne}^{\mathcal{H}_2}(V_k)\backslash\{V_i, V_j\} = \emptyset$. Clearly, for any $V \in \mathbf{V}_c\backslash\{V_i, V_j\}$, $\mathrm{Cov}(V, V_i) = 0$, which leads to contradiction.

  (ii) Suppose there exists $\{V_k, V_l\} \subset \mathbf{V}_c \cup \mathbf{V}_f\backslash\{V_i, V_j\}$ s.t. $V_k \in \mathrm{Pa}^{\mathcal{H}_2}(V_i)$ and $V_l \in \mathrm{Pa}^{\mathcal{H}_2}(V_j)$. If $\mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k)\backslash\{V_i, V_j\} \neq \emptyset$ and $\mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_l)\backslash\{V_i, V_j\} \neq \emptyset$, the proof is similar to case (1.b) of "if" part in proof of Thm. 1. Otherwise, let $\mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k)\backslash\{V_i, V_j\} = \emptyset$ without loss of generality, then we have $V_k \in \mathbf{V}_f \subset \mathbf{L}$ and $\mathrm{Ch}^{\mathcal{G}}(V_k) = \{V_i, V_j\}$ based on Cor. 4. Also, based on Asmp. 2(1), $\mathrm{Ch}^{\mathcal{G}}(V_k) \not\subset \mathrm{Ch}^{\mathcal{G}}(V_l)$, so $V_i \notin \mathrm{Ch}^{\mathcal{H}_2}(V_l)$, we have $\mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_l)\backslash\{V_i, V_j\} \neq \emptyset$ based on Cor. 4 and let $V_m \in \mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_l)\backslash\{V_i, V_j\}$. An illustrative example is shown as Fig. 12(i).

  - Suppose $V_i \notin \mathrm{De}^{\mathcal{H}_2}(V_l)$. As $m_{jl}m_{ml} \neq 0$ and $m_{il} = 0$, for any V s.t. V, V_i, V_j are correlated to each other, $\mathrm{R}(V_i, V_j|V) \not\perp\!\!\!\perp V_m$, which leads to contradiction.
  - Suppose $V_i \in \mathrm{De}^{\mathcal{H}_2}(V_l)$, besides $V_l \notin \mathrm{Pa}^{\mathcal{H}_2}(V_i)$ as mentioned above, we can also derive $V_l \notin \mathrm{Pa}^{\mathcal{H}_2}(V_k)$[6], so there exists $V_p \neq V_k$ s.t. $V_p \in \mathrm{De}^{\mathcal{H}_2}(V_l)$ and $V_i \in \mathrm{De}^{\mathcal{H}_2}(V_p)$. Based on Asmp. 2(1), $\mathrm{Ch}^{\mathcal{G}}(V_k) \not\subset \mathrm{Ch}^{\mathcal{G}}(V_p)$, so we have $\mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_p)\backslash\{V_i, V_j\} \neq \emptyset$ similarly to fn. 4. Let $V_q \in \mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_p)\backslash\{V_i, V_j\}$ (It is possible that $V_m = V_q$). An illustrative example is shown as Fig. 12(ii). If $V_j \notin \mathrm{De}^{\mathcal{H}_2}(V_p)$, $m_{ip}m_{qp} \neq 0$ and $m_{jp} = 0$, so for any V s.t. V, V_i, V_j are correlated to each other, $\mathrm{R}(V_i, V_j|V) \not\perp\!\!\!\perp V_q$, which leads to contradiction. Otherwise, $m_{il}m_{ip}m_{jl}m_{jp} \neq 0$. Since there exist two non-intersecting directed paths from $\{V_l, V_p\}$ to $\{V_i, V_j\}$ (e.g., $V_l \to V_j$ and $V_p \to \ldots \to V_i$), $m_{il}/m_{ip} \neq m_{jl}/m_{jp}$. Also, $m_{ml}m_{qp} \neq 0$, so for any V s.t. V, V_i, V_j are correlated to each other, $\mathrm{R}(V_i, V_j|V) \not\perp\!\!\!\perp V_m$ or $\mathrm{R}(V_i, V_j|V) \not\perp\!\!\!\perp V_q$, which leads to contradiction.

(c) Suppose $\mathrm{Ne}^{\mathcal{H}_2}(V_i) = \emptyset$ or $\mathrm{Ne}^{\mathcal{H}_2}(V_j) = \emptyset$. The proof is similar to case (1.c) of "if" part in proof of Thm. 1.

(2) Suppose $V_i \in \mathrm{Pa}^{\mathcal{H}_2}(V_j)$ or $V_j \in \mathrm{Pa}^{\mathcal{H}_2}(V_i)$, we take the former as an example without loss of generality. All possible cases are as follows.

  (a) Suppose $\mathrm{Ch}^{\mathcal{H}_2}(V_j) \neq \emptyset$. The proof is similar to case (2.a) of "if" part in proof of Thm. 1, except that we obtain $\mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k)\backslash\{V_i, V_j\} \neq \emptyset$ similarly to fn. 4.

  (b) Suppose $\mathrm{Pa}^{\mathcal{H}_2}(V_j)\backslash\{V_i\} = \emptyset$ and $\mathrm{Ch}^{\mathcal{H}_2}(V_j) = \emptyset$. The proof is similar to case (2.b) of "if" part in proof of Thm. 1.

[6] We can prove this by contradiction. Suppose $V_l \in \mathrm{Pa}^{\mathcal{H}_2}(V_k)$, then $\mathrm{Ch}^{\mathcal{G}}(V_l) \cup \{V_i\}\backslash\{V_k\}$ is a bottleneck from $\mathrm{Ch}^{\mathcal{G}}(V_l)$ to $\mathbf{O}$ and $|\mathrm{Ch}^{\mathcal{G}}(V_l)| = |\mathrm{Ch}^{\mathcal{G}}(V_l) \cup \{V_i\}\backslash\{V_k\}|$, contradicting Asmp. 2(2).

(c) Suppose $\mathrm{Ch}^{\mathcal{H}_2}(V_i)\backslash\{V_j\} \neq \emptyset$, $\mathrm{Pa}^{\mathcal{H}_2}(V_j)\backslash\{V_i\} \neq \emptyset$, and $\mathrm{Ch}^{\mathcal{H}_2}(V_j) = \emptyset$. The proof is similar to case (2.c) of "if" part in proof of Thm. 1, except that we obtain $\mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k)\backslash\{V_i, V_j\} \neq \emptyset$ similarly to fn. 4 and $\mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_l)\backslash\{V_i, V_j\} \neq \emptyset$ similarly to fn. 5.

(d) Suppose $\mathrm{Pa}^{\mathcal{H}_2}(V_i) \neq \emptyset$, $\mathrm{Ch}^{\mathcal{H}_2}(V_i)\backslash\{V_j\} = \emptyset$, $\mathrm{Pa}^{\mathcal{H}_2}(V_j)\backslash\{V_i\} \neq \emptyset$, and $\mathrm{Ch}^{\mathcal{H}_2}(V_j) = \emptyset$. The proof is similar to case (2.d) of "if" part in proof of Thm. 1, except that we obtain both $\mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k)\backslash\{V_i, V_j\} \neq \emptyset$ and $\mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_l)\backslash\{V_i, V_j\} \neq \emptyset$ similarly to fn. 5.

(e) Suppose $\mathrm{Pa}^{\mathcal{H}_2}(V_i) = \emptyset$, $\mathrm{Ch}^{\mathcal{H}_2}(V_i)\backslash\{V_j\} = \emptyset$, $\mathrm{Pa}^{\mathcal{H}_2}(V_j)\backslash\{V_i\} \neq \emptyset$, and $\mathrm{Ch}^{\mathcal{H}_2}(V_j) = \emptyset$. The proof is similar to case (2.e) of "if" part in proof of Thm. 1

□

Lemma 3. $\forall\{V_i, V_j\} \in \mathbb{S}$, $\mathrm{Ch}^{\mathcal{H}_1}(V_i) \subset \mathrm{PCh}^{\mathcal{G}}(V_i)$ *and* $\mathrm{Ch}^{\mathcal{H}_1}(V_j) \subset \mathrm{PCh}^{\mathcal{G}}(V_j)$.

Remark. This lemma means that if a variable V is in an identifiable pair, then there is $\mathrm{Ch}^{\mathcal{H}_1}(V) \subset \mathrm{PCh}^{\mathcal{G}}(V)$, which is consistent with the case where Asmp. 1 holds. This significantly simplifies the complexity of the proof of some following theoretical results. For instance, with this lemma, most proof strategies employed in the proof of Thm. 2 can be directly adapted to prove Thm. 9.

Proof. The proofs are as follows.

- Suppose $\{V_i, V_j\} \in \mathbb{S}_1$ and $V_i \in \mathrm{Pa}^{\mathcal{G}}(V_j)$. First, we can easily derive that $\mathrm{Ch}^{\mathcal{H}_1}(V_j) \subset \mathrm{PCh}^{\mathcal{G}}(V_j)$[7]. Second, we suppose $\mathrm{Ch}^{\mathcal{H}_1}(V_i) \not\subset \mathrm{PCh}^{\mathcal{G}}(V_i)$ and let $V_k \in \mathrm{Ne}^{\mathcal{H}_2}(V_i)\backslash\{V_j\}$. Similarly to fn. 4, we have $\mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k)\backslash\{V_i, V_j\} \neq \emptyset$ and let $V_l \in \mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k)\backslash\{V_i, V_j\}$. Clearly, there is $V_j \in \mathrm{P}^2\mathrm{De}^{\mathcal{G}}(V_i)$, $V_l \not\perp\!\!\!\perp V_i$, and $V_j \perp\!\!\!\perp V_l | V_i$, contradicting Cond. 3(2).
- Suppose $\{V_i, V_j\} \in \mathbb{S}_2$, similarly to fn. 7, we can easily derive that $\mathrm{Ch}^{\mathcal{H}_1}(V_i) \subset \mathrm{PCh}^{\mathcal{G}}(V_i)$ and $\mathrm{Ch}^{\mathcal{H}_1}(V_j) \subset \mathrm{PCh}^{\mathcal{G}}(V_j)$.
- Suppose $\{V_i, V_j\} \in \mathbb{S}_3$ and $V_i \in \mathrm{Pa}^{\mathcal{G}}(V_j)$. First, we can easily derive that $\mathrm{Ch}^{\mathcal{H}_1}(V_j) \subset \mathrm{PCh}^{\mathcal{G}}(V_j)$ similarly to fn. 7. Second, suppose $\mathrm{Ch}^{\mathcal{H}_1}(V_i) \not\subset \mathrm{PCh}^{\mathcal{G}}(V_i)$, based on Cond. 3(2), we have $\{\mathrm{Ch}^{\mathcal{H}_1}(V_i)\} = \mathrm{P}^3\mathrm{Ch}^{\mathcal{G}}(V_i)$, so $V_i \notin \mathbf{O}$, that is, $V_i \in \mathbf{L}$. Clearly, V_i is a I-PV. This leads to contradiction to Asmp. 2(3).

□

Theorem 9. $\forall\{V_i, V_j\} \in \mathbb{S}$, let $\{V_{i_1}, V_{i_2}\} \subset \mathrm{Ch}^{\mathcal{H}_1}(V_i)$.

(1) $\mathrm{R}(V_{i_1}, V_j | V_{i_2}) \perp\!\!\!\perp V_{i_2}$ iff $\{V_i, V_j\} \in \mathbb{S}_1$ and $V_i \in \mathrm{Pa}^{\mathcal{G}}(V_j)$.

(2) Suppose $\{V_i, V_j\} \notin \mathbb{S}_1$, $\exists\{V'_i, V'_j\} \in \mathbb{S}\backslash\{\{V_i, V_j\}\}$ s.t. $\{V'_i, V'_j\} \cap \{V_i, V_j\} \neq \emptyset$ only if (but not if) $\{V_i, V_j\} \in \mathbb{S}_2$.

(3) Suppose $\{V_i, V_j\} \notin \mathbb{S}_1$, $\exists\{V_k, V_l\} \subset \bigcup \mathrm{Ch}^{\mathcal{H}_1}(\mathbf{V}_c\backslash\{V_i, V_j\})$ s.t. $(V_{i_1}, V_{i_2}, V_j, V_k, V_l)$ satisfies the quintuple constraint only if (but not if) $\{V_i, V_j\} \in \mathbb{S}_3$ and $V_i \in \mathrm{Pa}^{\mathcal{G}}(V_j)$

Proof. Combined with Lem. 3, the proofs of (1), (2), and "only if" part of (3) are similar to Thm. 2. Here we focus on "not if" part of (3).

[7] Suppose $\mathrm{Ch}^{\mathcal{H}_1}(V_j) \not\subset \mathrm{PCh}^{\mathcal{G}}(V_j)$, based on Cond. 3(2), we have $\{\mathrm{Ch}^{\mathcal{H}_1}(V_j)\} = \mathrm{P}^3\mathrm{Ch}^{\mathcal{G}}(V_j)$, so $V_j \notin \mathbf{O}$, that is, $V_j \in \mathbf{L}$. Let $\mathrm{Ch}^{\mathcal{H}_1}(V_j) = \{V_k, V_l\}$ where $V_k \in \mathrm{Pa}^{\mathcal{G}}(V_l)$, then $\mathrm{Ch}^{\mathcal{G}}(V_j) = \mathrm{Ch}^{\mathcal{H}_1}(V_j) \cup \mathrm{Ch}^{\mathcal{H}_2}(V_j) = \{V_k, V_l\}$. There is $\mathrm{Ch}^{\mathcal{G}}(V_j) \subset \{V_k\} \cup \mathrm{Ch}^{\mathcal{G}}(V_k)$, contradicting Asmp. 2(1).

Suppose $\mathcal{G}_0$ is shown as Fig. 8(c), at the first iteration when $\mathbf{V}_c = \{O_2, ..., O_6\}$, $\{O_2, O_3\} \in \mathbb{S}_3$ and $O_2 \in \mathrm{Pa}^{\mathcal{G}}(O_3)$. Let $\{O_{2_1}, O_{2_2}\} \subset \mathrm{Ch}^{\mathcal{H}_1}(O_2)$, then O_{2_1}, O_{2_2}, O_3 can be expressed as

$$O_{2_1} = a_{21}a_{2_12}L_1 + a_{2_12}\epsilon_{O_2} + \epsilon_{O_{2_1}}, \tag{25}$$

$$O_{2_2} = a_{21}a_{2_22}L_1 + a_{2_22}\epsilon_{O_2} + \epsilon_{O_{2_2}}, \tag{26}$$

$$O_3 = (a_{21}a_{32} + a_{31})L_1 + a_{32}\epsilon_{O_2} + \epsilon_{O_3}. \tag{27}$$

Because $a_{31} \neq 0$, $a_{21}a_{2_12}/(a_{21}a_{32} + a_{31}) \neq a_{2_12}/a_{32}$. For any $\{O_i, O_j\} \in \bigcup \mathrm{Ch}^{\mathcal{H}_1}(\mathbf{V}_c \backslash \{O_2, O_3\})$, they can be expressed as

$$O_i = \lambda_i L_1 + (\gamma_i \epsilon_{O_4} + e'_i), \quad O_j = \lambda_j L_1 + (\gamma_j \epsilon_{O_4} + e'_j), \tag{28}$$

where $L_1, \epsilon_{O_2}, \epsilon_{O_{2_1}}, \epsilon_{O_{2_2}}, \epsilon_{O_3}, \gamma_i\epsilon_{O_4} + e'_i$ are independent of each other, $O_j \perp\!\!\!\perp \{\epsilon_{O_3}, \epsilon_{O_{2_1}}, \epsilon_{O_{2_2}}, \epsilon_{O_3}\}$ and $\mathrm{Cov}(O_j, L_1)\mathrm{Cov}(O_j, \gamma_i\epsilon_{O_4} + e'_i) \neq 0$. Based on Lem. 2(2.b), $(O_{2_1}, O_{2_2}, O_3, O_i, O_j)$ does not satisfy the quintuple constraint. □

Corollary 5. *Given $\{V_i, V_j\} \in \mathbb{S}_3$ and $V_i \in \mathrm{Pa}^{\mathcal{G}}(V_j)$, let $\mathrm{Pa}^{\mathcal{H}_2}(V_i) = \{V_h\}$ and $\{V_{i_1}, V_{i_2}\} \subset \mathrm{Ch}^{\mathcal{H}_1}(V_i)$.*

(1) If $V_h \in \mathbf{V}_c$, then $\exists\{V_k, V_l\} \subset \mathrm{Ch}^{\mathcal{H}_1}(\mathbf{V}_c \backslash \{V_i, V_j\})$ s.t. $(V_{i_1}, V_{i_2}, V_j, V_k, V_l)$ satisfies the quintuple constraint.

(2) If $\exists\{V_m, V_n\} \subset \mathbf{V}_c \backslash \{V_i, V_j\}$ s.t. $V_m \in \mathrm{P^2De}^{\mathcal{H}_2}(V_h)$, $V_n \not\perp\!\!\!\perp V_h$, and $V_m \perp\!\!\!\perp V_n | V_h$, then $\exists\{V_k, V_l\} \subset \mathrm{Ch}^{\mathcal{H}_1}(\mathbf{V}_c \backslash \{V_i, V_j\})$ s.t. $(V_{i_1}, V_{i_2}, V_j, V_k, V_l)$ satisfies the quintuple constraint.

Remark. Given $\{V_i, V_j\} \in \mathbb{S}_3$ and $V_i \in \mathrm{Pa}^{\mathcal{G}}(V_j)$, based on Rem. of Thm. 9 in the main text, both $\{V_i, V_j\} \in \tilde{\mathbb{S}}_2$ and $\{V_i, V_j\} \in \tilde{\mathbb{S}}_3$ are possible. This corollary provides two sufficient conditions that $\exists\{V_k, V_l\} \subset \mathrm{Ch}^{\mathcal{H}_1}(\mathbf{V}_c \backslash \{V_i, V_j\})$ s.t. $(V_{i_1}, V_{i_2}, V_j, V_k, V_l)$ satisfies the quintuple constraint, that is, $\{V_i, V_j\} \in \tilde{\mathbb{S}}_3$. The proof of the following Thm. 10 highly relies on this corollary.

Proof. The proofs are as follows.

(1) We first prove $\mathrm{Ch}^{\mathcal{H}_1}(V_h) \subset \mathrm{PCh}^{\mathcal{G}}(V_h)$ by contradiction. Suppose $\mathrm{Ch}^{\mathcal{H}_1}(V_h) \not\subset \mathrm{PCh}^{\mathcal{G}}(V_h)$, then based on Cond. 3(2), $\{\mathrm{Ch}^{\mathcal{H}_1}(V_h)\} = \mathrm{P^3Ch}^{\mathcal{G}}(V_h)$. In addition, since $\{V_i, V_j\} \in \mathbb{S}_3$, we have $\mathrm{Ch}^{\mathcal{H}_1}(V_i) \subset \mathrm{PCh}^{\mathcal{G}}(V_i)$ and $\mathrm{Ch}^{\mathcal{H}_1}(V_j) \subset \mathrm{PCh}^{\mathcal{G}}(V_j)$ based on Lem. 3, so $\{V_i, V_j\} \in \mathrm{P^3Ch}^{\mathcal{G}}(V_h) = \{\mathrm{Ch}^{\mathcal{H}_1}(V_h)\}$, which leads to contradiction. Therefore, $\mathrm{Ch}^{\mathcal{H}_1}(V_h) \subset \mathrm{PCh}^{\mathcal{G}}(V_h)$. Let $\{V_k, V_l\} \subset \mathrm{Ch}^{\mathcal{H}_1}(V_h)$, then the proof is similar to "'if' of (3)" part in proof of Thm. 2.

(2) Let $V_k \in \mathrm{Ch}^{\mathcal{H}_1}(V_m)$ and $V_l \in \mathrm{Ch}^{\mathcal{H}_1}(V_n)$, then the proof is similar to "'if' of (3)" part in proof of Thm. 2.

□

Theorem 10. (1) $\forall\{V_i, V_j\} \in \tilde{\mathbb{S}}_2$, $\bigcap \mathrm{Pa}^{\mathcal{G}}(\{V_i, V_j\}) \subset \mathbf{V}_c$ iff $\exists\{V'_i, V'_j\} \in \tilde{\mathbb{S}}_1$ s.t. $\{V_i, V_j\} \cap \{V'_i, V'_j\} \neq \emptyset$. (2) $\forall\{\{V_i, V_j\}, \{V'_i, V'_j\}\} \subset \tilde{\mathbb{S}}_2$, $\bigcap \mathrm{Pa}^{\mathcal{G}}(\{V_i, V_j\}) = \bigcap \mathrm{Pa}^{\mathcal{G}}(\{V'_i, V'_j\})$ iff $\exists\{V''_i, V''_j\} \in \tilde{\mathbb{S}}_2$ s.t. $\{V_i, V_j\} \cap \{V''_i, V''_j\} \neq \emptyset$ and $\{V'_i, V'_j\} \cap \{V''_i, V''_j\} \neq \emptyset$.

Proof. As mentioned in Rem. of Thm. 9 in the main text, $\tilde{\mathbb{S}}_1 = \mathbb{S}_1$, $\tilde{\mathbb{S}}_2 \supset \mathbb{S}_2$, $\tilde{\mathbb{S}}_3 \subset \mathbb{S}_3$.

- For any $\{V_i, V_j\} \in \mathbb{S}_2 \subset \tilde{\mathbb{S}}_2$, (1) can be derived from the definitions of $\mathbb{S}_1$ and $\mathbb{S}_2$.
- For $\{V_i, V_j\} \in \tilde{\mathbb{S}}_2 \backslash \mathbb{S}_2$, the proof of (1) is as follows. Clearly, $\{V_i, V_j\} \in \mathbb{S}_3$. First, based on the definition of $\mathbb{S}_1$, $\forall\{V'_i, V'_j\} \in \tilde{\mathbb{S}}_1 = \mathbb{S}_1$, $\{V_i, V_j\} \cap \{V'_i, V'_j\} = \emptyset$. Second, based on Cor. 5(1), $\bigcap \mathrm{Pa}^{\mathcal{H}_2}(\{V_i, V_j\}) \not\subset \mathbf{V}_c$, otherwise $\{V_i, V_j\} \in \tilde{\mathbb{S}}_3$, which leads to contradiction. This finishes the proof.
- For any $\{\{V_i, V_j\}, \{V'_i, V'_j\}\} \subset \mathbb{S}_2 \subset \tilde{\mathbb{S}}_2$, (2) can be derived from the definition of $\mathbb{S}_2$.

- For $\{V_i, V_j\} \in \tilde{\mathbb{S}}_2 \backslash \mathbb{S}_2$, the proof of (2) is as follows. Clearly, $\{V_i, V_j\} \in \mathbb{S}_3$. First, based on the definitions of $\mathbb{S}_2$ and $\mathbb{S}_3$, $\forall \{V_i', V_j'\} \in \tilde{\mathbb{S}}_2 \backslash \{\{V_i, V_j\}\} \subset \mathbb{S}_2 \cup \mathbb{S}_3 \backslash \{\{V_i, V_j\}\}$, $\{V_i, V_j\} \cap \{V_i', V_j'\} = \emptyset$. Second, we prove $\forall \{V_i', V_j'\} \in \tilde{\mathbb{S}}_2 \backslash \{\{V_i, V_j\}\}$, $\bigcap \mathrm{Pa}^{\mathcal{H}_2}(\{V_i, V_j\}) \neq \bigcap \mathrm{Pa}^{\mathcal{H}_2}(\{V_i', V_j'\})$ by contradiction. Let $\bigcap \mathrm{Pa}^{\mathcal{H}_2}(\{V_i, V_j\}) = \{V_h\}$ and suppose $\bigcap \mathrm{Pa}^{\mathcal{H}_2}(\{V_i', V_j'\}) = \{V_h\}$. First, we have $V_h \in \mathbf{V}_f \subset \mathbf{L}$, otherwise $\{V_i, V_j\} \in \tilde{\mathbb{S}}_3$ based on Cor. 5(1), which leads to contradiction. Second, we also have $\{V_i', V_j'\} \in \mathbb{S}_3$, otherwise let $\{V_i', V_j'\} = \{V_m, V_n\} \in \mathbb{S}_2$, we have $V_m \in \mathrm{P}^2\mathrm{De}^{\mathcal{G}}(V_h)$, $V_n \not\perp\!\!\!\perp V_h$, and $V_m \perp\!\!\!\perp V_n | V_h$, so $\{V_i, V_j\} \in \tilde{\mathbb{S}}_3$ based on Cor. 5(2), which leads to contradiction. Because V_h is not a II-PV based on Asmp. 2(3), there exists $V_k \in \mathrm{Ne}^{\mathcal{H}_2}(V_h) \backslash (\{V_i, V_j\} \cup \{V_i', V_j'\})$ and we can derive $\mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k) \backslash (\{V_i, V_j\} \cup \{V_i', V_j'\}) \neq \emptyset$[8]. Let $V_m \in \{V_i', V_j'\}$ and $V_n \in \mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k) \backslash (\{V_i, V_j\} \cup \{V_i', V_j'\})$, since $V_m \in \mathrm{P}^2\mathrm{De}^{\mathcal{G}}(V_k)$, $V_n \not\perp\!\!\!\perp V_k$, and $V_m \perp\!\!\!\perp V_n | V_k$, $\{V_i, V_j\} \in \tilde{\mathbb{S}}_3$ based on Cor. 5(2), which leads to contradiction.

$\square$

Proposition 4. *Cond. 3 is still valid after update.*

Proof. We denote $\mathbf{V}_p, \mathbf{V}_c, \mathbf{V}_f, \mathcal{H}_1, \mathcal{H}_2$ after update by $\mathbf{V}_p', \mathbf{V}_c', \mathbf{V}_f', \mathcal{H}_1', \mathcal{H}_2'$ respectively. While Cond. 3 is valid for $\mathbf{V}_p' \cap \mathbf{V}_p$ and $\mathbf{V}_c' \cap \mathbf{V}_c$ trivially, we focus on $\mathbf{V}_p' \backslash \mathbf{V}_p$ and $\mathbf{V}_c' \backslash \mathbf{V}_c$.

- If $V_j \in \mathbf{V}_p' \backslash \mathbf{V}_p$, then $V_j \in \mathbf{V}_c$ and there exists $V_i \in \mathbf{V}_c$ s.t. (1) $\{V_i, V_j\} \in \tilde{\mathbb{S}}_1$ and $V_i \in \mathrm{Pa}^{\mathcal{H}_2}(V_j)$ or (2) $\{V_i, V_j\} \in \tilde{\mathbb{S}}_2$. Based on Lem. 3, $\mathrm{Ch}^{\mathcal{H}_1}(V_j) \subset \mathrm{PCh}^{\mathcal{G}}(V_j)$, then the proof is similar to part 1 in proof of Prop. 2.
- If $V_j \in \mathbf{V}_c' \backslash \mathbf{V}_c$, then $V_j \in \mathbf{V}_f$, $|\mathrm{Ch}^{\mathcal{H}_1'}(V_j)| \geq 2$, and $\forall \{V_k, V_l\} \subset \mathrm{Ch}^{\mathcal{H}_1'}(V_j)$, $\{V_k, V_l\} \in \tilde{\mathbb{S}}_2$ and $\bigcap \mathrm{Pa}^{\mathcal{H}_2}(\{V_k, V_l\}) = \{V_j\}$. Also, we have $\forall V \in \mathrm{Ch}^{\mathcal{H}_1'}(V_j)$, $\mathrm{Ch}^{\mathcal{H}_1}(V) \subset \mathrm{PCh}^{\mathcal{G}}(V)$ based on Lem. 3. Furthermore, based on Thm. 10, there are two possible cases.
  - $\forall \{V_k, V_l\} \subset \mathrm{Ch}^{\mathcal{H}_1'}(V_j)$, $\{V_k, V_l\} \in \mathbb{S}_2$. In this case, it is trivial that $\mathrm{Ch}^{\mathcal{H}_1'}(V_j) \subset \mathrm{PCh}^{\mathcal{G}}(V_j)$.
  - $|\mathrm{Ch}^{\mathcal{H}_1'}(V_j)| = 2$ and $\mathrm{Ch}^{\mathcal{H}_1'}(V_j) \in \mathbb{S}_3$. In this case, it is trivial that $\mathrm{Ch}^{\mathcal{H}_1'}(V_j) \in \mathrm{P}^3\mathrm{Ch}^{\mathcal{G}}(V_j)$. Now we prove $\{\mathrm{Ch}^{\mathcal{H}_1'}(V_j)\} = \mathrm{P}^3\mathrm{Ch}^{\mathcal{G}}(V_j)$ by contradiction. Let $\mathrm{Ch}^{\mathcal{H}_1'}(V_j) = \{V_{j_1}, V_{j_2}\}$ and suppose there exists $\{V_k, V_l\} \in \mathrm{P}^3\mathrm{Ch}^{\mathcal{G}}(V_j) \backslash \{\{V_{j_1}, V_{j_2}\}\}$. Similarly to fn. 4, we have $\mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k) \backslash \{V_{j_1}, V_{j_2}\} \neq \emptyset$ and let $V_m \in \mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k) \backslash \{V_{j_1}, V_{j_2}\}$. Because V_j is not a II-PV based on Asmp. 2(3), there exists $V_i \in \mathrm{Ne}^{\mathcal{H}_2}(V_h) \backslash \{V_{j_1}, V_{j_2}, V_k, V_l\}$. Similarly to fn. 8, we have $\mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_i) \backslash \{V_{j_1}, V_{j_2}, V_m\} \neq \emptyset$ and let $V_n \in \mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_i) \backslash \{V_{j_1}, V_{j_2}, V_m\}$. Clearly, $V_m \in \mathrm{P}^2\mathrm{De}^{\mathcal{H}_2}(V_j)$, $V_n \not\perp\!\!\!\perp V_j$, and $V_m \perp\!\!\!\perp V_n | V_j$, so $\{V_{j_1}, V_{j_2}\} \in \tilde{\mathbb{S}}_3$ based on Cor. 5(2), which leads to contradiction. Therefore, $\{\mathrm{Ch}^{\mathcal{H}_1'}(V_j)\} = \mathrm{P}^3\mathrm{Ch}^{\mathcal{G}}(V_j)$. Likewise, $\nexists \{V_k, V_l\} \subset \mathbf{V}_c' \backslash \{V_j\}$ s.t. $V_k \in \mathrm{P}^2\mathrm{De}^{\mathcal{G}}(V_j)$, $V_l \not\perp\!\!\!\perp V_j$, and $V_k \perp\!\!\!\perp V_l | V_j$, otherwise there is also $\{V_{j_1}, V_{j_2}\} \in \tilde{\mathbb{S}}_3$, which leads to contradiction.

  Finally, it is trivial that $\mathrm{Pa}^{\mathcal{H}_1'}(V_j) = \emptyset$.

$\square$

[8] There are three possible cases. (1) If $V_k \in \mathbf{V}_c$, then $V_k \in \mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k) \backslash (\{V_i, V_j\} \cup \{V_i', V_j'\}) \neq \emptyset$. (2) If $V_k \in \mathbf{V}_f$ and $V_k \in \mathrm{Ch}^{\mathcal{H}_2}(V_h)$, then $\mathrm{De}^{\mathcal{H}_2}(V_k) \cap (\{V_i, V_j\} \cup \{V_i', V_j'\}) = \emptyset$, so $\mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k) \backslash (\{V_i, V_j\} \cup \{V_i', V_j'\}) \neq \emptyset$ based on Cor. 4. (3) If $V_k \in \mathbf{V}_f$ and $V_k \in \mathrm{Pa}^{\mathcal{H}_2}(V_h)$, then $\mathrm{De}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k) \backslash (\{V_i, V_j\} \cup \{V_i', V_j'\}) \cup \{V_h\}$ is a bottleneck from $\mathrm{Ch}^{\mathcal{G}}(V_k)$ to $\mathbf{O}$, so $|\mathrm{De}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k) \backslash (\{V_i, V_j\} \cup \{V_i', V_j'\}) \cup \{V_h\}| \geq |\mathrm{Ch}^{\mathcal{G}}(V_k)| \geq 2$ based on Asmp. 2(1,2), so $\mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_k) \backslash (\{V_i, V_j\} \cup \{V_i', V_j'\}) \neq \emptyset$.

Theorem 11. If Asmp. 1 is invalid, when $\tilde{\mathbb{S}}_1 \cup \tilde{\mathbb{S}}_2 = \emptyset$, $\mathbf{V}_f \neq \emptyset$ or there exists $L \in \mathbf{V}_c$ s.t. $\mathrm{Ch}^{\mathcal{H}_1}(L) \not\subset \mathrm{PCh}^{\mathcal{G}}(L)$.

Proof. The proofs are as follows.

- Suppose $\exists L_i \in \mathbf{L}$ s.t. $|\mathrm{PCh}^{\mathcal{G}}(L_i)| < 2$. If $\mathrm{P}^3\mathrm{Ch}^{\mathcal{G}}(L_i) \neq \emptyset$,
  - It is possible that $L_i \in \mathbf{V}_f$, e.g., when no pair in $\mathrm{P}^3\mathrm{Ch}^{\mathcal{G}}(L_i)$ is incorporated into $\tilde{\mathbb{S}}_2$.
  - It is possible that $L_i \in \mathbf{V}_c$, an example is shown as Fig. 8(d). In this case, there must be $\mathrm{Ch}^{\mathcal{H}_1}(L_i) \not\subset \mathrm{PCh}^{\mathcal{G}}(L_i)$ because $|\mathrm{PCh}^{\mathcal{G}}(L_i)| < 2$ but $|\mathrm{Ch}^{\mathcal{H}_1}(L_i)| \geq 2$ based on Cond. 3(2).
  - It is impossible that $L_i \in \mathbf{V}_p$. Since L_i is not a pure child of any other variable, if $L_i \in \mathbf{V}_p$, this leads to contradiction to Cond. 3(1).

  Otherwise, there is $L_i \in \mathbf{V}_f$ trivially.

- Suppose $\forall L \in \mathbf{L}$, $|\mathrm{PCh}^{\mathcal{G}}(L)| \geq 2$. Since Asmp. 1 is invalid, $\exists L_i \in \mathbf{L}$ s.t. $|\mathrm{Ne}^{\mathcal{G}}(L_i)| < 3$, that is, $|\mathrm{PCh}^{\mathcal{G}}(L_i)| = 2$ and $\mathrm{Ne}^{\mathcal{G}}(L_i) \backslash \mathrm{PCh}^{\mathcal{G}}(L_i) = \emptyset$. According to the definition of identifiable pairs (Def. 2), there is always $\mathrm{PCh}^{\mathcal{G}}(L_i) \notin \mathbb{S}$, so there is always $L_i \in \mathbf{V}_f$.

□

Corollary 6. *If Asmp. 1 is invalid, when $\tilde{\mathbb{S}}_1 \cup \tilde{\mathbb{S}}_2 = \emptyset$, (1) $\forall V_i \in \mathbf{V}_f, |\mathrm{De}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_i)| \geq 2$. (2) $\forall V_i \in \mathbf{V}_c$ s.t. $\mathrm{Ch}^{\mathcal{H}_1}(V_i) \not\subset \mathrm{PCh}^{\mathcal{G}}(V_i)$, $|\mathrm{De}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_i)| \geq 1$.*

Remark. This lemma means that at the end of stage 1, (1) for any $V_i \in \mathbf{V}_c$, V_i has at least two descendants in $\mathbf{V}_c$ and (2) for any $\forall V_i \in \mathbf{V}_c$ s.t. $\mathrm{Ch}^{\mathcal{H}_1}(V_i) \not\subset \mathrm{PCh}^{\mathcal{G}}(V_i)$, V_i has at least one descendant in $\mathbf{V}_c$. This corollary is important for the proofs of the following Thms. 12 and 13.

Proof. The proofs are as follows.

(1) This directly follows Cor. 4.

(2) Based on Cond. 3(2), $\{\mathrm{Ch}^{\mathcal{H}_1}(V_i)\} = \mathrm{P}^3\mathrm{Ch}^{\mathcal{G}}(V_i)$, then we can prove $\mathrm{Ch}^{\mathcal{H}_2}(V_i) \neq \emptyset$ by contradiction similarly to fn. 7. Let $V_j \in \mathrm{Ch}^{\mathcal{H}_2}(V_i)$, we can obtain $\mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_j) \neq \emptyset$ similarly to fn. 4, so $\mathrm{De}^{\mathcal{H}_2}_{\mathbf{V}_c}(V_i) \neq \emptyset$.

□

C.3.2 Proof of theoretical results in Sec. 4.2

Condition 4. (1) $\forall V \in \mathbf{V}_c \backslash \mathbf{U}_c, \mathrm{Ch}^{\mathcal{H}_1}(V_i) \subset \mathrm{PCh}^{\mathcal{G}}(V_i)$. (2) $\forall V \in \mathbf{U}_c \cup \mathbf{V}_f, \mathrm{De}^{\mathcal{H}_2}(V) \subset \mathbf{U}_c \cup \mathbf{V}_f$. (3) $\forall V_i \in \mathbf{U}_c$, X_{2i-1}, X_{2i} can be written as

$$X_{2i-1} = c_{i_1} \sum_{V_j \in \mathbf{U}_c \cup \mathbf{V}_f} m_{ij}\epsilon_{V_j} + e_{X_{2i-1}} + e'_{X_{2i-1}}, \quad X_{2i} = c_{i_2} \sum_{V_j \in \mathbf{U}_c \cup \mathbf{V}_f} m_{ij}\epsilon_{V_j} + e_{X_{2i}} + e'_{X_{2i}}, \tag{29}$$

where $\forall j, k, l$, (i) $\epsilon_{V_j} \perp\!\!\!\perp e_{X_k} \perp\!\!\!\perp e'_{X_l}$, (ii) $\{e_{X_{2j-1}}, e_{X_{2j}}\} \perp\!\!\!\perp \{e_{X_{2k-1}}, e_{X_{2k}}\}$ if $j \neq k$, (iii) $e_{X_{2j-1}} \perp\!\!\!\perp e_{X_{2j}}$ iff $\mathrm{Ch}^{\mathcal{H}_1}(V_j) \subset \mathrm{PCh}^{\mathcal{G}}(V_j)$, and (iv) $e'_{X_{2j-1}} \perp\!\!\!\perp e'_{X_{2k}}$.

Theorem 12. $\forall V_i \in \mathbf{U}_c$, $\mathrm{An}^{\mathcal{H}_2}(V_i) \cap (\mathbf{U}_c \cup \mathbf{V}_f) = \emptyset$ and $\mathrm{Ch}^{\mathcal{H}_1}(V_i) \subset \mathrm{PCh}^{\mathcal{G}}(V_i)$ iff $\forall V_j \in \mathbf{U}_c \backslash \{V_i\}$, $\mathrm{R}(X_{2j-1}, X_{2i-1}|X_{2i}) \perp\!\!\!\perp X_{2i}$.

Proof. When $|\mathbf{U}_c| = 1$, there is $\mathbf{V}_f = \emptyset$ and the only $V_i \in \mathbf{U}_c$ satisfies $\mathrm{Ch}^{\mathcal{H}_1}(V_i) \subset \mathrm{PCh}^{\mathcal{G}}(V_i)$, otherwise we can derive contradiction to Cor. 6. We focus on the case where $|\mathbf{U}_c| > 1$.

"Only if": The proof is similar to "only if" part in Thm. 5.

"If": We prove this part by contradiction. All possible cases are as follows.

- Suppose $\mathrm{Ch}^{\mathcal{H}_1}(V_i) \not\subset \mathrm{PCh}^{\mathcal{G}}(V_i)$. Based on Cond. 3(2), $\{\mathrm{Ch}^{\mathcal{H}_1}(V_i)\} = \mathrm{P}^3\mathrm{Ch}^{\mathcal{G}}(V_i)$. Let $\mathrm{Ch}^{\mathcal{H}_1}(V_i) = \{V_{i_1}, V_{i_2}\}$ where $V_{i_1} \in \mathrm{Pa}^{\mathcal{G}}(V_{i_2})$. Combining Cor. 6(2) with Cond. 4(2), $\mathrm{De}^{\mathcal{H}_2}_{\mathbf{U}_c}(V_i) \neq \emptyset$ and let $V_j \in \mathrm{De}^{\mathcal{H}_2}_{\mathbf{U}_c}(V_i)$. Since both X_{2i-1} and X_{2i} contain $\epsilon_{V_{i_1}}$ and X_{2j-1} does not contain $\epsilon_{V_{i_1}}$, $\mathrm{R}(X_{2j-1}, X_{2i-1}|X_{2i}) \not\perp X_{2i}$ based on Lem. 1(2), which leads to contradiction.

- Suppose $\mathrm{Ch}^{\mathcal{H}_1}(V_i) \subset \mathrm{PCh}^{\mathcal{G}}(V_i)$ and $\mathrm{An}^{\mathcal{H}_2}_{\mathbf{U}_c}(V_i) \neq \emptyset$, let $V_j \in \mathrm{An}^{\mathcal{H}_2}_{\mathbf{U}_c}(V_i)$. The proof is similar to "if" part in proof of Thm. 5.

- Suppose $\mathrm{Ch}^{\mathcal{H}_1}(V_i) \subset \mathrm{PCh}^{\mathcal{G}}(V_i)$, $\mathrm{An}^{\mathcal{H}_2}_{\mathbf{U}_c}(V_i) = \emptyset$, and $\mathrm{An}^{\mathcal{H}_2}_{\mathbf{V}_f}(V_i) \neq \emptyset$, let $V_k \in \mathrm{Pa}^{\mathcal{H}_2}_{\mathbf{V}_f}(V_i)$. Combining Cor. 6(1) with Cond. 4(2), $\mathrm{De}^{\mathcal{H}_2}_{\mathbf{U}_c}(V_k)\backslash\{V_i\} \neq \emptyset$. Besides, there exists $V_j \in \mathrm{De}^{\mathcal{H}_2}_{\mathbf{U}_c}(V_k)\backslash\{V_i\}$ s.t. there exists a directed path from V_k to V_j which does not include V_i. Conversely, note that $\mathbf{V}_c$ is a bottleneck from $\mathrm{Ch}^{\mathcal{G}}(V_k)$ to $\mathbf{O}$ as mentioned in proof of Cor. 4, if for each $V \in \mathrm{De}^{\mathcal{H}_2}_{\mathbf{U}_c}(V_k)\backslash\{V_i\}$, every directed path from V_k to V includes V_i, then $\{V_i\}$ is a bottleneck from $\mathrm{Ch}^{\mathcal{G}}(V_k)$ to $\mathbf{O}$, which leads to contradiction to Asmp. 2(1,2). If $V_j \notin \mathrm{De}^{\mathcal{H}_2}(V_i)$, then X_{2i-1} and X_{2i} both contain ϵ_{V_i} while X_{2j-1} does not contain ϵ_{V_i}, so $\mathrm{R}(X_{2j-1}, X_{2i-1}|X_{2i}) \not\perp X_{2i}$ based on Lem. 1(2), which leads to contradiction. Otherwise, if $V_j \in \mathrm{De}^{\mathcal{H}_2}(V_i)$, then X_{2i-1}, X_{2i} and X_{2j-1} all contain ϵ_{V_i} and ϵ_{V_k}, and there exist two non-intersecting paths from $\{V_k, V_i\}$ to $\{X_{2j-1}, X_{2i-1}\}$ (e.g., $V_k \to \ldots \to V_j \to \ldots \to X_{2j-1}$ and $V_i \to \ldots \to X_{2i-1}$), so $\mathrm{R}(X_{2j-1}, X_{2i-1}|X_{2i}) \not\perp X_{2i}$ based on Lem. 1(3), which leads to contradiction.

□

Proposition 5. *If we can find $V \in \mathbf{U}_c$ satisfying Thm. 12, Cond. 4 is still valid after removal.*

Proof. Based on Thm. 12, Cond. 4(1,2) holds trivially. The remaining proof is similar to the proof of Prop. 3. □

C.4 Proof of Theoretical Results in Sec. 4.3

Theorem 13. Suppose the observed variables are generated by a LiNGAM with latent variables satisfying the rank-faithfulness assumption and Asmp. 2, if Asmp. 1 is invalid, in the limit of infinite data, our algorithm raises an error.

Proof. Based on Thm. 11, at the end of stage 1, denote $\{L \in \mathbf{V}_c | \mathrm{Ch}^{\mathcal{H}_1}(L) \not\subset \mathrm{PCh}^{\mathcal{G}}(L)\}$ by $\mathbf{V}'_c$, if Asmp. 1 is invalid, $\mathbf{V}_f \cup \mathbf{V}'_c \neq \emptyset$. Based on Cor. 6, $|\bigcup \mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(\mathbf{V}_f \cup \mathbf{V}'_c)| \geq 2$. Based on Cond. 4(1,2), throughout stage 2, there is always $\bigcup \mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(\mathbf{V}_f \cup \mathbf{V}'_c) \subset \mathbf{U}_c$. When $\mathbf{U}_c = \bigcup \mathrm{GDe}^{\mathcal{H}_2}_{\mathbf{V}_c}(\mathbf{V}_f \cup \mathbf{V}'_c)$, there exists no $V_i \in \mathbf{U}_c$ s.t. $\mathrm{An}^{\mathcal{H}_2}(V_i) \cap (\mathbf{U}_c \cup \mathbf{V}_f) = \emptyset$ and $\mathrm{Ch}^{\mathcal{H}_1}(V_i) \subset \mathrm{PCh}^{\mathcal{G}}(V_i)$, that is, we cannot find a $V_i \in \mathbf{U}_c$ satisfying the independence condition in Thm. 12. Therefore, before $\mathbf{U}_c$ becomes an empty set, our algorithm raises an error. □

D Real-world Data

The ground-truth causal graph of multitasking behavior model is shown as Fig. 13(a), it satisfies Asmp. 1, on which our algorithm yields a correct result. Moreover, we add some edges (marked in red in Fig. 13(b)) into the ground-truth graph by replacing some single variable with the sum of multiple variables, the modified graph violates Asmp. 1, on which our algorithm raises an error.

E Algorithm

The details of our proposed algorithm are provided in Alg. 3 and 4.

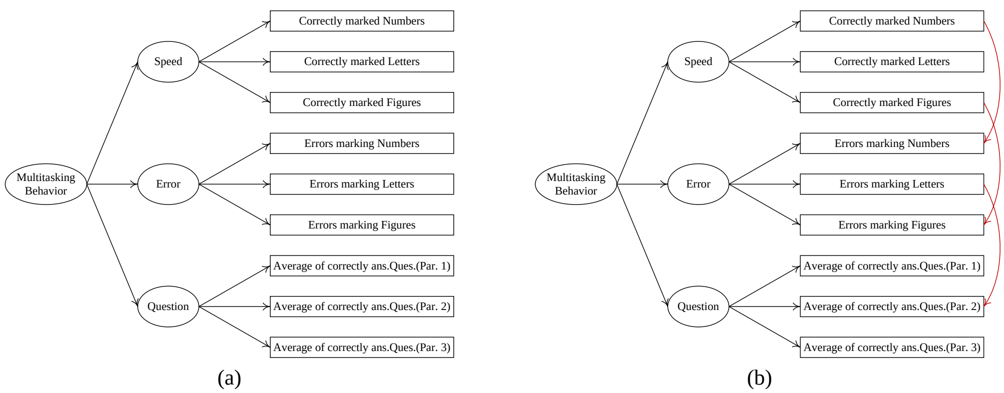


Figure 13: (a) ground-truth causal graph and (b) modified causal graph of multitasking behavior model. Rectangles represent observed variables while circles represent latent variables.

Algorithm 3: Stage 1: Identifying latent variables (detailed)

Input: Observed variables $\mathbf{O}_0$ and $\mathbf{O}_1$
Output: $\mathbf{V}_c$, $\mathbf{V}_p$, and $\mathcal{H}_1$

Initialize $\mathbf{V}_c$ as $\mathbf{O}_0$, $\mathbf{V}_p$ as $\mathbf{O}_1$, and let $V_1 \in \mathrm{Pa}^{\mathcal{H}_1}(V_2)$ iff $V_1 \in \mathrm{Pa}^{\mathcal{G}}(V_2)$, $V_1 \in \mathbf{O}_0$, and $V_2 \in \mathbf{O}_1$.
while *the current* $\mathbf{V}_c$ *is not identical to the previous* $\mathbf{V}_c$ **do**
  Assert Cond. 1 holds.
  // *Locating identifiable pairs. (Thm. 1)*
  $\mathbb{S} := \emptyset$.
  for $\{V_i, V_j\} \subset \mathbf{V}_c$ **do**
    if $\exists V_k \in \mathbf{V}_c \backslash \{V_i, V_j\}$ *s.t.* $\mathrm{Cov}(V_i, V_j)\,\mathrm{Cov}(V_i, V_k)\mathrm{Cov}(V_j, V_k) \neq 0$ *and* $\mathrm{R}(V_i, V_j | V_k) \perp\!\!\!\perp \mathbf{V}_c \backslash \{V_i, V_j\}$ **then**
      $\mathbb{S} := \mathbb{S} \cup \{\{V_i, V_j\}\}$.
    end
  end
  Assert $\mathbb{S}$ consists of all identifiable pairs
  // *Locating pure children from identifiable pairs. (Thm. 2)*
  $\mathbb{S}_1 := \emptyset, \mathbb{S}_2 := \emptyset, \mathbb{S}_3 := \emptyset$.
  for $\{V_i, V_j\} \in \mathbb{S}$ *where* $\{V_{i_1}, V_{i_2}\} \subset \mathrm{Ch}^{\mathcal{H}_1}(V_i)$ *and* $\{V_{j_1}, V_{j_2}\} \subset \mathrm{Ch}^{\mathcal{H}_1}(V_j)$ **do**
    if $\mathrm{R}(V_{i_1}, V_j | V_{i_2}) \perp\!\!\!\perp V_{i_2}$ **then**
      $\mathbb{S}_1 := \mathbb{S}_1 \cup \{\{V_i, V_j\}\}$ and $V_i \in \mathrm{Pa}^{\mathcal{G}}(V_j)$.
    else if $\mathrm{R}(V_{j_1}, V_i | V_{j_2}) \perp\!\!\!\perp V_{j_2}$ **then**
      $\mathbb{S}_1 := \mathbb{S}_1 \cup \{\{V_i, V_j\}\}$ and $V_j \in \mathrm{Pa}^{\mathcal{G}}(V_i)$.
    else if $\exists V_k \in \mathbf{V}_c \backslash \{V_i, V_j\}$ *s.t.* $\{V_i, V_k\} \in \mathbb{S}$ *or* $\{V_j, V_k\} \in \mathbb{S}$ **then**
      $\mathbb{S}_2 := \mathbb{S}_2 \cup \{\{V_i, V_j\}\}$.
    else if $\exists \{V_k, V_l\} \subset \bigcup \mathrm{Ch}^{\mathcal{H}_1}(\mathbf{V}_c \backslash \{V_i, V_j\})$ *s.t.* $(V_{i_1}, V_{i_2}, V_j, V_k, V_l)$ *satisfies the quintuple constraint* **then**
      $\mathbb{S}_3 := \mathbb{S}_3 \cup \{\{V_i, V_j\}\}$ and $V_i \in \mathrm{Pa}^{\mathcal{G}}(V_j)$.
    else if $\exists \{V_k, V_l\} \subset \bigcup \mathrm{Ch}^{\mathcal{H}_1}(\mathbf{V}_c \backslash \{V_i, V_j\})$ *s.t.* $(V_{j_1}, V_{j_2}, V_i, V_k, V_l)$ *satisfies the quintuple constraint* **then**
      $\mathbb{S}_3 := \mathbb{S}_3 \cup \{\{V_i, V_j\}\}$ and $V_j \in \mathrm{Pa}^{\mathcal{G}}(V_i)$.
    else
      $\mathbb{S}_2 := \mathbb{S}_2 \cup \{\{V_i, V_j\}\}$.
    end
  end
  Assert $\mathbb{S}$ is divided into $\mathbb{S}_1, \mathbb{S}_2, \mathbb{S}_3$, that is, $\mathbb{S} = \mathbb{S}_1 \cup \mathbb{S}_2 \cup \mathbb{S}_3$.
  // *Identifying pure children's parents. (Thm. 3)*
  for $\{V_i, V_j\} \in \mathbb{S}_2$ **do**
    if $\exists \{V_i', V_j'\} \in \mathbb{S}_1$ *s.t.* $\{V_i, V_j\} \cap \{V_i', V_j'\} \neq \emptyset$ **then**
      $\bigcap \mathrm{Pa}^{\mathcal{G}}(\{V_i, V_j\}) \subset \mathbf{V}_c$.
    else
      $\bigcap \mathrm{Pa}^{\mathcal{G}}(\{V_i, V_j\}) \subset \mathbf{V}_f$.
    end
    if $\exists \{V_i', V_j'\} \in \mathbb{S}_2$ *s.t.* $\{V_i, V_j\} \cap \{V_i', V_j'\} \neq \emptyset$ **then**
      $\bigcap \mathrm{Pa}^{\mathcal{G}}(\{V_i, V_j\}) = \bigcap \mathrm{Pa}^{\mathcal{G}}(\{V_i', V_j'\})$.
    end
  end
  Assert for each $\{V_i, V_j\} \in \mathbb{S}_2$, it is known whether $\bigcap \mathrm{Pa}^{\mathcal{G}}(\{V_i, V_j\}) \subset \mathbf{V}_f$; and for each $\{\{V_i, V_j\}, \{V_i', V_j'\}\} \subset \mathbb{S}_2$, it is known whether $\bigcap \mathrm{Pa}^{\mathcal{G}}(\{V_i, V_j\}) = \bigcap \mathrm{Pa}^{\mathcal{G}}(\{V_i', V_j'\})$.
  // *Updating* $\mathbf{V}_c$, $\mathbf{V}_p$, *and* $\mathcal{H}_1$.
  for $\{V_i, V_j\} \in \mathbb{S}_1$ *where* $V_i \in \mathrm{Pa}^{\mathcal{G}}(V_j)$ **do**
    $\mathbf{V}_c := \mathbf{V}_c \backslash \{V_j\}$, $\mathbf{V}_p := \mathbf{V}_p \cup \{V_j\}$, and $\mathcal{H}_1 := \mathcal{H}_1 \cup \{V_i \to V_j\}$.
  end
  for $\{V_i, V_j\} \in \mathbb{S}_2$ **do**
    if $\bigcap \mathrm{Pa}^{\mathcal{G}}(\{V_i, V_j\}) \subset \mathbf{V}_f$. **then**
      Find $\mathbb{S}_2' \subset \mathbb{S}_2$ s.t. $\forall \{V_i', V_j'\} \in \mathbb{S}_2'$, $\bigcap \mathrm{Pa}^{\mathcal{G}}(\{V_i, V_j\}) = \bigcap \mathrm{Pa}^{\mathcal{G}}(\{V_i', V_j'\})$.
      $\mathbb{S}_2 := \mathbb{S}_2 \backslash \mathbb{S}_2'$.
      Introduce a new latent variable L.
      $\mathbf{V}_c := \mathbf{V}_c \cup \{L\} \backslash \bigcup \mathbb{S}_2'$, $\mathbf{V}_p := \mathbf{V}_p \cup \bigcup \mathbb{S}_2'$, and $\mathcal{H}_1 := \mathcal{H}_1 \cup \{L \to V | V \in \bigcup \mathbb{S}_2'\}$.
    end
  end
end
Assert $\mathbf{V}_c \cup \mathbf{V}_p = \mathbf{V}$, that is, $\mathbf{V}_f = \emptyset$

Algorithm 4: Stage 2: Inferring causal relations (detailed)

Input: $\mathbf{V}_c$, $\mathbf{V}_p$, and $\mathcal{H}_1$ output by Alg. 3

Output: a complete causal structure $\mathcal{G}$

```
Initialize U_c as V_c and assign two observed surrogates X_{2i-1}, X_{2i} for each V_i ∈ U_c.
while |U_c| > 0 do
    flag:=0.
    for V_i ∈ U_c do
        // Identifying an root variable. (Thm. 5)
        if ∀V_j ∈ U_c\{V_i}, R(X_{2j-1}, X_{2i-1}|X_{2i}) ⫫ X_{2i} then
            Assert V_i is a root variable among U_c
            flag:=1.
            // Estimating the root variable's effects on others. (Thm. 6)
            Calculate sgn(m_{ij}), c_{i1} c_{i2} c_{j1} c_{j2} m_{ij}^2, and c_{i1} c_{i2} following Eq. (5).
            // Updating U_c and X_{2j-1}, X_{2j} for each V_j ∈ U_c.
            U_c := U_c\{V_i}, X_{2j-1} := R(X_{2j-1}, X_{2i-1}|X_{2i}), X_{2j} := X_{2j}.
            break
        end
    end
    if flag = 0 then
        raise error
    end
end
Calculate all m_{ij} and then recover H_2.
G := H_1 ∪ H_2
```