CONDITIONAL INDEPENDENT COMPONENT ANALYSIS FOR ESTIMATING CAUSAL STRUCTURE WITH LATENT VARIABLES

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ABSTRACT

Identifying latent variables and their induced causal structure is fundamental in various scientific fields. Existing approaches often rely on restrictive structural assumptions (e.g., purity) and may become invalid when these assumptions are violated. We introduce Conditional Independent Component Analysis (CICA), a new tool that extracts components that are conditionally independent given latent variables. Under mild conditions, CICA can be optimized using a tractable proxy such as rank-deficiency constraints. Building on CICA, we establish an identifiability theory for linear non-Gaussian acyclic models with latent variables: solving CICA and then applying an appropriate row permutation to the sparsest CICA solution enables recovery of the causal structure. Accordingly, we propose an estimation method based on the identifiability theory and substantiate the algorithm with experiments on both synthetic and real-world datasets.

1 INTRODUCTION

Understanding causal structures is essential in numerous scientific domains, such as biology (Woodward, 2010), psychology (Eronen, 2020), and economics (Hicks et al., 1980). To uncover the underlying causal structures in a data-driven manner, various methods have been proposed (Peters et al., 2017). Most traditional causal discovery methods rely on the causal sufficiency assumption (Spirtes et al., 2000), i.e., no latent confounders exist between any pair of observed variables. However, in many real-world applications, it is often infeasible to measure all the underlying causal variables. For example, in psychology, researchers investigate the impact of social behavior on mental health, while intelligence or personality may often act as latent confounders. It is difficult to precisely measure these variables, yet ignoring such latent confounders can lead to misleading conclusions. Generally, identifying the presence of latent variables and recovering the causal structure involving both observed and latent variables remains a significant challenge.

Some approaches attempt to address the challenge by exploiting conditional independence constraints, such as the FCI algorithm (Spirtes et al., 1995) and its variants (Colombo et al., 2012). However, their results capture only the causal relationships among observed variables. To further discover causal relationships between latent variables, additional parametric assumptions are typically required. For linear Gaussian causal models, several methods leverage rank-deficiency constraints to recover the underlying structure, including latent variables, up to the Markov equivalence class (Silva et al., 2006; Kummerfeld & Ramsey, 2016; Huang et al., 2022; Dong et al., 2023). To take into account higher-order statistics, (Xie et al., 2020) develops a generalized independent noise (GIN) condition and establishes its corresponding estimation algorithm for linear non-Gaussian data. TIN (Dai et al., 2022) defines the independent linear transformation subspace and its dimension can be used to further improve the identifiability of causal discovery with measurement error.

Although these methods have achieved some progress, they typically involve certain structural assumptions to simplify the problem. In particular, the purity assumption (Cai et al., 2019; Xie et al., 2020) rules out edges between observed variables. Violating these assumptions can lead to failures in determining the true causal graph. For example, in Fig. 1, the two graphs cannot be distinguished by most existing methods. Only a few methods can theoretically distinguish these two graphs, primarily overcomplete ICA (OICA) (Eriksson & Koivunen, 2004)-based methods and higher-order

Figure 1: An example of a non-identifiability issue of most existing methods.

cumulant-based methods (Schkoda et al., 2024; Chen et al., 2024). However, OICA typically relies on the expectation maximization (EM) procedure along with approximate inference, which is computationally prohibitive and prone to local optima (Cai et al., 2023). On the other hand, higher-order statistics can be very sensitive to outliers in the data (Hyvärinen & Oja, 2000), reliably estimating higher-order cumulants requires massive samples (Nikias & Mendel, 1993). This raises an important question: can we strike a better balance between identifiability and practical feasibility? Our findings indicate that this could be possible.

Concretely, by analyzing why GIN and TIN conditions fail to distinguish Fig. (1a) and (1b), we argue that relying solely on a one-sided projection $\omega^\top \mathbf{Y} \perp\!\!\!\perp \mathbf{Z}$ ($\mathbf{Y}, \mathbf{Z}$ are two subsets of observed variables) could be restricted. Instead, two-sided projections $\omega_1^\top \mathbf{Y} \perp\!\!\!\perp \omega_2^\top \mathbf{Z}$ may leave additional identifiable traces. Accordingly, we seek a unified procedure that estimates latent causal structure by searching for non-zero ω_1, ω_2 with $\omega_1^\top \mathbf{Y} \perp\!\!\!\perp \omega_2^\top \mathbf{Z}$. Motivated by this, we introduce a new tool named **conditional independent component analysis (CICA)**, which extracts components that are conditionally independent given latent variables. Under mild conditions, CICA can be optimized using a tractable proxy such as rank-deficiency constraints, which avoid involving the estimation of high-order cumulants like OICA or cumulant-based methods. Building on CICA, we establish an identifiability theory and estimation algorithm for linear non-Gaussian acyclic models with latent variables: by first solving CICA and then applying an appropriate row permutation to the sparsest CICA solution, we recover the underlying causal structure, achieving a more general identifiability result with a tolerable computational burden.

Contributions: (1) We introduce a novel principle, conditional independent component analysis (CICA), that extracts components that are conditionally independent given latent variables. (2) We establish an identification theory and an estimation algorithm that performs CICA and then selects row permutations of the sparsest CICA solutions to recover the underlying causal structure. (3) We conduct synthetic and real-world experiments to validate its identifiability guarantees.

2 Background

2.1 Problem Setup

We consider a linear latent variable causal model with DAG G, in which the observed variables $\mathbf{X} = \{X_i\}_{i=1}^m$ and latent variables $\mathbf{L} = \{L_i\}_{i=1}^d$ follow the data generating process:

$$\mathbf{L} = \mathbf{B}_{\mathbf{L},\mathbf{L}}\mathbf{L} + \mathbf{E}_{\mathbf{L}}, \qquad \mathbf{X} = \mathbf{B}_{\mathbf{X},\mathbf{L}}\mathbf{L} + \mathbf{B}_{\mathbf{X},\mathbf{X}}\mathbf{X} + \mathbf{E}_{\mathbf{X}}. \\ \mathbf{V} = \mathbf{A}\mathbf{E}, \text{ with } \mathbf{A} := (\mathbf{I} - \mathbf{B})^{-1}. \tag{1}$$

where $\mathbf{E}_{\mathbf{X}} = \{E_{X_i}\}_{i=1}^m$ and $\mathbf{E}_{\mathbf{L}} = \{E_{L_i}\}_{i=1}^d$ are mutually independent non-Gaussian exogenous noises. We use $V_i \in \mathbf{V}$ to denote a generic variable. $\mathbf{B}$ denotes the adjacency matrix, with the entry $\mathbf{B}_{j,i}$ representing the direct causal effect of V_i on V_j. $\mathbf{B}_{j,i} \neq 0$ if and only if V_i is a direct parent of V_j in G. Here, $\mathbf{V}$ can also be expressed directly as a linear combination of independent exogenous noises $\mathbf{E}$, through the mixing matrix $\mathbf{A}$.

Notations. For a matrix M, we denote by $M_{\mathbf{S},:}$ the rows in M indexed by set $\mathbf{S}$, and similarly by $M_{:,\mathbf{S}}$ the columns. In addition, let $\mathrm{GL}(m)$ be the invertible matrix $\mathbf{W} \in \mathbb{R}^{m\times m}$. Further, we use $\mathrm{Pa}(V_i), \mathrm{Ch}(V_i), \mathrm{Anc}(V_i), \mathrm{De}(V_i)$ as parents, children, ancestors and descendants of V_i, respectively. We use $\mathrm{LPa}(\mathbf{S})$ for a subset $\mathbf{S} \subseteq \mathbf{V}$ to denote the set that contains all the common latent parents of any two nodes in $\mathbf{S}$, excluding the variables in $\mathbf{S}$. By default, $\mathbf{Y}$ and $\mathbf{Z}$ denote two subsets of observed random variables.

2.2 Preliminaries

Definition 1 (GIN condition (Xie et al., 2020))**.** *Let $\mathbf{Y}$ and $\mathbf{Z}$ be two observed random vectors. Suppose that the variables follow a linear, non-Gaussian acyclic model (LiNGAM). We say $(\mathbf{Z}, \mathbf{Y})$ satisfies the GIN condition, if and only if the following two conditions are satisfied: 1) $\exists$ non-zero $\omega \in \mathbb{R}^{|\mathbf{Y}|}$ that solves the equation $\mathrm{cov}(\mathbf{Z}, \mathbf{Y})\omega = \mathbf{0}$, and 2) Any such solution ω makes the linear transformation $\omega^\top \mathbf{Y} \perp\!\!\!\perp \mathbf{Z}$.*

GIN condition needs to be equipped with enough pure children, which is defined as follows:

Definition 2 (Purity (Xie et al., 2024))**.** *Let $\widetilde{\mathbf{L}}$ be a set of latent variables, and $\mathbf{S}$ be a subset of descendant nodes of $\widetilde{\mathbf{L}}$, i.e., $\mathbf{S} \subseteq \mathrm{De}(\widetilde{\mathbf{L}})$. We say $\mathbf{S}$ is a pure set relative to $\widetilde{\mathbf{L}}$ iff i) $V_a \perp\!\!\!\perp V_b | \widetilde{\mathbf{L}}$ for any $V_a, V_b \in \mathbf{S}$, and ii) $\mathbf{S} \perp\!\!\!\perp \{\mathbf{V} \setminus \mathrm{De}(\widetilde{\mathbf{L}})\} | \widetilde{\mathbf{L}}$. In addition, we say that a variable $V_c \in \mathbf{S}$ relative to $\widetilde{\mathbf{L}}$ is a pure variable if $\mathbf{S}$ is a pure set relative to $\widetilde{\mathbf{L}}$. Specifically, if $\mathbf{S} \subseteq \mathrm{Ch}(\widetilde{\mathbf{L}})$, we say that each variable $V_c \in \mathbf{S}$ is a pure child relative to $\widetilde{\mathbf{L}}$.*

Definition 3 (TIN condition (Dai et al., 2022))**.** *Let $\mathbf{Z}$ and $\mathbf{Y}$ be two subsets of random variables. Denote the independent linear transformation subspace $\Omega_{\mathbf{Z};\mathbf{Y}} := \left\{\omega \in \mathbb{R}^{|\mathbf{Y}|} \mid \omega^\top \mathbf{Y} \perp\!\!\!\perp \mathbf{Z}\right\}$. The TIN condition of $\mathbf{Z}$ and $\mathbf{Y}$ is defined as: $\mathrm{TIN}(\mathbf{Z}, \mathbf{Y}) := |\mathbf{Y}| - \dim(\Omega_{\mathbf{Z};\mathbf{Y}})$, where $\dim(\Omega_{\mathbf{Z};\mathbf{Y}})$ denotes the dimension of the subspace $\Omega_{\mathbf{Z};\mathbf{Y}}$, i.e., the degree of freedom of ω.*

3 Method

In this section, we develop a principled framework for causal discovery in the presence of latent confounders. We first describe our motivation by analyzing why existing tools that rely on constructing independence fail (§3.1). We then formalize our proposed tool, conditional independent component analysis (CICA), and discuss its indeterminacy (§3.2), optimization criterion (§3.3). Next, we provide a comprehensive introduction to the identifiability guarantee of latent causal structure based on CICA (§3.4). Finally, we discuss the connection between CICA and independent subspace analysis (ISA) and why ISA is not informative in our settings (§3.5).

3.1 Motivation: beyond one-sided projections

Existing criteria such as GIN and TIN conditions are built on one-sided projections of the form $\omega^\top \mathbf{Y} \perp\!\!\!\perp \mathbf{Z}$. To ensure identifiability, these methods require that latent variables $\mathbf{L}$ have enough pure children (Xie et al., 2024). The rationale is that pure children are mutually conditionally independent given $\mathbf{L}$. With sufficient pure children, one can construct a linear combination of $\mathbf{Y}$ to remove the dependence entirely attributable to the common ancestors $\mathbf{L}$ and thus induce independence.

In contrast, in Fig. 1a and 1b, every pair of observed variables share not only L but also E_1. In this case, no one-sided projection of the form $\omega^\top \mathbf{Y} \perp\!\!\!\perp \mathbf{Z}$ with non-zero ω can eliminate both sources of dependence simultaneously. As a result, the GIN and TIN conditions fail to distinguish between the two graphs since both exhibit no non-degenerate independence pattern under one-sided projections.

This limitation highlights the insufficiency of these tools based on one-sided projections when recovering the latent causal structure in the presence of multiple latent influences. In fact, not all constructive independence patterns can be expressed as $\omega^\top \mathbf{Y} \perp\!\!\!\perp \mathbf{Z}$. A natural step forward is to consider two-sided projections of the form $\omega_1^\top \mathbf{Y} \perp\!\!\!\perp \omega_2^\top \mathbf{Z}$, to remove the dependence from both sides. The following lemma shows that the independence patterns in the form of $\omega^\top \mathbf{Y} \perp\!\!\!\perp \mathbf{Z}$ are a subset of those of $\omega_1^\top \mathbf{Y} \perp\!\!\!\perp \omega_2^\top \mathbf{Z}$.

Lemma 1. *Let $\mathbf{Z}$ and $\mathbf{Y}$ be two subsets of random variables. If $\omega_1^\top \mathbf{Y} \perp\!\!\!\perp \mathbf{Z}$ has a non-zero solution ω_1, then there must exist a non-zero vector ω_2 makes $\omega_1^\top \mathbf{Y} \perp\!\!\!\perp \omega_2^\top \mathbf{Z}$.*

Essentially, the richer the independence structure that a principle exploits, the stronger its identification power. As shown next, Fig. 1a and Fig. 1b fall into different equivalent classes when using the information contained in $\omega_1^\top \mathbf{Y} \perp\!\!\!\perp \omega_2^\top \mathbf{Z}$.

Remark 1. *In Fig. 1a, there always exist two non-zero vectors $\omega_1, \omega_2 \in \mathbb{R}^2$ such that $\omega_{1,1} X_2 + \omega_{1,2} X_3 \perp\!\!\!\perp \omega_{2,1} X_1 + \omega_{2,2} X_2$. In contrast, in Fig. 1b, no non-zero solution satisfies this independence constraint. Besides, in Fig. 1b, there always exist two non-zero vectors $\omega_1, \omega_2 \in \mathbb{R}^2$ such that $\omega_{1,1} X_2 + \omega_{1,2} X_3 \perp\!\!\!\perp \omega_{2,1} X_1 + \omega_{2,2} X_3$, whereas no non-zero solution exists in Fig. 1a.*

Motivated by these asymmetries, when two causal graphs cannot be distinguished using only a one-sided projection $\omega^\top \mathbf{Y} \perp\!\!\!\perp \mathbf{Z}$, two-sided projections $\omega_1^\top \mathbf{Y} \perp\!\!\!\perp \omega_2^\top \mathbf{Z}$ can leave additional identifiable traces for the causal direction. This prompts a natural question: Can we develop a unified procedure that searches for non-zero ω_1, ω_2 with $\omega_1^\top \mathbf{Y} \perp\!\!\!\perp \omega_2^\top \mathbf{Z}$ to enhance identifiability?

3.2 Conditional Independent Component Analysis

A direct route to construct $\omega_1^\top \mathbf{Y} \perp\!\!\!\perp \omega_2^\top \mathbf{Z}$ is to use overcomplete ICA (OICA), which separates more mutually independent sources from fewer observed signals. However, OICA is known to be computationally and statistically ineffective (Ding et al., 2019). An alternative solution is to brute-force searching for each "two-sided projection" (ω_1, ω_2). However, it is difficult to guarantee that all feasible (ω_1, ω_2) have been found.

Instead of fully separating all latent sources as in OICA, we propose to factor out the shared influences explicitly and only require independence conditional on a latent vector. Concretely, we seek an invertible transform $\mathbf{W}$ such that $\mathbf{Z} = \mathbf{W}\mathbf{X}$ has mutually independent coordinates given some latent $\mathbf{L} \in \mathbb{R}^p$. This approach is powerful for two reasons: 1. As we will show in Section 3.3, when p is known, this principle allows for more tractable optimization proxies, avoiding the statistical and computational burdens of OICA. 2. As we will prove in Lemma 3, any solution that satisfies this generative principle ($Z_i \perp\!\!\!\perp Z_j | \mathbf{L}$) provably induces the two-sided projections $\omega_1^\top \mathbf{Y} \perp\!\!\!\perp \omega_2^\top \mathbf{Z}$ required for identifiability. We formalize this core generative principle as follows:

Assumption 1 (Linear mixing with conditionally independent sources)**.** *Let $\mathbf{X}$ be an observed variable set with $|\mathbf{X}| = m$. There exist an invertible matrix $\mathbf{A} \in \mathbb{R}^{m\times m}$, p latent variables $\mathbf{L}$ with $\Sigma_\mathbf{L} \succ 0$, a matrix $\mathbf{M} \in \mathbb{R}^{m\times p}$, and noise variables $\mathbf{E} = (E_1, \ldots, E_m)^\top$ such that*

$$\mathbf{X} = \mathbf{A}\mathbf{S}, \qquad \mathbf{S} = \mathbf{M}\mathbf{L} + \mathbf{E}, \qquad \mathbf{E} \perp\!\!\!\perp \mathbf{L}. \tag{2}$$

$\{E_i\}$ are mutually independent with finite, non-zero variances, and at most one E_i is Gaussian. $\Sigma_\mathbf{E}$ is not a scalar multiple of the identity matrix $\mathbf{I} \in \mathbb{R}^{m\times m}$. Besides, $\mathbf{A}$ does not depend on $\mathbf{L}$.

Definition 4 (p-order Conditional Independent Component Analysis (CICA))**.** *Let $\mathbf{X}$ be an observed variable set with $|\mathbf{X}| = m$. An invertible matrix $\mathbf{W} \in \mathbb{R}^{m\times m}$ is called a p-order CICA solution for $\mathbf{X}$ if there exists p latent variables $\mathbf{L}$ (with $p \geq 0$) such that:*

*(i) (**Conditional independence**) Writing $\mathbf{Z} := \mathbf{W}\mathbf{X} = (Z_1, \ldots, Z_m)^\top$, the components are mutually conditionally independent given $\mathbf{L}$.*

*(ii) (**Minimality in** p) There exist no latent variables $\widetilde{\mathbf{L}}$ with $0 \leq |\widetilde{\mathbf{L}}| < p$ for which the conditional independence in (1) holds.*

When $p = 0$, condition (i) reduces to mutual independence of $\mathbf{Z}$, and CICA coincides with ICA. In addition, we introduce $p_{min}(\mathbf{X}) := \min\{k : k \in \mathbb{N}, k\text{-order CICA solution of } \mathbf{X} \text{ exists}\}$ to measure the size of the minimal latent conditional set of $\mathbf{X}$.

Lemma 2 (Indeterminacy of CICA)**.** *Given Assump. 1, let $\mathbf{X}$ be m observed variables, $\mathbf{W}_1, \mathbf{W}_2 \in \mathbb{R}^{m\times m}$ be two p-order CICA solutions for $\mathbf{X}$. The following two statements are equivalent:*

(i) There exists p latent variables $\mathbf{L}$ such that, writing $\mathbf{Z}^{(k)} := \mathbf{W}_k\mathbf{X}$, the components of $\mathbf{Z}^{(k)}$ are mutually conditionally independent given $\mathbf{L}$ for $k \in \{1, 2\}$.

(ii) There exist a permutation matrix $\mathbf{P}_\pi$ (for some permutation π of $[m]$) and a non-singular diagonal matrix $\mathbf{D}$ such that $\mathbf{W}_2 = \mathbf{P}_\pi\mathbf{D}\mathbf{W}_1$.

In particular, when $p = 0$ (the ICA case), (i) is understood with $\mathbf{L}$ degenerate, and the conclusion reduces to the classical permutation and scaling indeterminacy of ICA. Therefore, Lemma 2 tells us that CICA introduces an additional indeterminacy about the conditional set $\mathbf{L}$ compared to ICA. In addition, based on the CICA solution, one can naturally induce two-sided projections $\omega_1^\top \mathbf{Y} \perp\!\!\!\perp \omega_2^\top \mathbf{Z}$.

Lemma 3. *Let $\mathbf{X}$ be m observed variables, and $\mathbf{W}$ be a p-order CICA solution of $\mathbf{X}$. Let $\mathbf{X}' = \mathbf{W}\mathbf{X}$,$\mathbf{Y}$ and $\mathbf{Z}$ are two subsets of $\mathbf{X}'$, then if $\max\{|\mathbf{Y}|, |\mathbf{Z}|\} > p$, $\omega_1^\top \mathbf{Y}' \perp\!\!\!\perp \omega_2^\top \mathbf{Z}'$ has a non-zero solution (ω_1, ω_2) for $(\mathbf{Y}', \mathbf{Z}')$, where $\mathbf{Y}' = \{X_i | \sum_{X_k \in \mathbf{Y}} \mathbf{W}_{k,i} \neq 0\}$, $\mathbf{Z}'$ are defined similarly.*

Example 1. *The following structural causal model serves as an instantiation of Fig. 1a, where L, E_1, E_2, E_3 are independent non-Gaussian variables, a, b, c, u, v are non-zero coefficients. The identity matrix $\mathbf{I} \in \mathrm{GL}(3)$ is a 3-order CICA solution of $\mathbf{X}$ (the conditional set can be $\{L, E_1, E_2\}$). The right-hand side below shows an example of a 1-order CICA solution of $\mathbf{X}$ (the conditional set is $\{L\}$). The existence of L leads to the absence of a 0-order CICA (i.e., ICA) solution of $\mathbf{X}$.*

$$\begin{cases} X_1 = aL + E_1, \\ X_2 = bL + uX_1 + E_2, \\ X_3 = cL + vX_2 + E_3. \end{cases} \qquad \overbrace{\begin{bmatrix} 1 & 0 & 0 \\ -u & 1 & 0 \\ 0 & -v & 1 \end{bmatrix}}^{\mathbf{W}} \begin{bmatrix} X_1 \\ X_2 \\ X_3 \end{bmatrix} = \begin{bmatrix} a \\ b \\ c \end{bmatrix} L + \begin{bmatrix} E_1 \\ E_2 \\ E_3 \end{bmatrix}$$

Besides, we can construct two-sided projections $\omega_1^\top \mathbf{Y} \perp\!\!\!\perp \omega_2^\top \mathbf{Z}$ with non-zero ω_1, ω_2, based on the CICA solution of $\mathbf{X}$. Taking $\mathbf{Y} = \{X_1', X_2'\}$, $\mathbf{Z} = \{X_3'\}$ as an example, denoting $\mathbf{X}' = \mathbf{W}\mathbf{X}$, then we have $aX_2' - bX_1' \perp\!\!\!\perp X_3'$. i.e., $-(au + b)X_1 + bX_2 \perp\!\!\!\perp X_3 - vX_2$. A non-zero solution $\omega_1 = [-(au + b), b]^\top$, $\omega_2 = [-v, 1]^\top$ exists for $(\mathbf{Y}' = \{X_1, X_2\}, \mathbf{Z}' = \{X_2, X_3\})$.

3.3 Optimization Criterion for CICA

Since the conditional set is latent, the definition of CICA does not specify a testable optimization objective. A practical question arises: which optimization criterion should we use for CICA? Inspired by (Huang et al., 2022; Dong et al., 2023), we characterize conditional independence by introducing the following rank-deficiency constraint.

Lemma 4. *For an observed variable set $\mathbf{X}$ with $|\mathbf{X}| = m$, denote $p = p_{min}(\mathbf{X})$. Suppose $m \geq 2p + 2$, and set $\mathbf{X}' := \mathbf{W}\mathbf{X}$, then $\mathbf{W}$ is a p-order CICA solution of $\mathbf{X}$ if and only if for every pair of disjoint coordinate subsets $\mathbf{X_1}, \mathbf{X_2}$ of $\mathbf{X}'$ with $|\mathbf{X_1}| = |\mathbf{X_2}| = p + 1$, $\det(\Sigma_{\mathbf{X_1},\mathbf{X_2}}) = 0$, where $\Sigma := \mathrm{Cov}(\mathbf{X}')$ denotes the covariance matrix on $\mathbf{X}'$ and $\Sigma_{\mathbf{X_1},\mathbf{X_2}}$ is the $(p+1) \times (p+1)$ sub-matrix of Σ with rows indexed by $\mathbf{X_1}$ and columns by $\mathbf{X_2}$.*

In fact, here $m \geq 2p + 2$ is not a strict restriction; we can relax it by replacing the covariance matrix with a higher-order cumulant tensor. More details are included in Appendix B.3. When $p_{min}(\mathbf{X}) = 1$, we can use another proxy objective of CICA, equipped with a weaker condition.

Definition 5 (Triad constraint (Cai et al., 2019))**.** *Define the pseudo-residual of $\{X_i, X_j\}$ relative to X_k as $E_{(i,j|k)} := \mathrm{Cov}(X_j, X_k) \cdot X_i - \mathrm{Cov}(X_i, X_k) \cdot X_j$. We say that the pair of variables $\{X_i, X_j\}$ and X_k satisfy the Triad constraint if $E_{(i,j|k)} \perp\!\!\!\perp X_k$.*

Lemma 5. *For an observed variable set $\mathbf{X}$ with $|\mathbf{X}| = m$, suppose that $p_{min}(\mathbf{X}) = 1$ and $m \geq 3$ hold, set $\mathbf{X}' \triangleq \mathbf{W}\mathbf{X}$, then the invertible matrix $\mathbf{W}$ is a 1-order CICA solution of $\mathbf{X}$ if and only if for every ordered triple (X_i', X_j', X_k') of $\mathbf{X}'$, $\{X_i', X_j'\}$ and X_k' satisfies the Triad constraint.*

In both Lemma 4 and 5, we assume $p_{min}(\mathbf{X})$ is known, then characterize $p_{min}(\mathbf{X})$-order CICA using the zero-determinant and independence constraint, respectively. In our estimation algorithm, we can determine the value of $p_{min}(\mathbf{X})$ in principle, without requiring prior knowledge (see Lemma 11). Since both the determinant and dependence measures (e.g., HSIC (Gretton et al., 2005)) used in Def. 5 are differentiable, these lemmas actually provide an optimization criterion for CICA.

3.4 Identifiability of Latent Causal Structure based on CICA

In this section, we establish an identifiability theory for causal structure in the linear non-Gaussian acyclic models with latent variables. Once CICA is solved, when and how can the causal structure be recovered from the CICA solutions $\mathbf{W}$? First, we have the following basic assumptions.

Assumption 2 (Rank Faithfulness Assumption (Spirtes, 2013))**.** *Let a distribution P be (linearly) rank-faithful to a DAG G if every rank constraint on a sub-covariance matrix that holds in P is entailed by every free-parameter linear structural model with a path diagram equal to G.*

Assumption 2 holds generically, since the set of values of the free parameters of the SCM for which the rank is not faithful is of Lebesgue measure 0 (Spirtes, 2013).

Condition 1. *Each latent variable in G has at least three neighbors and two children (which can be latent or observed).*

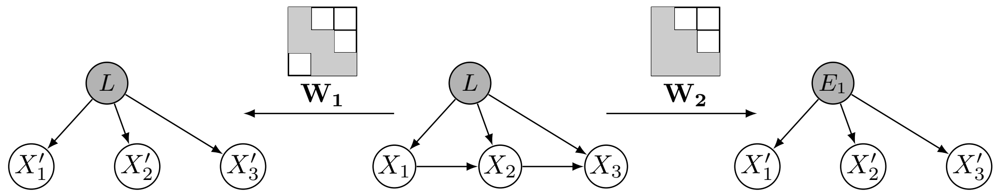

Figure 2: An example of different 1-order CICA solutions for $\mathbf{X}$. $\mathbf{W_1}$ is a 1-order CICA solution that renders $\mathbf{X}'$ conditionally independent given L, while $\mathbf{W_2}$ renders $\mathbf{X}'$ conditionally independent given E_1, the exogenous noise of X_1. The gray/white rectangle denotes non-zero/zero entries.

In this section, for the sake of brevity, we will primarily discuss the results under the one-factor scenario. Most results can be extended into the multi-factor scenario directly. We provide more discussion on the multi-factor scenario in Appendix B.4.

To identify the causal structure based on CICA, we must resolve all inherent indeterminacies. (Shimizu et al., 2006) demonstrates that the permutation and scaling indeterminacy in ICA can be fixed by acyclicity. As stated in Lemma 2, CICA introduces an additional indeterminacy: the choice of the latent conditional set. If $\mathbf{W}$ is a CICA solution of observed variables $\mathbf{X}$, the conditional set does not need to coincide with the latent confounders. Instead, it may correspond to the exogenous noise of the observed variables. Therefore, to solve the indeterminacy of the latent conditional set, we must further identify the CICA solution that aligns with the ground-truth causal structure.

Lemma 6. $\mathbf{I} - \mathbf{B}_{\mathbf{X},\mathbf{X}}$ *is a* $p_{min}(\mathbf{X})$*-order CICA solution of* $\mathbf{X}$ *with latent conditional set* $\mathrm{LPa}(\mathbf{X})$.

Lemma 7. *Suppose* $\mathbf{W}$ *is a* $p_{min}(\mathbf{X})$*-order CICA solution of* $\mathbf{X}$ *whose latent conditional set is* $\mathrm{LPa}(\mathbf{X})$*, there exists a unique row permutation matrix* $\mathbf{P}$ *that makes* $\mathbf{PW}$ *whose diagonal elements have non-zero values, simultaneously.*

As shown in Fig. 2, for $\mathbf{X} = \{X_1, X_2, X_3\}$, $\mathbf{W_1}$ is a 1-order CICA solution of $\mathbf{X}$ given L, thus $\mathbf{W_1} \sim \mathbf{I} - \mathbf{B}_{\mathbf{X},\mathbf{X}}$ according to Lemma 2. In contrast, the ambiguity of the latent conditional set allows alternative solutions, such as $\mathbf{W_2}$, to also qualify as feasible CICA solutions of $\mathbf{X}$, although without a direct correspondence to $\mathbf{B}_{\mathbf{X},\mathbf{X}}$. Essentially, $\mathbf{W_2}\mathbf{X}$ can be interpreted as swapping the roles of L and E_1 on $\mathbf{W_1}\mathbf{X}$. Although conditional independence is preserved after swapping the latent variables, the sparsity of the solution matrix changes. Specifically, it becomes denser. This observation highlights that sparsity can serve as an additional discriminative signal: the sparsest CICA solution better aligns with the underlying causal structure.

Lemma 8. $\mathbf{I} - \mathbf{B}_{\mathbf{X},\mathbf{X}} \in \arg\min\{\|\mathbf{W}\|_0 : \mathbf{W}$ *is a* $p_{min}(\mathbf{X})$*-order CICA solution of* $\mathbf{X}\}$.

Lemma 8 shows that $\mathbf{I} - \mathbf{B}_{\mathbf{X},\mathbf{X}}$ is a $p_{min}(\mathbf{X})$-order CICA solution of $\mathbf{X}$ with the minimum number of non-zero entries. Notably, we do not assume that real-world causal structure is maximally sparse. On the contrary, it can be arbitrarily dense. The minimal sparsity principle is not a prior assumption/convenient choice we impose on the causal structure. Instead, it is a provable theoretical property that emerges from the CICA framework itself, which we then exploit for identifiability. To ensure identifiability, we seek conditions under which $\mathbf{I} - \mathbf{B}_{\mathbf{X},\mathbf{X}}$ is the unique sparsest $p_{min}(\mathbf{X})$-order CICA solution of $\mathbf{X}$, up to some permutation and scale indeterminacies.

Condition 2. *For any* $X_i \in \mathbf{X}$*,* $\exists X_j \in \mathbf{X} \setminus \{X_i\}$ *with* $\mathrm{LPa}(\{X_i, X_j\}) \neq \emptyset$*,* $X_i \not\to X_j$.

Example 2. *In the figure on the left below, since* X_1 *is not the parent of* X_3*,* X_2 *and* X_3 *are not the parents of* X_1*, then Condition 2 holds. In contrast, in the figure on the right below,* X_1 *is both the parent of* X_2 *and* X_3*, thus Condition 2 does not hold.*

Lemma 9. *If Condition 2 holds,* $\mathbf{W} \in \arg\min\{\|\tilde{\mathbf{W}}\|_0 : \tilde{\mathbf{W}}$ *is a* $p_{min}(\mathbf{X})$*-order CICA solution of* $\mathbf{X}\}$ *if and only if we can find a permutation matrix* $\mathbf{P}$ *and non-singular diagonal matrix* $\mathbf{D}$ *that makes* $\mathbf{W} = \mathbf{PD}(\mathbf{I} - \mathbf{B}_{\mathbf{X},\mathbf{X}})$.

Under Condition 2, Lemma 9 establishes that the sparsest $p_{min}(\mathbf{X})$-order CICA solution recovers $\mathbf{I}-\mathbf{B}_{\mathbf{X},\mathbf{X}}$ up to permutation and scale indeterminacies. By Lemma 7, the remaining gap can be eliminated by row permutation. Consequently, $\mathbf{B}_{\mathbf{X},\mathbf{X}}$ is uniquely identified, including both the causal graph among the observed variables and its edge coefficients.

Conversely, when Condition 2 does not hold, $\mathbf{I}-\mathbf{B}_{\mathbf{X},\mathbf{X}}$ is non-identifiable: there exists a distinct $p_{min}(\mathbf{X})$-order CICA solution $\mathbf{W}'$ with an equal number of non-zero entries. Surprisingly, although $\mathbf{W}'$ has different parameters from $\mathbf{I}-\mathbf{B}_{\mathbf{X},\mathbf{X}}$, their support matrix remains the same. Therefore, the causal structure among observed variables is identifiable, which we summarized as follows.

Theorem 1. *All latent variables in $\mathrm{LPa}(\mathbf{X})$ can be identified. Besides, the causal edges of $\mathrm{LPa}(\mathbf{X})$ to $\mathbf{X}$ and the causal edges between the observed variables are also identifiable.*

When the variables form a hierarchical structure and some latent variables may have no observed children, due to the linearity assumption and the transitivity of linear causal relations, we can use a certain observed descendant of the latent variables to implement CICA and apply Theorem 1 recursively. The question is, which one is suitable to serve as a surrogate for the latent variable?

Lemma 10. *Let L be a latent variable discovered in the current iteration. Denote $\mathbf{S}=\mathrm{Ch}(L)$. Let S_k have the highest causal order in $\mathbf{S}$ whose index in $\mathbf{S}$ is k, and $\mathbf{W}$ be the sparsest $p_{min}(\mathbf{S})$-order CICA solution of $\mathbf{S}$. $\mathbf{P}$ is the permutation matrix that makes $\mathbf{PW}$ have non-zero diagonal elements, simultaneously. Denote $\mathbf{Z}=\mathbf{PWS}$, then the value of Z_k can be a suitable surrogate for L.*

Example 3. *Taking Fig. 1a as an example, denote $\mathbf{W}$ as the sparsest 1-order CICA solution of $\mathbf{X}=\{X_1,X_2,X_3\}$, $\mathbf{P}$ is the permutation matrix that makes $\mathbf{PW}$ whose diagonal elements have non-zero values, simultaneously. Let $\mathbf{Z}=\mathbf{PWX}$. As X_1 is the variable that has the highest causal order in $\mathrm{Ch}(L)$, then we can take the value of Z_1 as the surrogate of L.*

Theorem 2. *Suppose Condition 1 holds, then the underlying causal graph G is fully identifiable, including both latent variables and their causal relationships.*

Based on the identifiability guarantee, we develop an estimation algorithm named CICA-LiNGAM to recover the latent causal structure from the CICA solution. Suppose that some observed variables $\mathbf{S}$ form a causal cluster, we can determine the value of $p_{min}(\mathbf{S})$ using the GIN condition. Here we say that an observed variable set $\mathbf{S}$ is a causal cluster if the variables in $\mathbf{S}$ partially share the same latent parents that satisfy $\mathbf{S}=\mathrm{Ch}(\mathrm{LPa}(\mathbf{S}))$, or $\mathrm{LPa}(\mathbf{S})$ d-separates $\mathbf{S}$ and $\mathrm{Ch}(\mathrm{LPa}(\mathbf{S}))\setminus\mathbf{S}$. The causal cluster serves as a basic unit that helps us quickly locate the latent variables. The following lemma states a basic criterion for identifying causal clusters from active variables $\mathbf{A}$ (active variables contain some variables that may form causal clusters in the bottom-up recursive procedure).

Lemma 11 (Identifying Causal Clusters (Xie et al., 2022))**.** *Let $\mathbf{A}$ be the active variable set and $\mathbf{S}\subset\mathbf{A}$. Then $\mathbf{S}$ is a causal cluster with $|\mathrm{LPa}(\mathbf{S})=p_{min}(\mathbf{S})=1$ if: 1) for any subset $\tilde{\mathbf{S}}$ of $\mathbf{Y}$ with $|\tilde{\mathbf{S}}|=2$, $(\mathbf{A}\setminus\mathbf{S},\tilde{\mathbf{S}})$ follows the GIN condition, and 2) no proper subset of $\mathbf{S}$ satisfies 1).*

Algorithm 1 CICA-LiNGAM

Require: Observed variables $\mathbf{X}$.
Ensure: Fully identified causal structure G on $\mathbf{X}$ and discovered latent variables.

```
1: Initialize active variable set A = X and G = ∅.
2: while A ≠ ∅ do
3:     Identify causal clusters in the current active variable set A (Lemma 11).
4:     Obtain the sparsest CICA solution W of each cluster (Lemma 4 or 5).
5:     Find a permutation matrix P to make the diagonal elements of PW non-zero (Lemma 7).
6:     Obtain causal structure within a causal cluster (Theorem 1).
7:     Merge clusters share the common latent parent (Proposition 1 in Appendix B).
8:     Determine whether new latent variables should be introduced (Corollary 2 in Appendix B).
9:     Update the active variable set A according to Lemma 10.
10: end while
11: Return G.
```

The algorithm adopts a recursive procedure. In each iteration, it performs four steps: i) identify causal clusters (line 3); ii) infer the causal structure within each cluster based on the sparsest CICA solution (lines 4$\sim$6); iii) merge the clusters share the common latent parent and determine how many new latent variables are required for these clusters in the current iteration (lines 7∼8, details see Appendix B); and iv) update the active variable set accordingly (line 9).

3.5 CONNECTION WITH ISA

Local ISA-LiNG (Dai et al., 2024) leverages independent subspace analysis (ISA) instead of OICA for local causal discovery. Inspired by this, we then ask whether ISA remains a suitable surrogate of OICA in the presence of latent confounders and what the relationship is between CICA and ISA. To answer these questions, we first review the basic terminology of ISA.

Definition 6 (Irreducible)**.** *An m-dim random vector $\mathbf{Z}$ is irreducible if it contains no lower-dim independent components. In other words, no invertible matrix $\mathbf{W} \in \mathrm{GL}(m)$ can decompose $\mathbf{W}\mathbf{Z} = (\mathbf{Z}_1', \mathbf{Z}_2')^\top$ into $\mathbf{Z}_1' \perp\!\!\!\perp \mathbf{Z}_2'$.*

Definition 7 (ISA solution (Theis, 2006))**.** *For an m-dim random vector $\mathbf{X}$, an invertible matrix $\mathbf{W}$ is called an independent subspace analysis (ISA) solution of $\mathbf{Y}$ if $\mathbf{W}\mathbf{X} = (\mathbf{Z}_1^\top, \dots, \mathbf{Z}_k^\top)^\top$ consists of mutually independent, irreducible random vectors $\mathbf{Z}_i$. The corresponding partition $\mathbf{\Gamma}_{\mathbf{W}}$ of the indices $[m]$ is called the ISA partition associated with $\mathbf{W}$.*

Although ISA seeks separation "as independent as possible", the following theorem shows that ISA is actually not informative enough in the presence of latent confounders.

Theorem 3 (Interpretations of ISA in LiNGAM model)**.** *Let the graph obtained after removing all the outgoing edges of $\mathbf{X}$ in $\mathcal{G}$ be named by $\mathcal{G}'$, which form several connected components of observed variables $\mathbf{X}'_{C_1}, \mathbf{X}'_{C_2}, \cdots, \mathbf{X}'_{C_k}$, where k be the number of connected components in $\mathcal{G}'$. For an ISA solution $\mathbf{W}$, let $\mathbf{W}\mathbf{X} = (\mathbf{Z}_1^\top, \dots, \mathbf{Z}_k^\top)^\top$. Then there is a permutation π of $[k]$ s.t. for any $i \in [k]$, $\exists \mathbf{W}_i \in \mathrm{GL}(|C_i|)$ makes $\mathbf{Z}_{\pi(i)} = \mathbf{W}_i \mathbf{X}'_{C_i}$.*

Example 4. *Here we present a concrete example to aid in understanding Theorem 3. After removing all outgoing edges of $\mathbf{X}$ in $\mathcal{G}$ (the graph in Fig. 4a), $\mathcal{G}'$ (the graph in Fig. 4b) form three connected components of observed variables, $\{X_1'\}$, $\{X_2', X_4'\}$ and $\{X_3', X_5'\}$. Then $\mathbf{W}\mathbf{X} = (\mathbf{Z}_1^\top, \mathbf{Z}_2^\top, \mathbf{Z}_3^\top)^\top, \exists \pi, \mathbf{W}_1, \mathbf{W}_2, \mathbf{W}_3$, s.t. $\mathbf{Z}_{\pi(1)} = \mathbf{W}_1 X_1', \mathbf{Z}_{\pi(2)} = \mathbf{W}_2 X'_{[2,4]}, \mathbf{Z}_{\pi(3)} = \mathbf{W}_3 X'_{[3,5]}$.*

Figure 4: An example to understand the procedure of ISA in the LiNGAM model.

According to Lemma 3, any matrix $\mathbf{W} \in \mathrm{GL}(3)$ is an ISA solution of Fig. 1a and 1b. Therefore, they are "ISA equivalent", which we summarize in the following remark.

Remark 2. *The two causal graphs in Fig. 1a and Fig. 1b cannot be identified by ISA.*

The fundamental reason why ISA fails to be informative in the presence of latent confounders is that, although it seeks components that are "as independent as possible", ISA does not impose constraints within each irreducible subspace. Consequently, regardless of how variables are connected within a subspace, the corresponding graphs belong to the same equivalence class under ISA. In contrast, the absence of constraints within each subspace can be addressed by CICA. For example, the sparsest 1-order CICA solution on $\{X_2, X_4\}$ makes the edge $X_2 \to X_4$ identifiable. In summary, solving CICA on each subspace can be a good complement to ISA.

4 EXPERIMENTS

In this section, we present simulation studies on synthetic data to demonstrate that our algorithm effectively identifies latent variables and latent causal structure. Due to space limitations, real-world experiments on personality psychology data are presented in Appendix C.

We generate data from some typical graph structures that satisfy Condition 1 (see Fig. 5). We consider different sample sizes $N = 5k, 10k, 20k$. The causal strengths $B_{i,j}$ are generated uniformly

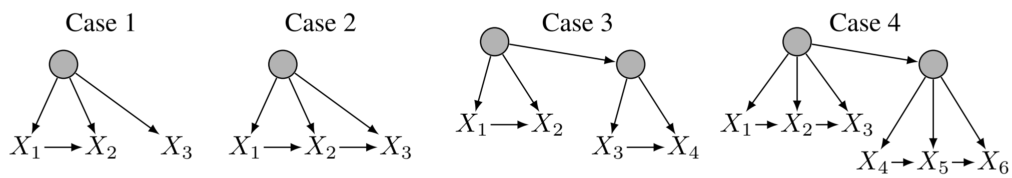

Figure 5: Causal structures used in synthetic experiments.

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

Graph	Method	Error in Latent Variables ↓			Correct-Ordering Rate ↑			F1-Score ↑		
		5k	10k	20k	5k	10k	20k	5k	10k	20k
Case 1	CDHS	0.30±0.46	0.20±0.40	0.40±0.49	**0.65±0.45**	**0.80±0.40**	0.60±0.49	0.67±0.45	**0.80±0.40**	0.60±0.49
	LaHME	0.00±0.00	0.10±0.30	0.00±0.00	0.50±0.00	0.45±0.15	0.50±0.00	0.67±0.00	0.60±0.20	0.67±0.00
	PO-LiNGAM	0.00±0.00	0.00±0.00	0.00±0.00	0.50±0.00	0.50±0.00	0.50±0.00	0.66±0.03	0.67±0.00	0.67±0.00
	RLCD	1.00±0.00	1.00±0.00	1.00±0.00	0.00±0.00	0.00±0.00	0.00±0.00	0.00±0.00	0.00±0.00	0.00±0.00
	Ours	**0.00±0.00**	**0.00±0.00**	**0.00±0.00**	0.65±0.25	0.60±0.35	**0.75±0.25**	**0.75±0.25**	0.67±0.38	**0.77±0.46**
Case 2	CDHS	1.00±0.00	1.00±0.00	1.00±0.00	0.00±0.00	0.00±0.00	0.00±0.00	0.00±0.00	0.00±0.00	0.00±0.00
	LaHME	1.00±0.00	1.00±0.00	1.00±0.00	0.00±0.00	0.00±0.00	0.00±0.00	0.00±0.00	0.00±0.00	0.00±0.00
	PO-LiNGAM	1.00±0.00	1.00±0.00	1.00±0.00	0.00±0.00	0.00±0.00	0.00±0.00	0.00±0.00	0.00±0.00	0.00±0.00
	RLCD	1.00±0.00	1.00±0.00	1.00±0.00	0.00±0.00	0.00±0.00	0.00±0.00	0.00±0.00	0.00±0.00	0.00±0.00
	Ours	**0.00±0.00**	**0.00±0.00**	**0.00±0.00**	**0.60±0.25**	**0.60±0.25**	**0.66±0.27**	**0.67±0.44**	**0.67±0.44**	**0.72±0.48**
Case 3	CDHS	2.00±0.00	1.90±0.30	2.00±0.00	0.00±0.00	0.00±0.00	0.00±0.00	0.00±0.00	0.00±0.00	0.00±0.00
	LaHME	0.00±0.00	0.20±0.60	0.10±0.30	0.44±0.00	0.40±0.13	0.40±0.13	0.73±0.00	0.65±0.22	0.65±0.22
	PO-LiNGAM	0.00±0.00	**0.00±0.00**	0.20±0.60	0.44±0.00	0.44±0.00	0.40±0.13	0.73±0.00	**0.73±0.00**	0.65±0.22
	RLCD	0.10±0.30	0.10±0.30	**0.00±0.00**	0.60±0.25	0.60±0.25	0.58±0.16	0.70±0.24	0.70±0.24	0.73±0.08
	Ours	**0.00±0.00**	0.20±0.60	0.10±0.00	**0.66±0.18**	**0.61±0.31**	**0.61±0.31**	**0.78±0.31**	0.72±0.35	**0.78±0.31**
Case 4	CDHS	2.00±0.00	2.00±0.00	2.00±0.00	0.00±0.00	0.00±0.00	0.00±0.00	0.00±0.00	0.00±0.00	0.00±0.00
	LaHME	0.25±0.54	0.20±0.40	0.10±0.44	0.30±0.15	0.30±0.15	0.36±0.08	0.56±0.28	0.56±0.28	0.67±0.15
	PO-LiNGAM	2.00±0.00	2.00±0.00	2.00±0.00	0.00±0.00	0.00±0.00	0.00±0.00	0.00±0.00	0.00±0.00	0.00±0.00
	RLCD	0.50±0.81	1.10±0.83	0.70±0.90	0.28±0.19	0.11±0.17	0.20±0.17	0.30±0.22	0.13±0.20	0.23±0.20
	Ours	**0.25±0.54**	**0.20±0.40**	**0.10±0.44**	**0.52±0.27**	**0.52±0.27**	**0.68±0.39**	**0.68±0.43**	**0.68±0.43**	**0.74±0.40**

from $[-2, -0.5] \cup [0.5, 2]$, and the non-Gaussian noise terms are generated from the square of exponential distributions. In each setting, the results are obtained after averaging the values in the 10 tests. We report both the average results and standard errors. We consider the following four methods as baselines for comparing: RLCD (Dong et al., 2023), PO-LiNGAM (Jin et al., 2023), LaHME (Xie et al., 2024), CDHS (Li et al., 2025). To evaluate the precision of the estimated graph, we used the following three metrics as (Li & Liu, 2025). 1) Error in Latent Variables: the absolute difference between the estimated number of latent variables and the ground-truth one; 2) Correct Ordering Rate: the number of correctly estimated causal orderings divided by that of ground-truth causal orderings; 3) F1 score of causal edges.

The experimental results are summarized in Table 1. For CDHS, the algorithm fails in the fully impure setting as its "Homologous Surrogates" condition (Li et al., 2025) is violated, preventing any valid output. While LaHME and PO-LiNGAM are relatively stable on key evaluation metrics, they are unable to produce correct results in fully impure scenarios (e.g., cases 2 and 4) because their clustering step fails. RLCD is inapplicable to cases 1 and 2, as its underlying rank test requires at least four observed variables; it also struggled to resolve the causal structure in the remaining scenarios. In contrast, our proposed algorithm demonstrated optimal performance across all cases. It consistently identified and characterized the impure connections among the observed variables, showcasing its advantages in handling impure structures.

5 Conclusion

In this paper, we introduce a new tool, Conditional Independent Component Analysis (CICA), which aims to identify components that are mutually independent given a certain number of latent variables. CICA naturally induces two-sided projections $\omega_1^\top \mathbf{Y} \perp\!\!\!\perp \omega_2^\top \mathbf{Z}$, which carry a richer identification signal than one-sided projections $\omega^\top \mathbf{Y} \perp\!\!\!\perp \mathbf{Z}$ used in GIN/TIN, thus improving the identifiability in latent causal structure learning. Although CICA involves additional indeterminacy on the latent conditional set, we show that sparsity resolves this ambiguity and yields full identification of the latent variables and causal relationships. Building on our theoretical results, we derive an estimation algorithm for latent causal structure recovery. Synthetic and real-world experiments show the superiority of our methods in dealing with impure structures.

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Organization of Appendices

A Definitions, Examples, and Proofs

A.1 Definitions

Definition 8 (Treks (Sullivant et al., 2010)). *In $\mathcal{G}$, a trek from X to Y is an ordered pair of directed paths (P_1, P_2) where P_1 has a sink X, P_2 has a sink Y, and both P_1 and P_2 have the same source Z.*

Definition 9 (T-separation (Sullivant et al., 2010)). *Let $\mathbf{A}, \mathbf{B}, \mathbf{C_A}$, and $\mathbf{C_B}$ be four subsets of $\mathbf{V}_\mathcal{G}$ in graph $\mathcal{G}$ (not necessarilly disjoint). $(\mathbf{C_A}, \mathbf{C_B})$ t-separates $\mathbf{A}$ from $\mathbf{B}$ if for every trek (P_1, P_2) from a vertex in $\mathbf{A}$ to a vertex in $\mathbf{B}$, either P_1 contains a vertex in $\mathbf{C_A}$ or P_2 contains a vertex in $\mathbf{C_B}$.*

Lemma 12 (Rank and T-separation (Sullivant et al., 2010)). *Given two sets of variables $\mathbf{A}$ and $\mathbf{B}$ from a linear model with graph $\mathcal{G}$, we have $\mathrm{rank}\,(\Sigma_{\mathbf{A},\mathbf{B}}) = \min\{|\mathbf{C_A}| + |\mathbf{C_B}| : (\mathbf{C_A}, \mathbf{C_B})$ t-separates $\mathbf{A}$ from $\mathbf{B}$ in $\mathcal{G}\}$, where $\Sigma_{\mathbf{A},\mathbf{B}}$ is the cross-covariance over $\mathbf{A}$ and $\mathbf{B}$.*

A.2 Examples

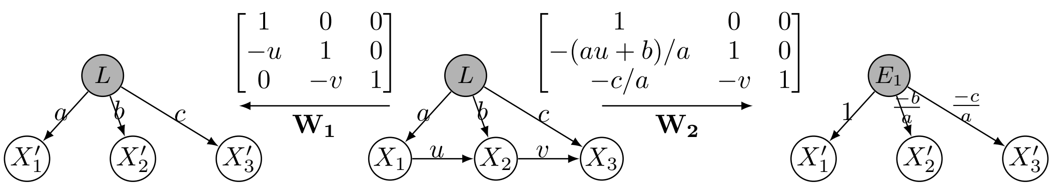


Figure 6: An example of different CICA solutions for $\mathbf{X}$. $\mathbf{W_1}$ is a CICA solution that renders $\mathbf{X}'$ conditionally independent given L, while $\mathbf{W_2}$ renders $\mathbf{X}'$ conditionally independent given E_1, the exogenous noise of X_1. The gray/white rectangle denotes non-zero/zero entries.

A.3 Proof

A.3.1 Preliminaries

Lemma 13 (Darmois-Skitovich Theorem (Darmois, 1953)). *Given n independent scalar random variables $X_1, \ldots, X_n$ that are not necessarily identically distributed. Consider two linear statistics $L_1 = \sum \alpha_i X_i$, $L_2 = \sum \beta_i X_i$, where α_i, β_i are constant coefficients. L_1 and L_2 are independent if and only if the random variables X_j for which $\alpha_j \beta_j \neq 0$ follow a normal distribution.*

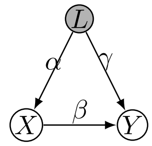
Lemma 14 (Graphical implication of TIN (Dai et al., 2022)). *Let $\mathbf{Z}$, $\mathbf{Y}$ be two subsets of variables, we have:*

$$\mathrm{TIN}(\mathbf{Z}, \mathbf{Y}) = \min\{|\mathbf{S}| \mid \mathbf{S} \textit{ is a vertex cut from } \mathrm{Anc}(\mathbf{Z}) \textit{ to } \mathbf{Y}\}. \tag{3}$$

In a linear non-Gaussian system, the Darmois–Skitovich theorem (Darmois, 1953) plays a key role in determining the independence of two linear statistics. It tells us that two linear combinations of independent non-Gaussian variables are independent if they do not share any non-Gaussian component. As $\omega^\top \mathbf{X}$ is a linear combination of independent noises of $\mathbf{V}$, characterizing all possible independence that can be constructed from observational data requires understanding which noise combinations can be represented by $\omega^\top \mathbf{X}$. To this end, we introduce a new definition that describes the noise combinations attainable through linear combinations of observed variables.

Definition 10 (Constructible Noise Combination). *A noise combination $\mathbf{Z} \subseteq \mathbf{E}$, which consists of some independent noises of variables in $\mathbf{V}$. The noise combination $\mathbf{Z}$ is constructible by some observed variables $\mathbf{X}$ if there exists a coefficient vector ω such that $\omega^\top \mathbf{X}$ is a linear combination of the noise variables in $\mathbf{Z}$ with non-zero coefficients, i.e., $\omega^\top \mathbf{X} = \sum_{E_i \in \mathbf{Z}} \nu_i E_i (\nu_i \neq 0)$. In other words, $\omega^\top \mathbf{X}$ contains and only contains noise variables in $\mathbf{Z}$.*

Example 5. *In the figure below, L is the latent confounder of two observed variables X and Y. We have $\emptyset, \{E_L, E_X\}, \{E_L, E_Y\}, \{E_X, E_Y\}$ and $\{E_L, E_X, E_Y\}$ are constructible while the other noise combinations are not.*



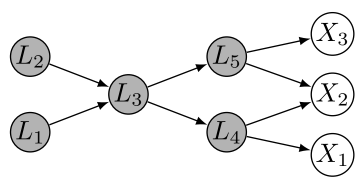
$$\begin{pmatrix} X \\ Y \end{pmatrix} = \begin{pmatrix} \alpha & 1 & 0 \\ \alpha\beta + \gamma & \beta & 1 \end{pmatrix} \begin{pmatrix} E_L \\ E_X \\ E_Y \end{pmatrix}$$

$\emptyset$	$\{E_L\}$	$\{E_X\}$	$\{E_Y\}$	$\{E_L, E_X\}$	$\{E_L, E_Y\}$	$\{E_X, E_Y\}$	$\{E_L, E_X, E_Y\}$
✓	×	×	×	✓	✓	✓	✓

Table 2: All constructive noise combinations of the graph above.

Definition 11 (Bottleneck)**.** *Let* $\mathbf{J}, \mathbf{K}$ *and* $\mathbf{B}$ *be three subsets of* $\mathbf{V}$ *that are not necessarily disjoint. We say that* $\mathbf{B}$ *is a bottleneck from* $\mathbf{J}$ *to* $\mathbf{K}$ *if, for every* $j \in \mathbf{J}$ *and every* $k \in \mathbf{K}$*, each directed path from* j *to* k *includes some* $b \in \mathbf{B}$*.*

Definition 12 (Latest Minimal bottleneck (LM bottleneck))**.** *Let* $\mathbf{J}, \mathbf{K}$ *and* $\mathbf{B}$ *be three subsets of* $\mathbf{V}$ *that are not necessarily disjoint. We say that a bottleneck* $\mathbf{B}$ *from* $\mathbf{J}$ *to* $\mathbf{K}$ *called minimal if every bottleneck* $\mathbf{B}'$ *from* J *to* K *has* $|\mathbf{B}'| \geq |\mathbf{B}|$*. Furthermore,* $\mathbf{B}$ *is the (topologically) latest minimal bottleneck (LM bottleneck) from* $\mathbf{J}$ *to* $\mathbf{K}$ *if for every minimal bottleneck* $\mathbf{B}'$ *from* $\mathbf{J}$ *to* $\mathbf{K}$*,* $\mathbf{B}$ *is the bottleneck from* $\mathbf{B}'$ *to* $\mathbf{K}$*.*



Example 6. *In the figure above,* $\{L_3\}$ *is a minimal bottleneck from* $\{L_1, L_2\}$ *to* $\mathbf{X}$*. More precisely, it is also the corresponding LM bottleneck.* $\{L_3, L_5\}$ *is a minimal bottleneck from* $\{L_1, L_5\}$ *to* $\mathbf{X}$ *but it is not the corresponding LM bottleneck. Instead, it should be* $\{L_4, L_5\}$*.*

Definition 13. *We define the LM bottleneck-dominated set of* $\mathbf{B}$ *with respect to* $\mathbf{K}$ *as the set of all nodes in* $\mathbf{V}$ *such that* $\mathbf{B}$ *is the LM bottleneck from the node to* $\mathbf{K}$*. Formally,*

$$\mathcal{D}_{\mathbf{B},\to\mathbf{K}} := \{v \in \mathbf{V} | \mathbf{B} \text{ is the LM bottleneck from } v \text{ to } \mathbf{K}\} \tag{4}$$

This is the maximal set of nodes for which $\mathbf{B}$ serves as a bottleneck toward $\mathbf{K}$.

Lemma 15. *Let* $\mathbf{J}, \mathbf{K} \subseteq \mathbf{V}$ *that are not necessarily disjoint. The LM bottleneck from* $\mathbf{J}$ *to* $\mathbf{K}$ *always exists and is unique.*

Proof. Build the standard vertex–splitting network $G' = (\mathbf{V}', \mathbf{E}')$ with capacities as follows. For each $v \in \mathbf{V}$, create two nodes v^-, v^+ and add a unit–capacity edge $v^- \to v^+$. For each $u \to v \in \mathbf{E}$, add an infinite–capacity edge $u^+ \to v^-$. Add a source s and a sink t; for each $j \in \mathbf{J}$ add an infinite–capacity edge $s \to j^-$, and for each $k \in \mathbf{K}$ add an infinite–capacity edge $k^+ \to t$.

Then for any $\mathbf{B} \subseteq \mathbf{V}$, $\mathbf{B}$ is a bottleneck from $\mathbf{J}$ to $\mathbf{K}$ $\iff$ $C(\mathbf{B}) := \{v^- \to v^+ : v \in \mathbf{B}\}$ is an s–t cut in G'. Moreover, the capacity of $C(\mathbf{B})$ equals $|\mathbf{B}|$. Indeed, every path $j \rightsquigarrow k$ in G lifts to a path $s \rightsquigarrow j^- \rightsquigarrow \cdots \rightsquigarrow k^+ \rightsquigarrow t$ in G' that necessarily traverses the split edge $x^- \to x^+$ for each visited x; cutting precisely the split edges in $C(\mathbf{B})$ blocks all lifted s–t paths iff every $j \rightsquigarrow k$ path in G meets $\mathbf{B}$. Since only split edges have finite capacity, the cut capacity is $|\mathbf{B}|$.

Therefore, a minimal bottleneck (of smallest cardinality) exists because it corresponds to a minimum s–t cut in the finite network G'.

Let f be any maximum flow on G' and let R_f be the residual network. Define

$$T_f := \{\, x \in \mathcal{V}' : t \text{ can reach } x \text{ in } R_f \,\}, \qquad S_f := \mathcal{V}' \setminus T_f.$$

Standard max–flow theory implies that (S_f, T_f) is a minimum s–t cut, and that T_f is inclusion–wise maximal among the sink sides of all minimum cuts (the "closest-to-t" minimum cut); in particular,

T_f is unique. For completeness: if (S', T') is any minimum cut, then edges from T' to S' carry zero residual capacity and edges from S' to T' are saturated; hence every node reachable from t in R_f must lie in T', so $T' \subseteq T_f$.

Map the t-closest minimum cut back to a vertex set:

$$\mathbf{B}^\star := \{ v \in \mathbf{V} : v^- \in S_f \text{ and } v^+ \in T_f \}.$$

By construction, $C(\mathbf{B}^\star)$ is the cut (S_f, T_f), hence $\mathbf{B}^\star$ is a minimal bottleneck.

Let $\mathbf{B}'$ be any other minimal bottleneck, and let (S', T') be its corresponding minimum cut in G'. From the previous paragraph $T' \subseteq T_f$ (equivalently $S_f \subseteq S'$). Take any path $b' \rightsquigarrow k$ in G with $b' \in \mathbf{B}'$ and $k \in \mathbf{K}$; its lift in G' goes from $b'^- \in S' \supseteq S_f$ to $k^+ \in T_f$, hence must cross the cut (S_f, T_f) through some split edge $v^- \to v^+$ with $v \in \mathbf{B}^\star$. Therefore every $b' \rightsquigarrow k$ path passes through $\mathbf{B}^\star$, i.e., $\mathbf{B}^\star$ is a bottleneck from $\mathbf{B}'$ to $\mathbf{K}$. Since $\mathbf{B}'$ was an arbitrary minimal bottleneck, $\mathbf{B}^\star$ is the latest minimal (LM) bottleneck.

If $\widetilde{\mathbf{B}}$ is another LM bottleneck with minimum cut $(\widetilde{S}, \widetilde{T})$, then by the same argument its sink side $\widetilde{T}$ must contain the sink side of every minimum cut, hence $\widetilde{T} = T_f$ by the maximality/uniqueness of T_f. Thus $\widetilde{\mathbf{B}} = \mathbf{B}^\star$. In summary, the LM bottleneck from $\mathbf{J}$ to $\mathbf{K}$ exists and is unique. □

Lemma 16. *A variable set $\mathbf{V_b} \subseteq \mathbf{V}$ is an LM bottleneck from some variable set $\mathbf{V_s}$ to $\mathbf{X}$ if and only if $\mathbf{V_b}$ itself is the LM bottleneck from $\mathbf{V_b}$ to $\mathbf{X}$.*

Proof. If $\mathbf{V}_b$ is the LM bottleneck from some $\mathbf{V}_s$ to $\mathbf{X}$, then $\mathbf{V}_b$ is the LM bottleneck from $\mathbf{V}_b$ to $\mathbf{X}$. Since $\mathbf{V}_b$ is a bottleneck from $\mathbf{V}_s$ to $\mathbf{X}$, every $\mathbf{V}_s \rightsquigarrow \mathbf{X}$ path meets $\mathbf{V}_b$. Consequently $\mathbf{V}_b$ is trivially a bottleneck from $\mathbf{V}_b$ to $\mathbf{X}$ (every $v \in \mathbf{V}_b$–$\mathbf{X}$ path contains $v \in \mathbf{V}_b$ at its first node).

We show that $\mathbf{V}_b$ is minimal for the pair $(\mathbf{V}_b, \mathbf{X})$. Assume, for contradiction, that there exists a bottleneck $\mathbf{C}$ from $\mathbf{V}_b$ to $\mathbf{X}$ with $|\mathbf{C}| < |\mathbf{V}_b|$. Then for any $s \in \mathbf{V}_s$ and $x \in \mathbf{X}$, each $s \rightsquigarrow x$ path first hits $\mathbf{V}_b$ and, from that hit, must pass $\mathbf{C}$ (because $\mathbf{C}$ meets every $\mathbf{V}_b \rightsquigarrow \mathbf{X}$ path). Hence $\mathbf{C}$ is also a bottleneck from $\mathbf{V}_s$ to $\mathbf{X}$, contradicting the minimality of $\mathbf{V}_b$ for $(\mathbf{V}_s, \mathbf{X})$.

It remains to verify the latest property for $(\mathbf{V}_b, \mathbf{X})$. Let $\mathbf{C}$ be any minimal bottleneck from $\mathbf{V}_b$ to $\mathbf{X}$. We claim that every $\mathbf{C} \rightsquigarrow \mathbf{X}$ path meets $\mathbf{V}_b$. Indeed, otherwise there would exist $c \in \mathbf{C}$ and $x \in \mathbf{X}$ with a path $c \rightsquigarrow x$ avoiding $\mathbf{V}_b$. Concatenate a path $s \rightsquigarrow c$ with $s \in \mathbf{V}_s$ whose internal nodes avoid $\mathbf{V}_b$ (which exists because $\mathbf{V}_b$ is minimal for $(\mathbf{V}_s, \mathbf{X})$; otherwise c would be redundant in $\mathbf{C}$), and then follow the $c \rightsquigarrow x$ path; this would give an $\mathbf{V}_s \rightsquigarrow \mathbf{X}$ path avoiding $\mathbf{V}_b$, contradicting that $\mathbf{V}_b$ is a bottleneck from $\mathbf{V}_s$ to $\mathbf{X}$. Thus $\mathbf{V}_b$ is a bottleneck from $\mathbf{C}$ to $\mathbf{X}$; since $\mathbf{C}$ was arbitrary minimal for $(\mathbf{V}_b, \mathbf{X})$, $\mathbf{V}_b$ is the LM bottleneck from $\mathbf{V}_b$ to $\mathbf{X}$.

If $\mathbf{V}_b$ is the LM bottleneck from $\mathbf{V}_b$ to $\mathbf{X}$, then $\mathbf{V}_b$ is the LM bottleneck from some $\mathbf{V}_s$ to $\mathbf{X}$. Take $\mathbf{V}_s := \mathbf{V}_b$. By assumption, $\mathbf{V}_b$ is a (latest) minimal bottleneck for $(\mathbf{V}_b, \mathbf{X})$; in particular it is a bottleneck from $\mathbf{V}_s$ to $\mathbf{X}$ and, for every minimal bottleneck $\mathbf{C}$ from $\mathbf{V}_s$ to $\mathbf{X}$, every $\mathbf{C} \rightsquigarrow \mathbf{X}$ path meets $\mathbf{V}_b$. Hence $\mathbf{V}_b$ is the LM bottleneck from $\mathbf{V}_s$ to $\mathbf{X}$. □

Theorem 4 (Graphical criteria of the constructible noise combination)**.** *Any noise combination α is constructible by $\mathbf{X}$ if and only if (i) $\exists \mathbf{T} \subseteq \mathbf{V}$ s.t. $\mathbf{T}$ is the LM bottleneck of $\mathbf{T}$ to $\mathbf{X}$ in $\mathcal{G}$. (ii) $\forall V_i \in \mathbf{V}$, $\alpha_i = 0 \Longleftrightarrow \mathbf{T}$ is a bottleneck from V_i to $\mathbf{X}$ in $\mathcal{G}$.*

Proof. Constructibility $\Longrightarrow$ (i)–(ii). Assume α is constructible, let $\mathbf{S} := \{ i \in \mathbf{V} : \alpha_i \neq 0 \}$ be the support of α. By Lemma 15, the LM bottleneck $\mathbf{T}^\star$ from $\mathbf{S}$ to $\mathbf{X}$ exists and is unique; by Lemma 16, $\mathbf{T}^\star$ is also the LM bottleneck from $\mathbf{T}^\star$ to $\mathbf{X}$. This gives (i).

It remains to show (ii). Fix $i \in \mathbf{V}$. If $\alpha_i = 0$, then $\mathbf{T}^\star$ is a bottleneck from V_i to $\mathbf{X}$. Suppose to the contrary that there exists a directed path $P : i \rightsquigarrow x$ avoiding $\mathbf{T}^\star$ (with $x \in \mathbf{X}$). Since $\mathbf{T}^\star$ is the LM bottleneck from $\mathbf{S}$ to $\mathbf{X}$, it is, by definition, the bottleneck from every minimal bottleneck for $(\mathbf{S}, \mathbf{X})$ to $\mathbf{X}$; in particular, P can be concatenated with an $\mathbf{S} \rightsquigarrow i$ path that avoids $\mathbf{T}^\star$ up to i (otherwise i would be separated from $\mathbf{S}$ by $\mathbf{T}^\star$ and α_i would inherit a nonzero contribution through i's first hit in $\mathbf{T}^\star$). Consequently there exists at least one directed path from $\mathbf{S}$ to x that avoids $\mathbf{T}^\star$ and can be continued by P, contradicting that $\mathbf{T}^\star$ intercepts all $\mathbf{S} \rightsquigarrow \mathbf{X}$ paths. Hence every $i \rightsquigarrow \mathbf{X}$ path hits $\mathbf{T}^\star$, i.e., $\mathbf{T}^\star$ is a bottleneck from V_i to $\mathbf{X}$.

If $\alpha_i \neq 0$, then $\mathbf{T}^\star$ is not a bottleneck from V_i to $\mathbf{X}$. If every $i \rightsquigarrow x$ path met $\mathbf{T}^\star$, then any ω whose latent terms have been canceled via constraints indexed by $\mathbf{T}^\star$ would give $\nu_i = 0$ (all contributions must pass through $\mathbf{T}^\star$ and are nullified), contradicting $\alpha_i \neq 0$. Thus i has a path to some $x \in \mathbf{X}$ that avoids $\mathbf{T}^\star$.

Combining the two implications yields (ii) with $\mathbf{T} = \mathbf{T}^\star$.

($\Leftarrow$) (i)–(ii) $\Longrightarrow$ constructibility. Assume (i)–(ii) hold for some $\mathbf{T} \subseteq \mathbf{V}$. Let

$$\mathbf{S} \;:=\; \{\, i \in \mathbf{V} :\; \alpha_i \neq 0 \,\} \;=\; \{\, i \in \mathbf{V} :\; \mathbf{T} \text{ is not a bottleneck from } V_i \text{ to } \mathbf{X} \,\}.$$

By (i) and Lemma 16, $\mathbf{T}$ is the LM bottleneck from $\mathbf{T}$ to $\mathbf{X}$ and, therefore, from $\mathbf{S}$ to $\mathbf{X}$ as well (latest with respect to any minimal bottleneck for $(\mathbf{S}, \mathbf{X})$).

Consider the vertex–splitting network G' used in Lemma 15. Let (S_f, T_f) be the unique t-closest minimum cut in G' (induced by any maximum flow); it induces $\mathbf{T}$ by $\mathbf{T} = \{v \in \mathbf{V} : v^- \in S_f,\ v^+ \in T_f\}$. Choose $|\,\mathbf{T}\,|$ distinct nodes $\{x_1, \ldots, x_{|\mathbf{T}|}\} \subseteq \mathbf{X}$ reached by the $|\mathbf{T}|$ vertex–disjoint paths guaranteed by Menger's theorem from $\mathbf{T}$ to $\mathbf{X}$ (tightness of the cut). Define ω supported on $\{x_1, \ldots, x_{|\mathbf{T}|}\}$ as the unique solution to the linear system that zeroes the contributions flowing through $\mathbf{T}$ (the $|\mathbf{T}| \times |\mathbf{T}|$ system is non-singular because the $\mathbf{T} \rightsquigarrow \{x_\ell\}$ paths are vertex-disjoint). Then 1) for any i such that $\mathbf{T}$ is a bottleneck from V_i to $\mathbf{X}$, every $i \rightsquigarrow \mathbf{X}$ path must traverse some $t \in \mathbf{T}$, hence its contribution to ν_i is canceled by construction; thus $\nu_i = 0$. 2) for any i such that $\mathbf{T}$ is not a bottleneck from V_i to $\mathbf{X}$, there exists a path $P : i \rightsquigarrow x$ that avoids $\mathbf{T}$. Since our constraints only cancel flows that pass through $\mathbf{T}$, the term corresponding to P survives so $\nu_i \neq 0$.

Finally, impose additional linear constraints (orthogonality) on ω to remove latent terms (these constraints are independent of the $\mathbf{T}$-cancellation because the latter acts only on flows that cross $\mathbf{T}$), which is always possible as we only eliminate $|\mathbf{T}|$ directions associated with the cut while retaining degrees of freedom on $\mathbf{X}$. Thus α is constructible by $\mathbf{X}$. □

Corollary 1. *Any noise combination α is constructible by $\tilde{\mathbf{X}} \subseteq \mathbf{X}$ if and only if (i) $\exists \mathbf{T} \subseteq \mathbf{V}$ s.t. $\mathbf{T}$ is the LM bottleneck of $\mathbf{T}$ to $\mathbf{X}$ in $\mathcal{G}$. (ii) $\forall V_i \in \mathbf{V}$, $\alpha_i = 0 \Longleftrightarrow \mathbf{T}$ is a bottleneck from V_i to $\mathbf{X}$ in $\mathcal{G}$.*

A.3.2 Illustration of Non-identifiability Issue on Fig. 1a and 1b

Z \ Y	$\{X_1\}$	$\{X_2\}$	$\{X_3\}$	$\{X_1, X_2\}$	$\{X_1, X_3\}$	$\{X_2, X_3\}$	$\{X_1, X_2, X_3\}$
$\{X_1\}$	1	1	1	2	2	2	2
$\{X_2\}$	1	1	1	2	2	2	3
$\{X_3\}$	1	1	1	2	2	2	3

Table 3: TIN value of different $\mathbf{Y}$ and $\mathbf{Z}$ of Fig. 1a

Z \ Y	$\{X_1\}$	$\{X_2\}$	$\{X_3\}$	$\{X_1, X_2\}$	$\{X_1, X_3\}$	$\{X_2, X_3\}$	$\{X_1, X_2, X_3\}$
$\{X_1\}$	1	1	1	2	2	2	2
$\{X_2\}$	1	1	1	2	2	2	3
$\{X_3\}$	1	1	1	2	2	2	3

Table 4: TIN value of different $\mathbf{Y}$ and $\mathbf{Z}$ of Fig. 1b

Proof. We use $\mathcal{G}_1$ and $\mathcal{G}_2$ to represent the causal graph in Fig. 1a, and Fig. 1b, respectively. By some simple calculations, we can find that both $\mathcal{G}_1$ and $\mathcal{G}_2$ have no rank-deficiency constraints. Thus, for each pair of $(\mathbf{Z}, \mathbf{Y})$, $\text{rank}_{\mathcal{G}_1}(\Sigma_{\mathbf{Z},\mathbf{Y}}) = \min(\mathbf{Z}, \mathbf{Y}) = \text{rank}_{\mathcal{G}_2}(\Sigma_{\mathbf{Z},\mathbf{Y}})$. In addition, as we can see in Table 3 and 4, $\mathcal{G}_1$ and $\mathcal{G}_2$ have the same TIN value for each $(\mathbf{Z}, \mathbf{Y})$. As $\text{GIN}(\mathbf{Z}, \mathbf{Y})$ is satisfied if and only if $\text{TIN}(\mathbf{Z}, \mathbf{Y}) = \text{rank}(\Sigma_{\mathbf{Z},\mathbf{Y}}) < |\mathbf{Y}|$ (Dai et al., 2022), whether the GIN condition is satisfied for a certain pair $(\mathbf{Z}, \mathbf{Y})$ keeps the same in $\mathcal{G}_1$ and $\mathcal{G}_2$. □

A.3.3 Proof of Lemma 1

Proof. $\mathrm{NS}(\mathbf{Z}) = \mathrm{Anc}(\mathbf{Z})$. By Theorem 4, $\mathrm{Anc}(\mathbf{Z})$ is constructible. Therefore, according to the definition of constructible noise combination, we can always find a non-zero coefficient ω_2 such that $\mathrm{NS}(\omega_2^\top \mathbf{Z}) = \mathrm{Anc}(\mathbf{Z})$. Since $\omega_1^\top \mathbf{Y} \perp\!\!\!\perp \mathbf{Z}$, we naturally obtain $\omega_1^\top \mathbf{Y} \perp\!\!\!\perp \omega_2^\top \mathbf{Z}$. □

A.3.4 Proof of Remark 1

Proof. By Theorem 4, we can enumerate all constructive noise combinations by finding all LM bottlenecks. All LM bottlenecks can be identified by testing for Lemma 16. All constructive noise combinations by $\{X_1, X_2\}$, $\{X_1, X_3\}$ and $\{X_2, X_3\}$ in Fig. 1a are shown in Tab. 5. All constructive noise combinations by $\{X_1, X_2\}$, $\{X_1, X_3\}$ and $\{X_2, X_3\}$ in Fig. 1b are shown in Tab. 6.

$\mathbf{Z} = \{X_1, X_2\}$	$\emptyset$	$\{L\}$	$\{X_1\}$	$\{X_2\}$
	$\{E_L, E_1, E_2\}$	$\{E_1, E_2\}$	$\{E_L, E_2\}$	$\{E_L, E_1\}$
$\mathbf{Z} = \{X_1, X_3\}$	$\emptyset$	$\{L\}$	$\{X_1\}$	$\{X_3\}$
	$\{E_L, E_1, E_2, E_3\}$	$\{E_1, E_2, E_3\}$	$\{E_L, E_2, E_3\}$	$\{E_L, E_1, E_2\}$
$\mathbf{Z} = \{X_2, X_3\}$	$\emptyset$	$\{L\}$	$\{X_2\}$	$\{X_3\}$
	$\{E_L, E_1, E_2, E_3\}$	$\{E_1, E_2, E_3\}$	$\{E_L, E_3\}$	$\{E_L, E_1, E_2\}$

Table 5: All constructive noise combinations by $\{X_1, X_2\}$, $\{X_1, X_3\}$ and $\{X_2, X_3\}$ in Fig. 1a. Each constructive noise combination is shown together with its corresponding LM bottleneck in a pairwise manner.

$\mathbf{Z} = \{X_1, X_2\}$	$\emptyset$	$\{L\}$	$\{X_1\}$	$\{X_2\}$
	$\{E_L, E_1, E_2, E_3\}$	$\{E_1, E_2, E_3\}$	$\{E_L, E_2, E_3\}$	$\{E_L, E_1, E_3\}$
$\mathbf{Z} = \{X_1, X_3\}$	$\emptyset$	$\{L\}$	$\{X_1\}$	$\{X_3\}$
	$\{E_L, E_1, E_3\}$	$\{E_1, E_3\}$	$\{E_L, E_3\}$	$\{E_L, E_1\}$
$\mathbf{Z} = \{X_2, X_3\}$	$\emptyset$	$\{L\}$	$\{X_2\}$	$\{X_3\}$
	$\{E_L, E_1, E_2, E_3\}$	$\{E_1, E_2, E_3\}$	$\{E_L, E_1, E_3\}$	$\{E_L, E_2\}$

Table 6: All constructive noise combinations by $\{X_1, X_2\}$, $\{X_1, X_3\}$ and $\{X_2, X_3\}$ in Fig. 1b. Each constructive noise combination is shown together with its corresponding LM bottleneck in a pairwise manner.

From Tab. 5, when $\mathbf{Z} = \{X_1, X_2\}, \mathbf{Y} = \{X_2, X_3\}$, we can construct $\mathrm{NS}(\omega_1^\top \mathbf{Z}) = \{E_1, E_2\}$ and $\mathrm{NS}(\omega_2^\top \mathbf{Y}) = \{E_L, E_3\}$ with non-zero $\omega_1, \omega_2 \in \mathbb{R}^2$. In contrast, in Tab. 6, each pair of constructive noise combinations by $\mathbf{Z}$ and $\mathbf{Y}$ has shared noise components, thus cannot be independent. The conclusion for $\mathbf{Z} = \{X_1, X_3\}$ and $\mathbf{Y} = \{X_2, X_3\}$ can be analyzed similarly.

□

A.3.5 Proof of Lemma 2

Lemma 2 (Indeterminacy of CICA). *Given Assump. 1, let $\mathbf{X}$ be m observed variables, $\mathbf{W}_1, \mathbf{W}_2 \in \mathbb{R}^{m\times m}$ be two p-order CICA solutions for $\mathbf{X}$. The following two statements are equivalent:*

- *(i) There exists p latent variables $\mathbf{L}$ such that, writing $\mathbf{Z}^{(k)} := \mathbf{W}_k\mathbf{X}$, the components of $\mathbf{Z}^{(k)}$ are mutually conditionally independent given $\mathbf{L}$ for $k \in \{1, 2\}$.*
- *(ii) There exist a permutation matrix $\mathbf{P}_\pi$ (for some permutation π of $[m]$) and a non-singular diagonal matrix $\mathbf{D}$ such that $\mathbf{W}_2 = \mathbf{P}_\pi \mathbf{D} \mathbf{W}_1$.*

Proof. Under Assumption 1 there exist an invertible $\mathbf{A} \in \mathbb{R}^{m\times m}$, a latent vector $\mathbf{L} \in \mathbb{R}^p$, a matrix $\mathbf{M} \in \mathbb{R}^{m\times p}$, and a noise $\mathbf{E} = (E_1, \ldots, E_m)^\top$ with mutually independent coordinates, $\mathbf{E} \perp\!\!\!\perp \mathbf{L}$, finite non-zero variances, and with at most one Gaussian coordinate, such that $\mathbf{X} = \mathbf{A}\mathbf{S}$ and $\mathbf{S} = \mathbf{M}\mathbf{L} + \mathbf{E}$. For $k \in \{1, 2\}$ write $\mathbf{Z}^{(k)} := \mathbf{W}_k\mathbf{X}$ and set $\mathbf{B}_k := \mathbf{W}_k\mathbf{A}$ (hence $\mathbf{Z}^{(k)} = \mathbf{B}_k\mathbf{S}$).

For every ℓ, $\mathbf{Z}^{(k)} \mid \{\mathbf{L}=\ell\} = \mathbf{B}_k(\mathbf{ML}+\mathbf{E}) \mid \{\mathbf{L}=\ell\} = (\mathbf{B}_k\mathbf{M})\,\ell \;+\; \mathbf{B}_k\mathbf{E}$. Thus, for each k, the coordinates of $\mathbf{Z}^{(k)}$ are mutually independent given $\mathbf{L}$ if and only if the coordinates of $\mathbf{B}_k\mathbf{E}$ are mutually independent (a deterministic shift $(\mathbf{B}_k\mathbf{M})\ell$ does not affect independence). In particular, we have an ICA model with independent sources $\mathbf{E}$ and mixing matrices $\mathbf{B}_k$.

($\Rightarrow$) Assume (i) holds: there exists a single latent $\mathbf{L}$ such that $\mathbf{Z}^{(k)}$ has mutually independent coordinates conditional on $\mathbf{L}$ for $k=1,2$. By the reduction above, both $\mathbf{B}_1\mathbf{E}$ and $\mathbf{B}_2\mathbf{E}$ have mutually independent coordinates. Since $\mathbf{E}$ has mutually independent coordinates with at most one Gaussian, the standard ICA identifiability implies that the only invertible linear maps sending $\mathbf{E}$ to a vector with independent coordinates are permutation–scalings. Concretely, there exists a permutation matrix $\mathbf{P}_\pi$ and a non-singular diagonal matrix $\mathbf{D}$ such that $\mathbf{B}_2 = \mathbf{P}_\pi\mathbf{D}\,\mathbf{B}_1$. Multiplying on the right by $\mathbf{A}^{-1}$ (recall $\mathbf{B}_k = \mathbf{W}_k\mathbf{A}$) yields $\mathbf{W}_2 = \mathbf{P}_\pi\mathbf{D}\,\mathbf{W}_1$.

($\Leftarrow$) Assume (ii) holds: $\mathbf{W}_2 = \mathbf{P}_\pi\mathbf{D}\,\mathbf{W}_1$ with $\mathbf{P}_\pi$ a permutation and $\mathbf{D}$ diagonal nonsingular. Let $\mathbf{L}$ be any latent vector for which $\mathbf{W}_1$ is a p-order CICA solution (which exists by assumption that $\mathbf{W}_1$ is a CICA solution). Then for almost every ℓ,

$$\mathbf{Z}^{(2)} \mid \{\mathbf{L}=\ell\} = \mathbf{W}_2\mathbf{X} \mid \{\mathbf{L}=\ell\} = \mathbf{P}_\pi\mathbf{D}\,\mathbf{W}_1\mathbf{X} \mid \{\mathbf{L}=\ell\} = \mathbf{P}_\pi\mathbf{D}\,\mathbf{Z}^{(1)} \mid \{\mathbf{L}=\ell\}.$$

Since permutation and nonzero per-coordinate scaling preserve mutual independence of coordinates, the coordinates of $\mathbf{Z}^{(2)}$ are mutually independent given $\mathbf{L}$ whenever those of $\mathbf{Z}^{(1)}$ are. Hence (i) holds. Therefore, the two statements are equivalent. $\square$

A.3.6 PROOF OF LEMMA 3

Lemma 3. *Let $\mathbf{X}$ be m observed variables, and $\mathbf{W}$ be a p-order CICA solution of $\mathbf{X}$. Let $\mathbf{X}' = \mathbf{WX}$, $\mathbf{Y}$ and $\mathbf{Z}$ are two subsets of $\mathbf{X}'$, then if $\max\{|\mathbf{Y}|, |\mathbf{Z}|\} > p$, $\omega_1^\top\mathbf{Y}' \perp\!\!\!\perp \omega_2^\top\mathbf{Z}'$ has a non-zero solution (ω_1, ω_2) for $(\mathbf{Y}', \mathbf{Z}')$, where $\mathbf{Y}' = \{X_i | \sum_{X_k\in\mathbf{Y}} \mathbf{W}_{k,i} \neq 0\}$, $\mathbf{Z}'$ are defined similarly.*

Proof. $\mathbf{Y} = \mathbf{W}_{\mathbf{Y},:}\mathbf{Y}'$, $\mathbf{Z} = \mathbf{W}_{\mathbf{Z},:}\mathbf{Z}'$, $\mathbf{Y}$ and $\mathbf{Z}$ are conditional independent given p latent variables. Since $\max\{|\mathbf{Y}|, |\mathbf{Z}|\} > p$, without losing generality, we assume $|\mathbf{Y}| > p$. Then we can find a non-zero ω_1 that $\omega_1^\top\mathbf{Y} \perp\!\!\!\perp \mathbf{Z}$. By Lemma 1, there exist a non-zero ω_2 that makes $\omega_1^\top\mathbf{Y} \perp\!\!\!\perp \omega_2^\top\mathbf{Z}$. Thus, $\omega_1^\top\mathbf{W}_{\mathbf{Y},:}\mathbf{Y}' \perp\!\!\!\perp \omega_2^\top\mathbf{W}_{\mathbf{Z},:}\mathbf{Z}'$. $\square$

A.3.7 PROOF OF LEMMA 4

Lemma 4. *For an observed variable set $\mathbf{X}$ with $|\mathbf{X}| = m$, denote $p = p_{min}(\mathbf{X})$. Suppose $m \geq 2p+2$, and set $\mathbf{X}' := \mathbf{WX}$, then $\mathbf{W}$ is a p-order CICA solution of $\mathbf{X}$ if and only if for every pair of disjoint coordinate subsets $\mathbf{X_1}, \mathbf{X_2}$ of $\mathbf{X}'$ with $|\mathbf{X_1}| = |\mathbf{X_2}| = p+1$, $\det(\Sigma_{\mathbf{X_1},\mathbf{X_2}}) = 0$, where $\Sigma := \mathrm{Cov}(\mathbf{X}')$ denotes the covariance matrix on $\mathbf{X}'$ and $\Sigma_{\mathbf{X_1},\mathbf{X_2}}$ is the $(p+1)\times(p+1)$ sub-matrix of Σ with rows indexed by $\mathbf{X_1}$ and columns by $\mathbf{X_2}$.*

Proof. ($\Rightarrow$) Necessity. If W is a p-order CICA solution, there exist a p-dimensional latent vector L and independent noises $E = (E_1, \ldots, E_m)$ (independent of L) such that $Z_i = a_i^\top L + E_i, i = 1, \ldots, m$. Hence $\Sigma = \underbrace{A\Sigma_L A^\top}_{\text{rank}\leq p} + \underbrace{(\mathrm{diag}(\mathrm{Var}(E_i))}_{\text{diagonal}}$. For disjoint $\mathbf{X}_1, \mathbf{X}_2$ the diagonal term vanishes, so $\Sigma_{\mathbf{X}_1,\mathbf{X}_2} = A_{\mathbf{X}_1}\Sigma_L A_{\mathbf{X}_2}^\top$ has rank at most p. Therefore $\det(\Sigma_{\mathbf{X}_1,\mathbf{X}_2}) = 0$ for every such pair.

($\Leftarrow$) Sufficiency. Assume that for every disjoint $\mathbf{X}_1, \mathbf{X}_2$ of size $p+1$, $\mathrm{rank}(\Sigma_{\mathbf{X_1},\mathbf{X_2}}) \leq p$ (equivalently, all $(p+1)$-minors vanish). By the trek separation theorem, for each such pair there exists a t-separating pair (L_1, L_2) with $|L_1| + |L_2| \leq p$ that t-separates $\mathbf{X_1}$ from $\mathbf{X_2}$. Since $p = p_{\min}(X)$, no separator of size $< p$ works uniformly; hence the minimum size is exactly p for all these pairs.

Consider some $(\mathbf{X}_A, \mathbf{X}_B)$ with $X_A \cap X_b = \emptyset$ and both $|X_A|$ and $|X_b|$ equals $p+1$, let (L_1, L_2) be a minimal t-separator for this pair, so $|L_1| + |L_2| = p$. We claim that (L_1, L_2) t-separates every other disjoint $(\mathbf{X}_C, \mathbf{X}_D)$ with $|\cdot| = p+1$ and is minimal for that pair as well. Suppose (L_1, L_2) does not t-separate $\mathbf{X}_C$ from $\mathbf{X}_D$. Then there exists a trek from some $c \in \mathbf{X}_C$ to $d \in \mathbf{X}_D$ avoiding $L_1 \cup L_2$. Because $|L_1| + |L_2| = p$ while $|\mathbf{X}_A| = |\mathbf{X}_B| = p+1$, Menger's theorem for treks imply that there are p vertex-disjoint treks connecting $\mathbf{X}_A \setminus \{a\}$ to $\mathbf{X}_B \setminus \{b\}$ for some $a \in \mathbf{X}_A$, $b \in \mathbf{X}_B$, all avoiding $L_1 \cup L_2$. Together with the trek $c \rightsquigarrow d$ (also avoiding $L_1 \cup L_2$) we obtain $p{+}1$ vertex-disjoint treks between the modified sets $\mathbf{X}'_A = (\mathbf{X}_A \setminus \{a\}) \cup \{c\}$ and $\mathbf{X}'_B = (\mathbf{X}_B \setminus \{b\}) \cup \{d\}$, hence $\mathrm{rank}(\Sigma_{\mathbf{X}'_A,\mathbf{X}'_B}) \geq p+1$, contradicting our hypothesis. Thus (L_1, L_2) t-separates every such pair. If for some $(\mathbf{X}_C, \mathbf{X}_D)$ there were a smaller separator (L'_1, L'_2) with $|L'_1| + |L'_2| < p$, then $\mathrm{rank}(\Sigma_{\mathbf{X}_C,\mathbf{X}_D}) \leq |L'_1| + |L'_2| < p$, again contradicting the assumption that all those ranks equal p by minimality of $p = p_{\min}(X)$. Hence the same (L_1, L_2) is a minimal t-separator (of size p) for every such pair. We fix this global separator (L_1, L_2).

Let $i \neq j$ be nodes outside $L_1 \cup L_2$. If there existed a trek from i to j avoiding $L_1 \cup L_2$, then by the same replacement argument as above we could build $p{+}1$ vertex-disjoint treks between some disjoint $(p{+}1)$-subsets, forcing a cross-rank $\geq p+1$, which is a contradiction. Therefore, every trek from i to j meets $L_1 \cup L_2$, i.e., all covariance between distinct observed coordinates flows through (L_1, L_2). Equivalently, Σ admits a decomposition $\Sigma = A\,\Sigma_L\,A^\top + D$ with $\mathrm{rank}(A\Sigma_L A^\top) \leq p$ and diagonal D collecting variances.

Under Assumption 1, noises are mutually independent and independent of the latents. The diagonal D found in Step 2 implies that each observed coordinate has a unique private noise, and distinct coordinates share no private noise. Therefore, we may write, for some p-vector L, $Z_i = a_i^\top L + E_i, E = (E_1, \ldots, E_m)$ mutually independent, $E \perp\!\!\!\perp L$. Thus the coordinates of Z are mutually independent given L, i.e., W is a p-order CICA solution.

Combining both directions proves the equivalence. □

A.3.8 PROOF OF LEMMA 5

Lemma 5. *For an observed variable set $\mathbf{X}$ with $|\mathbf{X}| = m$, suppose that $p_{min}(\mathbf{X}) = 1$ and $m \geq 3$ hold, set $\mathbf{X}' \triangleq \mathbf{W}\mathbf{X}$, then the invertible matrix $\mathbf{W}$ is a 1-order CICA solution of $\mathbf{X}$ if and only if for every ordered triple (X'_i, X'_j, X'_k) of $\mathbf{X}'$, $\{X'_i, X'_j\}$ and X'_k satisfies the Triad constraint.*

Proof. ($\Rightarrow$) Necessity. If $\mathbf{W}$ is a 1-order CICA solution, then for some latent L we have $Z_i = \tilde{m}_i L + \tilde{E}_i$ with $\tilde{E} = (\tilde{E}_1, \ldots, \tilde{E}_m)$ mutually independent, $\tilde{E} \perp\!\!\!\perp L$, and $\mathrm{Var}(\tilde{E}_i) \in (0, \infty)$. For $i \neq j \neq k$, $\mathrm{Cov}(Z_j, Z_k) = \tilde{m}_j \tilde{m}_k \mathrm{Var}(L)$ and hence

$$E_{(i,j|k)} = \tilde{m}_k \mathrm{Var}(L)\,(\tilde{m}_j Z_i - \tilde{m}_i Z_j) = \tilde{m}_k \mathrm{Var}(L)\,(\tilde{m}_j \tilde{E}_i - \tilde{m}_i \tilde{E}_j),$$

which depends only on $(\tilde{E}_i, \tilde{E}_j)$ and is independent of $Z_k = \tilde{m}_k L + \tilde{E}_k$. Thus the Triad constraint holds for all distinct triples.

($\Leftarrow$) Sufficiency. Assume the Triad constraint holds for every distinct (i, j, k). Fix k and set

$$\beta_{ik} := \frac{\mathrm{Cov}(Z_i, Z_k)}{\mathrm{Var}(Z_k)}, \qquad E_i^{(k)} := Z_i - \beta_{ik} Z_k \quad (i \neq k).$$

Then for any distinct i, j, k, $E_{(i,j|k)} = \mathrm{Var}(Z_k)\big(\beta_{jk} E_i^{(k)} - \beta_{ik} E_j^{(k)}\big) \perp\!\!\!\perp Z_k$. Varying (i, j), the family of non-degenerate linear forms $\{\beta_{jk} E_i^{(k)} - \beta_{ik} E_j^{(k)}\}_{i \neq j \neq k}$ is independent of Z_k. By the classical characterization of independence of linear forms for non-Gaussian sources, this is only possible if the vector $E^{(k)} = (E_i^{(k)})_{i \neq k}$ has mutually independent coordinates and is independent of Z_k. Therefore, we obtain a one-factor representation

$$Z_i = \beta_{ik}\, L + E_i^{(k)}, \qquad L := Z_k, \qquad E^{(k)} \perp\!\!\!\perp L, \text{ and } \{E_i^{(k)}\}_{i \neq k} \text{ mutually independent,}$$

which means the coordinates of Z are mutually independent given L. Hence W is a 1-order CICA solution. Combining both directions proves the claim. □

A.3.9 PROOF OF LEMMA 6

Lemma 6. $\mathbf{I} - \mathbf{B}_{\mathbf{X},\mathbf{X}}$ *is a $p_{min}(\mathbf{X})$-order CICA solution of $\mathbf{X}$ with latent conditional set* $\mathrm{LPa}(\mathbf{X})$.

Proof. In the setting of our paper, $\mathbf{A}^{-1}_{\mathbf{X},\mathbf{X}} = \mathbf{I} - \mathbf{B}_{\mathbf{X},\mathbf{X}}$. In the proof of Theorem 3, we prove that $\mathbf{A}^{-1}_{\mathbf{X},\mathbf{X}}\mathbf{X}$ deletes all the outgoing edges from $\mathbf{X}$ graphically. Therefore, $\mathbf{A}^{-1}_{\mathbf{X},\mathbf{X}}\mathbf{X}$ is conditional independent given $\mathrm{LPa}(\mathbf{X})$. Given Condition 1 holds, $p_{min}(\mathbf{X}) = |\,\mathrm{LPa}(\mathbf{X})|$. Thus, $\mathbf{I} - \mathbf{B}_{\mathbf{X},\mathbf{X}}$ is a $p_{min}(\mathbf{X})$-order CICA solution of $\mathbf{X}$ with latent conditional set $\mathrm{LPa}(\mathbf{X})$. □

A.3.10 PROOF OF LEMMA 7

Lemma 7. *Suppose* $\mathbf{W}$ *is a* $p_{min}(\mathbf{X})$*-order CICA solution of* $\mathbf{X}$ *whose latent conditional set is* $\mathrm{LPa}(\mathbf{X})$*, there exists a unique row permutation matrix* $\mathbf{P}$ *that makes* $\mathbf{PW}$ *whose diagonal elements have non-zero values, simultaneously.*

Proof. By Lemma 2 and Lemma 6, we can find a permutation matrix $\mathbf{P}$ and non-singular diagonal matrix $\mathbf{D}$ that makes $\mathbf{W} = \mathbf{PD}(\mathbf{I} - \mathbf{B}_{\mathbf{X},\mathbf{X}})$. Subsequent proofs can be analogized to Lemma 1 in (Shimizu et al., 2006). □

A.3.11 PROOF OF LEMMA 8

Lemma 8. $\mathbf{I} - \mathbf{B}_{\mathbf{X},\mathbf{X}} \in \arg\min\{\|\mathbf{W}\|_0 : \mathbf{W}$ *is a* $p_{min}(\mathbf{X})$*-order CICA solution of* $\mathbf{X}\}$. .

Proof. For $\omega \in \mathbb{R}^m$, denote $\mathbf{X}' = \alpha^\top \mathbf{E} = \omega^\top \mathbf{X} = \omega^\top \mathbf{AE} = \omega^\top (\mathbf{I} - \mathbf{B}_{\mathbf{X},\mathbf{X}})\mathbf{E}$, where $\alpha \in \mathbb{R}^{m+d}$. As $\mathbf{A}_{\mathbf{X},\mathbf{X}}$ is a non-singular matrix, denote the row indices corresponding to $\mathbf{X}$ as $\alpha^{\mathbf{X}}$ for convenience, then we have $\mathbf{A}_{\mathbf{X},\mathbf{X}}^\top \omega = \alpha^{\mathbf{X}}$, $\omega = \mathbf{A}_{\mathbf{X},\mathbf{X}}^{-T} \alpha^{\mathbf{X}} = (\mathbf{I} - \mathbf{B}_{\mathbf{X},\mathbf{X}})^T \alpha^{\mathbf{X}} = \alpha^{\mathbf{X}} - \mathbf{B}_{\mathbf{X},\mathbf{X}}^T \alpha^{\mathbf{X}}$. $\alpha^{\mathbf{L}}$ is defined similarly, then $\alpha^{\mathbf{L}} = \mathbf{A}_{\mathbf{L},\mathbf{X}}^\top \omega = \mathbf{A}_{\mathbf{L},\mathbf{X}}^\top (\mathbf{I} - \mathbf{B}_{\mathbf{X},\mathbf{X}})^T \alpha^{\mathbf{X}}$. In summary, we can represent ω and $\alpha^{\mathbf{L}}$ as the linear combination of $\alpha^{\mathbf{X}}$:

$$\left[\frac{\alpha^{\mathbf{L}}}{\alpha^{\mathbf{X}}}\right] = \left[\frac{\mathbf{A}_{\mathbf{L},\mathbf{X}}^\top}{\mathbf{A}_{\mathbf{X},\mathbf{X}}^\top}\right]\omega \qquad \Longrightarrow \qquad \left[\frac{\alpha^{\mathbf{L}}}{\omega}\right] = \left[\frac{\mathbf{A}_{\mathbf{L},\mathbf{X}}^\top \mathbf{A}_{\mathbf{X},\mathbf{X}}^{-\mathbf{T}}}{\mathbf{A}_{\mathbf{X},\mathbf{X}}^{-\mathbf{T}}}\right]\alpha^{\mathbf{X}} \tag{5}$$

Here, since we focus mainly on the sparsity of $\mathbf{W}$ (i.e., $\|\mathbf{W}\|_0$) rather than the specific value in $\mathbf{W}$, we use 0 to represent a value 0, and $\times$ represents a nonzero value as (Ghassami et al., 2020).

According to Lemma 5, X' is conditionally independent given a latent variable. Then, for $\mathbf{W} = \mathbf{A}_{\mathbf{X},\mathbf{X}}^{-1}$, denote its corresponding noise coefficients of observed variables $\alpha_X = [\alpha_{X,1}, \alpha_{X,2}, \cdots, \alpha_{X,m}]$, we have $\alpha_{X,i} = [\underbrace{0, \cdots, 0}_{(i-1)\text{-times}}, \times, \underbrace{0, \cdots, 0}_{(m-i)\text{-times}}]^\top$, $\alpha_{L,i} = [\times, \cdots, \times]^\top$. For other feasible solutions except for $\mathbf{A}_{\mathbf{X},\mathbf{X}}^{-1}$, it corresponds to choosing d variables in $d + m$ independent noises.

If $\mathbf{W}$ is a 1-order CICA solution whose latent conditional set is $\mathrm{LPa}(\mathbf{X})$, then we can find a permutation matrix $\mathbf{P}$ and non-singular diagonal matrix $\mathbf{D}$ that makes $\mathbf{W} = \mathbf{PDA}_{\mathbf{X},\mathbf{X}}^{-1}$. As the permutation matrix $\mathbf{P}$ and non-singular diagonal matrix $\mathbf{D}$ do not change the sparsity pattern of $\mathbf{W}$, we can analyze $\mathbf{W} = \mathbf{A}_{\mathbf{X},\mathbf{X}}^{-1}$ directly for convenience.

For the j-th row of $\mathbf{W}$, we have exactly one $\times$ in each column of $\alpha^{\mathbf{X}}$. As $\mathbf{A}_{\mathbf{X},\mathbf{X}}^{-1} = \mathbf{I} - \mathbf{B}_{\mathbf{X},\mathbf{X}}$, $\mathbf{W} = (\mathbf{I} - \mathbf{B}_{\mathbf{X},\mathbf{X}}^\top)\alpha^{\mathbf{X}}$. For $\forall t \in [m]$, $\mathbf{W}_{j,t} = (\mathbf{I}_{j,:} - \mathbf{B}_{j,\mathbf{X}})\alpha_{:,t}^{\mathbf{X}} = (\mathbf{I}_{j,t} - \mathbf{B}_{j,t})\alpha_{t,t}^{\mathbf{X}}$.

Case (i): If $t = j$ ($\mathbf{I}_{j,t} \neq 0$), then $\mathbf{W}_{j,j} = \alpha_{j,j}^{\mathbf{X}} = \times$.

Case (ii): If $X_t \in \mathrm{Pa}(X_j)$ ($\mathbf{B}_{j,t} \neq 0$), then $\mathbf{W}_{j,t} = -\mathbf{B}_{j,t}\alpha_{t,t}^{\mathbf{X}} = \times$.

Case (iii): If X_t does not fall into any of the two cases above, then $\mathbf{W}_{j,t} = 0$.

In summary, $\forall t \in [m]$, $\mathbf{W}_{j,t} \neq 0 \Longleftrightarrow X_t \in \{X_j\} \cup \mathrm{Pa}(X_j)$. Thus, $\|\mathbf{W}\|_0 = |\mathbf{X}| + |\mathbf{G}_{\mathbf{X}}|$.

If $\mathbf{W}$ is a 1-order CICA solution whose latent conditional set is not $\mathrm{LPa}(\mathbf{X})$, then $\mathbf{X}'$ is conditionally independent given another latent variable than L. Without loss of generality, we assume that $\mathbf{X}'$ is conditionally independent given the exogenous noise of X_k, E_k. Therefore, $E_k \in \mathrm{NS}(X_j')$ for any $j \in [m]$. In other words, we have $\alpha_{\mathbf{X},j} \in \mathbb{R}^m$ has a $\times$ in its k-th position. Besides, exact only one $\alpha_{\mathbf{X},j}$ has a $\times$ in j-th position for $j \in [m] \setminus \{k\}$. On the other hand, we have $\alpha^{\mathbf{L}} = [\underbrace{0, \cdots, 0}_{(k-1)\text{-times}}, \times, \underbrace{0, \cdots, 0}_{(m-k)\text{-times}}]$. Essentially, in this scenario we exchange the position between E_L and E_k compared to $\mathbf{W} \sim \mathbf{A}_{\mathbf{X},\mathbf{X}}^{-1}$.

For example, Equ. (6) presents an example of $\alpha^{\mathbf{X}}$ when $k = 3$.

$$\begin{bmatrix} \times & 0 & 0 & 0 & \cdots & 0 \\ 0 & \times & 0 & 0 & \cdots & 0 \\ \times & \times & \times & \times & \cdots & \times \\ 0 & 0 & 0 & \times & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & \times \end{bmatrix} \tag{6}$$

Based on the expression of $\alpha^{\mathbf{X}}$ above, we can now check the sparsity of $\|\mathbf{W}\|$ of each row.

For the k-th row of $\mathbf{W}$, we have exactly one $\times$ in $\alpha^{\mathbf{X}}_{:,k}$, in the k-th rows. In addition, $\alpha^{\mathbf{L}}_{:,k} = \times$. Therefore, the support of $\alpha^{\mathbf{L}}_{:,k}$ is exactly the same as in the scenario $\mathbf{W} \sim \mathbf{A}^{-1}_{\mathbf{X},\mathbf{X}}$.

For the j-th column of $\mathbf{W}$ with $j \neq k$, we have two $\times$ in $\alpha^{\mathbf{X}}_{:,j}$, in the j-th and k-th rows, respectively. As $\mathbf{A}^{-1}_{\mathbf{X},\mathbf{X}} = \mathbf{I} - \mathbf{B}_{\mathbf{X},\mathbf{X}}$, $\mathbf{W} = (\mathbf{I} - \mathbf{B}^{\top}_{\mathbf{X},\mathbf{X}})\alpha^{\mathbf{X}}$. For $\forall t \in [m]$, $\mathbf{W}_{t,j} \neq 0 \iff (\mathbf{I}_{t,:} - \mathbf{B}_{t,\mathbf{X}})\alpha^{\mathbf{X}}_{:,j} \neq 0 \iff (\mathbf{I}_{t,j} - \mathbf{B}_{t,j})\alpha^{\mathbf{X}}_{j,j} + (\mathbf{I}_{t,k} - \mathbf{B}_{t,k})\alpha^{\mathbf{X}}_{k,j} \neq 0$.

Case (i): If $t = j$ ($\mathbf{I}_{t,j} \neq 0, \mathbf{I}_{t,k} = 0$), then $\mathbf{W}_{t,j} = (\mathbf{I}_{j,j} - \mathbf{B}_{j,j})\alpha^{\mathbf{X}}_{j,j} + (\mathbf{I}_{j,k} - \mathbf{B}_{j,k})\alpha^{\mathbf{X}}_{k,j} = \alpha^{\mathbf{X}}_{j,j} - \mathbf{B}_{j,k}\alpha^{\mathbf{X}}_{k,j}$. On the other hand,

$$\begin{aligned} \alpha^{\mathbf{L}}_{:,j} &= \mathbf{A}^{\top}_{\mathbf{L},\mathbf{X}}(\mathbf{I} - \mathbf{B}^{\top}_{\mathbf{X},\mathbf{X}})\alpha^{\mathbf{X}}_{:,j} \\ &= \mathbf{A}^{\top}_{\mathbf{L},\mathbf{X}}(\mathbf{I}_{:,j} - \mathbf{B}^{\top}_{\mathbf{X},j})\alpha^{\mathbf{X}}_{j,j} + \mathbf{A}^{\top}_{\mathbf{L},\mathbf{X}}(\mathbf{I}_{:,k} - \mathbf{B}^{\top}_{\mathbf{X},k})\alpha^{\mathbf{X}}_{k,j} \\ &= (\mathbf{A}^{\top}_{\mathbf{L},j} - \mathbf{A}^{\top}_{\mathbf{L},\mathbf{X}}\mathbf{B}^{\top}_{\mathbf{X},j})\alpha^{\mathbf{X}}_{j,j} + (\mathbf{A}^{\top}_{\mathbf{L},k} - \mathbf{A}^{\top}_{\mathbf{L},\mathbf{X}}\mathbf{B}^{\top}_{\mathbf{X},k})\alpha^{\mathbf{X}}_{k,j} \\ &= 0 \end{aligned}$$

If $\mathbf{W}_{j,j} = 0$, as $\alpha^{\mathbf{X}}_{j,j}$ and $\alpha^{\mathbf{X}}_{k,j}$ are non-zero, then the following system of equations has a non-zero solution $x_1 = \alpha^{\mathbf{X}}_{j,j}, x_2 = \alpha^{\mathbf{X}}_{k,j}$.

$$\begin{cases} x_1 - \mathbf{B}_{j,k}x_2 = 0 \\ (\mathbf{A}^{\top}_{\mathbf{L},j} - \mathbf{A}^{\top}_{\mathbf{L},\mathbf{X}}\mathbf{B}^{\top}_{\mathbf{X},j})x_1 + (\mathbf{A}^{\top}_{\mathbf{L},k} - \mathbf{A}^{\top}_{\mathbf{L},\mathbf{X}}\mathbf{B}^{\top}_{\mathbf{X},k})x_2 = 0 \end{cases} \tag{7}$$

Therefore, we have the determinant of the coefficient matrix being zero, that is, $(\mathbf{A}^{\top}_{\mathbf{L},k} - \mathbf{A}^{\top}_{\mathbf{L},\mathbf{X}}\mathbf{B}^{\top}_{\mathbf{X},k}) + (\mathbf{A}^{\top}_{\mathbf{L},j} - \mathbf{A}^{\top}_{\mathbf{L},\mathbf{X}}\mathbf{B}^{\top}_{\mathbf{X},j})\mathbf{B}_{j,k} = 0$. Here, $\mathbf{A}^{\top}_{\mathbf{L},k} - \mathbf{A}^{\top}_{\mathbf{L},\mathbf{X}}\mathbf{B}^{\top}_{\mathbf{X},k}$ measures the total causal effects of L to X_k without passing through other observed variables, $(\mathbf{A}^{\top}_{\mathbf{L},j} - \mathbf{A}^{\top}_{\mathbf{L},\mathbf{X}}\mathbf{B}^{\top}_{\mathbf{X},j})\mathbf{B}_{j,k}$ measures the total causal effects of L to X_k without passing through $\mathbf{X} \setminus \{X_j\}$ and end with X_j. Therefore, the causal effect of L on X_k is zero given all observed variables other than X_j and X_k. In other words, $L \perp\!\!\!\perp X_k | \mathbf{X} \setminus \{X_k, X_j\}$ and $\mathrm{Rank}(\Sigma_{L,X_k|\mathbf{X}\setminus\{X_k,X_j\}}) = 0$. However, this rank constraint is not a generic constraint, which violates the rank faithfulness assumption. Therefore, we have $\mathbf{W}_{j,j} \neq 0$ in contradiction.

Case (ii): If $t = k$ ($\mathbf{I}_{t,j} = 0, \mathbf{I}_{t,k} \neq 0$), then $\mathbf{W}_{t,j} = (\mathbf{I}_{k,j} - \mathbf{B}_{k,j})\alpha^{\mathbf{X}}_{j,j} + (\mathbf{I}_{k,k} - \mathbf{B}_{k,k})\alpha^{\mathbf{X}}_{k,j} = -\mathbf{B}_{k,j}\alpha^{\mathbf{X}}_{j,j} + \alpha^{\mathbf{X}}_{k,j}$. Similarly to case (i), if $\mathbf{W}_{k,j} = 0$, we have $(\mathbf{A}^{\top}_{\mathbf{L},k} - \mathbf{A}^{\top}_{\mathbf{L},\mathbf{X}}\mathbf{B}^{\top}_{\mathbf{X},k})\mathbf{B}_{k,j} + (\mathbf{A}^{\top}_{\mathbf{L},j} - \mathbf{A}^{\top}_{\mathbf{L},\mathbf{X}}\mathbf{B}^{\top}_{\mathbf{X},j}) = 0$, which means the causal effect of L on X_j is zero given all observed variables other than X_j and X_k. It implies $\mathrm{Rank}(\Sigma_{L,X_j|\mathbf{X}\setminus\{X_k,X_j\}}) = 0$. As this rank constraint is not a generic constraint and violates the rank faithfulness assumption, we have $\mathbf{W}_{k,j} \neq 0$.

Case (iii): If $X_t \in \mathrm{Ch}(X_j) \setminus \{X_k\}$ ($\mathbf{B}_{t,j} \neq 0$), then $\mathbf{W}_{t,j} = -\mathbf{B}_{t,j}\alpha^{\mathbf{X}}_{j,j} - \mathbf{B}_{t,k}\alpha^{\mathbf{X}}_{k,j}$. Similarly to case (i), if $\mathbf{W}_{t,j} = 0$, we have $(\mathbf{A}^{\top}_{\mathbf{L},k} - \mathbf{A}^{\top}_{\mathbf{L},\mathbf{X}}\mathbf{B}^{\top}_{\mathbf{X},k})\mathbf{B}_{t,j} = (\mathbf{A}^{\top}_{\mathbf{L},j} - \mathbf{A}^{\top}_{\mathbf{L},\mathbf{X}}\mathbf{B}^{\top}_{\mathbf{X},j})\mathbf{B}_{t,k}$. Then $\mathrm{Rank}(\Sigma_{\{L,X_t\},\{X_k,X_j\}|\mathbf{X}\setminus\{X_t,X_k,X_j\}}) = 1$, which violates the rank faithfulness assumption. Therefore, we have $\mathbf{W}_{t,j} \neq 0$.

Case (iv): If $X_t \in \mathrm{Ch}(X_k) \setminus \{X_j\}$ ($\mathbf{B}_{t,k} \neq 0$), then $\mathbf{W}_{t,j} = -\mathbf{B}_{t,j}\alpha^{\mathbf{X}}_{j,j} - \mathbf{B}_{t,k}\alpha^{\mathbf{X}}_{k,j}$. Similarly to case (iii), if $\mathbf{W}_{t,j} = 0$, we have $(\mathbf{A}^{\top}_{\mathbf{L},k} - \mathbf{A}^{\top}_{\mathbf{L},\mathbf{X}}\mathbf{B}^{\top}_{\mathbf{X},k})\mathbf{B}_{t,j} = (\mathbf{A}^{\top}_{\mathbf{L},j} - \mathbf{A}^{\top}_{\mathbf{L},\mathbf{X}}\mathbf{B}^{\top}_{\mathbf{X},j})\mathbf{B}_{t,k}$. Therefore, we can prove $\mathbf{W}_{t,j} \neq 0$ as $\mathrm{Rank}(\Sigma_{\{L,X_t\},\{X_k,X_j\}|\mathbf{X}\setminus\{X_t,X_k,X_j\}}) = 1$ violates the rank faithfulness assumption.

Case (v): If X_t does not fall into any of the four cases above, then $\mathbf{W}_{t,j} = 0$.

In summary, $\forall t \in [m] \setminus \{k\}$, $\mathbf{W}_{t,j} \neq 0 \iff X_t \in \{X_j, X_k\} \cup \mathrm{Ch}(X_j) \cup \mathrm{Ch}(X_k)$. As $\{X_j\} \cup \mathrm{Ch}(X_j) \subseteq \{X_j, X_k\} \cup \mathrm{Ch}(X_j) \cup \mathrm{Ch}(X_k)$, we have $\|\mathbf{A}_{\mathbf{X},\mathbf{X}}^{-1}\|_0 \leq \|\mathbf{W}\|_0$. Therefore, $\mathbf{I} - \mathbf{B}_{\mathbf{X},\mathbf{X}} \in \arg\min\{\|\mathbf{W}\|_0 : \mathbf{W}$ is a $p_{min}(\mathbf{X})$-order CICA solution of $\mathbf{X}\}$. □

A.3.12 Proof of Lemma 9

Lemma 9. *If Condition 2 holds,* $\mathbf{W} \in \arg\min\{\|\tilde{\mathbf{W}}\|_0 : \tilde{\mathbf{W}}$ *is a* $p_{min}(\mathbf{X})$*-order CICA solution of* $\mathbf{X}\}$ *if and only if we can find a permutation matrix* $\mathbf{P}$ *and non-singular diagonal matrix* $\mathbf{D}$ *that makes* $\mathbf{W} = \mathbf{PD}(\mathbf{I} - \mathbf{B}_{\mathbf{X},\mathbf{X}})$.

Proof. First, during the proof in Lemma 8 we obtain the following results. If $\mathbf{W}$ is a 1-order CICA solution whose latent conditional set is $\mathrm{LPa}(\mathbf{X})$, $\forall t \in [m] \setminus \{k\}$, $\mathbf{W}_{t,j} \neq 0 \iff X_t \in \{X_j\} \cup \mathrm{Ch}(X_j)$. If $\mathbf{W}$ is a 1-order CICA solution whose latent conditional set is not $\mathrm{LPa}(\mathbf{X})$, $\forall t \in [m] \setminus \{k\}$, $\mathbf{W}_{t,j} \neq 0 \iff X_t \in \{X_j, X_k\} \cup \mathrm{Ch}(X_j) \cup \mathrm{Ch}(X_k)$. If $X_k \in \mathrm{Ch}(X_j)$ and $\mathrm{Ch}(X_k) = \emptyset$, $\{X_j, X_k\} \cup \mathrm{Ch}(X_j) \cup \mathrm{Ch}(X_k) = \{X_j\} \cup \mathrm{Ch}(X_j)$, thus $\mathbf{W}_{t,j}$ has the exactly same sparsity pattern. If Condition 2 holds, then there exist a X_j such that the constraint $X_k \in \mathrm{Ch}(X_j)$ and $\mathrm{Ch}(X_k) = \emptyset$ does not hold, $\{X_j\} \cup \mathrm{Ch}(X_j) \subsetneq \{X_j, X_k\} \cup \mathrm{Ch}(X_j) \cup \mathrm{Ch}(X_k)$, then the CICA solution whose latent conditional set is $\mathrm{LPa}(\mathbf{X})$ has a strictly small number of non-zero entries. □

A.3.13 Proof of Theorem 1

Theorem 1. *All latent variables in* $\mathrm{LPa}(\mathbf{X})$ *can be identified. Besides, the causal edges of* $\mathrm{LPa}(\mathbf{X})$ *to* $\mathbf{X}$ *and the causal edges between the observed variables are also identifiable.*

Proof. By Lemma 8, if Condition 2 is satisfied, we can identify $\mathbf{I} - \mathbf{B}_{\mathbf{X},\mathbf{X}}$ by adding sparsity constraints and induce the causal structure. On the other hand, if Condition 2 is not satisfied, $\mathbf{I} - \mathbf{B}_{\mathbf{X},\mathbf{X}}$ is not identifiable. That is, we can find another p-order CICA solution $\mathbf{W}'$ with the same number of non-zero entries as $\mathbf{I} - \mathbf{B}_{\mathbf{X},\mathbf{X}}$. Review the results obtained in the proof of Lemma 8, $\forall t \in [m] \setminus \{k\}$, $\mathbf{W}_{t,j} \neq 0 \iff X_t \in \{X_j, X_k\} \cup \mathrm{Ch}(X_j) \cup \mathrm{Ch}(X_k)$. If $X_k \in \mathrm{Ch}(X_j)$ and $\mathrm{Ch}(X_k) = \emptyset$, $\{X_j, X_k\} \cup \mathrm{Ch}(X_j) \cup \mathrm{Ch}(X_k) = \{X_j\} \cup \mathrm{Ch}(X_j)$, thus $\mathbf{W}_{t,j}$ has the exactly same sparsity pattern. If the constraint $X_k \in \mathrm{Ch}(X_j)$ and $\mathrm{Ch}(X_k) = \emptyset$ holds for every X_j (Condition 2 does not hold), then the whole $\mathbf{W}$ exist exactly same sparsity pattern. In other words, although $\mathbf{W}'$ has different parameters with $\mathbf{I} - \mathbf{B}_{\mathbf{S},\mathbf{S}}$, their support matrix remains the same. Therefore, in both cases, the causal structure among observed variables $\mathbf{B}_{\mathbf{X},\mathbf{X}}$ within a causal cluster is identifiable. Given Condition 1 holds, $p_{min}(\mathbf{X}) = |\,\mathrm{LPa}(\mathbf{X})|$, thus we can identify each latent variable in $\mathrm{LPa}(\mathbf{X})$. Putting all these partial results together, all the latent variables in $\mathrm{LPa}(\mathbf{X})$, the causal edges of $\mathrm{LPa}(\mathbf{X})$ to $\mathbf{X}$ and the causal edges between the observed variables can be identified.

A.3.14 Proof of Lemma 10

Lemma 10. *Let* L *be a latent variable discovered in the current iteration. Denote* $\mathbf{S} = \mathrm{Ch}(L)$. *Let* S_k *have the highest causal order in* $\mathbf{S}$ *whose index in* $\mathbf{S}$ *is* k, *and* $\mathbf{W}$ *be the sparsest* $p_{min}(\mathbf{S})$*-order CICA solution of* $\mathbf{S}$. $\mathbf{P}$ *is the permutation matrix that makes* $\mathbf{PW}$ *have non-zero diagonal elements, simultaneously. Denote* $\mathbf{Z} = \mathbf{PWS}$*, then the value of* Z_k *can be a suitable surrogate for* L.

Proof. By Lemma 8, if Condition 2 is satisfied, we can identify $\mathbf{I} - \mathbf{B}_{\mathbf{X},\mathbf{X}}$ by adding sparsity constraints and induce the causal structure. Then $\mathbf{PW}$ deletes all outgoing edges from $\mathbf{S}$ and makes Z_k a pure child of L. As shown in (Xie et al., 2024), it can be a suitable surrogate for L. On the other hand, if Condition 2 is not satisfied, $\mathbf{I} - \mathbf{B}_{\mathbf{X},\mathbf{X}}$ is not identifiable. Review the results obtained in the proof of Lemma 8, $\forall t \in [m] \setminus \{k\}$, $\mathbf{W}_{t,j} \neq 0 \iff X_t \in \{X_j, X_k\} \cup \mathrm{Ch}(X_j) \cup \mathrm{Ch}(X_k)$. If $X_k \in \mathrm{Ch}(X_j)$ and $\mathrm{Ch}(X_k) = \emptyset$, $\{X_j, X_k\} \cup \mathrm{Ch}(X_j) \cup \mathrm{Ch}(X_k) = \{X_j\} \cup \mathrm{Ch}(X_j)$, thus $\mathbf{W}_{t,j}$ has the exactly same sparsity pattern. If the constraint $X_k \in \mathrm{Ch}(X_j)$ and $\mathrm{Ch}(X_k) = \emptyset$ holds for every X_j (Condition 2 does not hold), then the whole $\mathbf{W}$ exist exactly same sparsity pattern. In other words, although $\mathbf{W}'$ has different parameters with $\mathbf{I} - \mathbf{B}_{\mathbf{S},\mathbf{S}}$, their support matrix remains the same. Essentially, $\mathbf{W}'\mathbf{S}$ can be interpreted as swapping the roles of L and E_k on $\mathbf{I} - \mathbf{B}_{\mathbf{S},\mathbf{S}}\mathbf{S}$. Although L is not contained in the latent conditional set, it is still included in Z_k. Therefore, in both cases, Z_k can be a suitable surrogate for L. □

A.3.15 Proof of Theorem 2

Theorem 2. *Suppose Condition 1 holds, then the underlying causal graph G is fully identifiable, including both latent variables and their causal relationships.*

Proof. Denote $\mathrm{Dis}(V_i)$ the length of the longest direct path from V_i to $\mathbf{X}$. $\forall X_i \in \mathbf{X}, \mathrm{Dis}(X_i) = 0$. We collect $\mathbf{Y_k} = \{V_i | \mathrm{Dis}(V_i) \leq k\}$. The proof is based on mathematical induction:

(1) Base: for $k = 1$, we use Theorem 1 to identify the common latent parents of observed variables and related causal edges. In other words, we can correctly identify the induced sub-graph of G with nodes in $\mathbf{Y_1}$.

(2) Induction: assume we have correctly identified the induced sub-graph of G with nodes in $\{V_i | \mathrm{Dis}(V_i) \leq k\}$, then using Lemma 10 to find the suitable surrogate for latent variables in $\mathbf{Y_k} \setminus \mathbf{Y_{k-1}}$, we can continue to use Theorem 1 to local the latent variables in $\mathbf{Y_{k+1}}$ and related causal edges, which concludes the induction.

Therefore, the underlying causal graph G is fully identifiable, including both latent variables and their causal relationships. □

A.3.16 Proof of Theorem 3

Theorem 3. *Let the graph obtained after removing all the outgoing edges of $\mathbf{X}$ in $\mathcal{G}$ be named by $\mathcal{G}'$, which form several connected components of observed variables $\mathbf{X}'_{C_1}, \mathbf{X}'_{C_2}, \cdots, \mathbf{X}'_{C_k}$, where k be the number of connected components in $\mathcal{G}'$. For an ISA solution $\mathbf{W}$, let $\mathbf{W}\mathbf{X} = (\mathbf{Z}_1^\top, \ldots, \mathbf{Z}_k^\top)^\top$. Then there is a permutation π of $[k]$ s.t. for any $i \in [k]$, $\exists \mathbf{W}_i \in \mathrm{GL}(|C_i|)$ makes $\mathbf{Z}_{\pi(i)} = \mathbf{W}_i \mathbf{X}'_{C_i}$.*

Proof. Based on the Schur complement, we have

$$\mathbf{A}^{-1}_{\mathbf{X},\mathbf{X}} = (\mathbf{I} - \mathbf{B}_{\mathbf{X},\mathbf{X}}) - \mathbf{B}_{\mathbf{X},\mathbf{L}}(\mathbf{I} - \mathbf{B}_{\mathbf{L},\mathbf{L}})^{-1}\mathbf{B}_{\mathbf{L},\mathbf{X}} \tag{8}$$

Denote $\mathbf{Z} = \mathbf{A}^{-1}_{\mathbf{X},\mathbf{X}}\mathbf{X}$. Then we have $\mathcal{NS}(\mathbf{Z}_i) = \{E_j | L_j$ has a directed path to X_i whose intermediate nodes, if exist, are all latent nodes$\}$. The reasons are as follows.

$$\begin{aligned} Z_i &= \sum_{j=1}^{|X|} (\mathbf{A}^{-1}_{\mathbf{X},\mathbf{X}})_{i,j} X_j \\ &= \sum_{j=1}^{|X|} ((\mathbf{I} - \mathbf{B}_{\mathbf{X},\mathbf{X}}) - \mathbf{B}_{\mathbf{X},\mathbf{L}}(\mathbf{I} - \mathbf{B}_{\mathbf{L},\mathbf{L}})^{-1}\mathbf{B}_{\mathbf{L},\mathbf{X}})_{i,j} X_j \\ &= X_i - \sum_{X_j \in \mathbf{X} \setminus \{X_i\}} (\mathbf{B}_{i,j} + \mathbf{B}_{i,\mathbf{L}}(\mathbf{I} - \mathbf{B}_{\mathbf{L},\mathbf{L}})^{-1}\mathbf{B}_{\mathbf{L},j}) X_j \end{aligned} \tag{9}$$

Considering all directed paths into X_i, we categorize them into different groups according to the topologically last observed nodes before X_i on this path. For example, if there is a path $P_1 : X_t \to L_1 \to X_k \to L_2 \to X_i$, we put this path into the group corresponding to X_k, named $\mathcal{G}[X_k]$. If there are no observed nodes before X_i in this path, we put this path in the group corresponding to $\emptyset$, named $\mathcal{G}[\emptyset]$. In total, there are $|X|$ groups: $\bigcup_{X_k \in \mathbf{X} \setminus \{X_i\}} \mathcal{G}[X_k] \cup \mathcal{G}[\emptyset]$.

X_i is a cumulative sum of all directed paths into X_i. The contribution of each directed path in this sum is the noise of the start point times the path coefficient. Obviously, any path will be placed in the group $\bigcup_{X_k \in \mathbf{X} \setminus \{X_i\}} \mathcal{G}[X_k] \cup \mathcal{G}[\emptyset]$. Then, consider what the subtrahend in the last line of Equ. (9) denotes. $\mathbf{B}_{i,j}$ denotes the direct causal effect from X_j to X_i, $\mathbf{B}_{i,\mathbf{L}}(\mathbf{I} - \mathbf{B}_{\mathbf{L},\mathbf{L}})^{-1}\mathbf{B}_{\mathbf{L},j}$ denotes the indirect causal effect from X_j to X_i through latent variables. Consequently, $(\mathbf{B}_{i,j} + \mathbf{B}_{i,\mathbf{L}}(\mathbf{I} - \mathbf{B}_{\mathbf{L},\mathbf{L}})^{-1}\mathbf{B}_{\mathbf{L},j})X_j$ includes all causal effects in X_i from $\mathrm{Anc}(X_i)$ whose last observed node before X_i in the causal path is X_j. This term is exactly the sum of causal effects on X_i by paths in $\mathcal{G}[X_j]$. As a consequence, Z_i equals the sum of causal effects on X_i by the paths in $\mathcal{G}[\emptyset]$. That is, those directed paths whose intermediate nodes are all latent.

Therefore, $\mathbf{A}^{-1}_{\mathbf{X},\mathbf{X}}$ deletes all the outgoing edges from $\mathbf{X}$ and forms several connected components which correspond to the subspace in ISA's definition. Since ISA does not pose any constraints within a subspace, any invertible matrix is valid. Since ISA exists block permutation indeterminacy (Theis, 2006), then we can conclude that there is a permutation π of $[k]$ s.t. for any $i \in [k]$, $\exists \mathbf{W}_i \in \mathrm{GL}(|C_i|)$ makes $\mathbf{Z}_{\pi(i)} = \mathbf{W}_i \mathbf{X}'_{C_i}$. □

A.3.17 PROOF OF REMARK 2

Remark 2. *The two causal graphs in Fig. 1a and Fig. 1b cannot be identified by ISA.*

Proof. For the causal graphs in Fig. 1a and 1b, after removing all the outgoing edges of $\mathbf{X}$, X_1, X_2, X_3 are still connected due to the existence of L. According to Theorem 3, $\forall$ $\mathbf{W} \in \mathrm{GL}(3)$ is an ISA solution in both causal graphs. Consequently, the two causal graphs in Fig. 1a and Fig. 1b cannot be identified by ISA. □

B ILLUSTRATIONS OF ALGORITHMS

B.1 MERGING RULES

Proposition 1 (Merging Rules)**.** *Let $\mathbf{A}$ be the active variable set and C_1 and C_2 be two causal clusters. C_1 and C_2 share the common latent parent, if one of the following rules holds.*

R1. 1) C_1 and C_2 are both pure clusters, and 2) for any subset $\tilde{C} \subseteq C_1 \cup C_2$ with $|\tilde{C}| = 2$, $(\mathbf{A}\backslash\tilde{C}, \tilde{C})$ follows the GIN condition.

R2. 1) One of the clusters is a pure cluster and the other is not, e.g., C_1 is pure and C_2 is impure, and 2) $\forall$ $V_i \in C_1$ and $\forall$ $V_j \in C_2$, $(\mathbf{A}\backslash\{C_2, V_i\}, \{V_i, V_j\})$ follows the GIN condition.

R3. 1) C_1 and C_2 both are impure clusters, and 2) for $\forall$ $\tilde{C} \subseteq C_1 \cup C_2$ with $|\tilde{C}| = 2$, $(\mathbf{A}\backslash\{C_1 \cup C_2\}, \tilde{C})$ follows the GIN condition.

Otherwise, C_1 and C_2 do not share the common latent parent.

Corollary 2. *Let L_1 be a latent variable that was introduced in previous iterations, C_2 be a new cluster, and $\mathbf{A}$ be the active variable set in the current iteration. Suppose cluster C_1 was a subset of $\mathrm{Ch}(L_1)$ found in previous iterations. Then C_1 and C_2 share the common latent parent L_1 if setting $\mathbf{A} = \mathbf{A} \cup C_1 \backslash L_1$ be the active set, one of the three rules in Proposition 2 holds. Otherwise, C_1 and C_2 do not share the common latent parent.*

B.2 PSEUDO CODE

Algorithm 2 CICA-LiNGAM

Require: Observed variables $\mathbf{X}$.
Ensure: Fully identified causal structure G.
1: Initialize active variable set $\mathbf{A} = \mathbf{X}$ and $G = \emptyset$.
2: **while** $\mathbf{A} \neq \emptyset$ **do**
3: $\mathbf{C} \leftarrow$ FindCausalClusters($\mathbf{A}$); (see Algorithm 3)
4: $G \leftarrow$ SparseCICA($\mathbf{C}, G$); (see Algorithm 4)
5: $G \leftarrow$ DetermineLatentVariables($\mathbf{C}$, $\mathbf{A}$, G). (see Algorithm 5)
6: $\mathbf{A} \leftarrow$ UpdateActiveData($\mathbf{A}, G$). (see Algorithm 6)
7: **end while**
8: Return G.

B.3 DISCUSSION OF OPTIMIZATION CRITERION OF CICA

Definition 14 (Cumulant (Brillinger, 2001))**.** *Let $X = (X_1, X_2, \ldots, X_n)$ be a random vector of length n. The k-th order cumulant tensor of X is defined as a $n \times \cdots \times n$ (k times) table, $\mathcal{C}^{(k)}$,*

Algorithm 3 Finding Causal Clusters

Require: Active variable set $\mathbf{A}$.
Ensure: The set of causal clusters $\mathbf{C}$.

```
1: Initialize C = ∅ and the group size GrLen = 2;
2: while |A| ≥ GrLen + 1 do
3:     repeat
4:         Select a subset Y from A such that |Y| = GrLen;
5:         if (A \ Y, Ỹ) follows GIN condition for ∀Ỹ ∈ Y such that |Ỹ| = 2 then
6:             Add Y into C;
7:         end if
8:     until All subsets with group length GrLen in A have been selected;
9:     A = A \ C; GrLen = GrLen + 1;
10: end while
11: Return C;
```

Algorithm 4 Sparse CICA

Require: The set of causal clusters $\mathbf{C}$, and partial graph G.
Ensure: Updated partial graph G.

```
1: for each C_i ∈ C do
2:     W ← sparsest CICA solution on C_i;
3:     P ← the permutation matrix that makes diag(PW) non-zero simultaneously;
4:     W̃ ← divide each row of PW by its corresponding diagonal element;
5:     Compute an estimate B̂ using B̂ = I − W̃;
6:     Update G := G ∪ {j → i | B̂_{i,j} ≠ 0};
7: end for
8: Return G;
```

whose entry at position $(i_1, \cdots, i_k)$ is

$$\mathcal{C}^{(k)}_{i_1,\cdots,i_k} = \mathrm{cum}(X_{i_1}, \ldots, X_{i_k}) = \sum_{(D_1,\ldots,D_h)} (-1)^{h-1}(h-1)!\mathbb{E}\left[\prod_{j\in D_i} X_j\right] \cdots \mathbb{E}\left[\prod_{j\in D_h} X_j\right],$$

where the sum is taken over all partitions $(D_1, \ldots, D_h)$ of the set $\{i_1, \ldots, i_k\}$.

A p-dimensional shared subspace leaves a low-rank fingerprint not only in covariance but also in higher-order cumulants. In the covariance view, identifiability comes from the fact that cross-covariance blocks live in a space of rank at most p; equivalently, all $(p+1)$-minors vanish. The same logic transfers to cumulants: when we form cumulant matrices by linearly contracting the fourth-order cumulant tensor, the contribution of the shared factors still spans at most p independent directions. Hence, these cumulant blocks also satisfy a rank deficiency property.

This viewpoint treats cumulants as providing additional low-rank views of the same latent structure. Because there are many ways to contract a cumulant tensor, we obtain many rank constraints without needing two large disjoint coordinate subsets, which loosens the requirement on m. At the same time, the framework strictly contains the second-order case: if we "degrade" the cumulant to order two, we recover the original covariance criterion. In short, moving from covariance to cumulants preserves the rank-deficiency principle while supplying more constraints and thereby stronger identifiability with fewer observed variables.

B.4 Discussion on Multi-factor Scenario

Proposition 2 (Merging Rules)**.** *Let $\mathbf{A}$ be the active variable set and $\mathbf{C}_1$ and $\mathbf{C}_2$ be two causal clusters. Then the following rules hold.*

R1. *If $|\,\mathrm{LPa}(\mathbf{C}_1)| = |\,\mathrm{LPa}(\mathbf{C}_2)|$, and for any subset $\tilde{\mathbf{C}} \subseteq \{\mathbf{C}_1 \cup \mathbf{C}_2\}$ with $|\tilde{\mathbf{C}}| = |\,\mathrm{LPa}(\mathbf{C}_1)| + 1$, $(\mathbf{A} \cup \{\mathbf{C}_1 \cup \mathbf{C}_2 \setminus \tilde{\mathbf{C}}\}, \tilde{\mathbf{C}})$ follows the GIN condition, then $\mathbf{C}_1$ and $\mathbf{C}_2$ share the same set of latent variables as parents, i.e., $\mathrm{LPa}(\mathbf{C}_1) = \mathrm{LPa}(\mathbf{C}_2)$.*

Algorithm 5 Determine Latent Variables

Require: A cluster set $\mathbf{C}$, active variable set $\mathbf{A}$, and partial graph G.
Ensure: Updated partial graph G.

1: $\mathbf{C} \leftarrow$ Merge clusters from $\mathbf{C}$ according to Rules $R1$ and $R2$ of Proposition 1;
2: **for** each $C_i \in \mathbf{C}$ **do**
3:   **if** L_j and C_i satisfy $R3$ of Corollary 2 **then**
4:     $G \leftarrow G \cup \{L_j \to V_i \mid V_i \in C_i\}$;
5:   **else**
6:     Introduce a new latent variable L_k to $\mathbf{L}$;
7:     $G \leftarrow G \cup \{L_j \to V_i \mid V_i \in C_i\}$;
8:   **end if**
9: **end for**
10: Return G;

Algorithm 6 Update Active Data

Require: Current active variable set $\mathbf{A}$, partial graph G.
Ensure: Updated active variable set $\mathbf{A}$.

1: **if** no new latent variable introduced in G **then**
2:   $\mathbf{A} \leftarrow \varnothing$;
3: **else**
4:   **for** each new latent variable $L_i \in G$ **do**
5:     Initialize the value of L_i according to Lemma 10;
6:     Add L_i into $\mathbf{A}$ and delete $\mathrm{Ch}(L_i)$ from $\mathbf{A}$;
7:   **end for**
8: **end if**

R2. *If* $|\mathrm{LPa}(\mathbf{C}_1)| \neq |\mathrm{LPa}(\mathbf{C}_2)|$ *(suppose* $|\mathrm{LPa}(\mathbf{C}_1)| > |\mathrm{LPa}(\mathbf{C}_2)|$*), and* $\forall \tilde{\mathbf{C}} \subseteq \mathbf{C}_1$ *with* $|\tilde{\mathbf{C}}| = |\mathrm{LPa}(\mathbf{C}_1)|$ *and* $\forall V_i \in \mathbf{C}_2 \setminus \tilde{\mathbf{C}}$, $(\mathcal{A} \cup \{\mathbf{C}_1 \cup \mathbf{C}_2 \setminus \{\tilde{\mathbf{C}}, V_i\}\}, \{\tilde{\mathbf{C}}, V_i\})$ *follows the GIN condition, then the common parents of* $\mathbf{C}_1$ *contain the common parents of* $\mathbf{C}_2$*, i.e.,* $\mathrm{LPa}(\mathbf{C}_2) \subseteq \mathrm{LPa}(\mathbf{C}_1)$.

Otherwise, $\mathbf{C}_1$ *and* $\mathbf{C}_2$ *do not share any common latent variables as parents.*

Corollary 3. *Let* $\tilde{\mathbf{L}}$ *be a latent variable set that has been introduced in the previous iterations,* $\mathbf{C}_2$ *be a new cluster, and* $\mathbf{A}$ *be the active variable set in the current iteration. Further, let* $\mathbf{C}_1$ *be the set of children of* $\tilde{\mathbf{L}}$ *that have been found. Then the following rules hold.*

R3. *If* $|L(\mathbf{C}_2)| = |\tilde{\mathbf{L}}|$*, and for any* $\tilde{\mathbf{C}} \subseteq \mathbf{C}_1$ *with* $|\tilde{\mathbf{C}}| = |\tilde{\mathbf{L}}|$*, and any* $V_i \in \mathbf{C}_2 \setminus \tilde{\mathbf{C}}$, $(\mathbf{A} \setminus \tilde{\mathbf{L}} \cup \{\mathbf{C}_1 \cup \mathbf{C}_2\} \setminus \{\tilde{\mathbf{C}}, V_i\}, \{\tilde{\mathbf{C}}, V_i\})$ *follows the GIN condition, then the common latent parents of* $\mathbf{C}_2$ *are* $\tilde{\mathbf{L}}$*, i.e.,* $L(\mathbf{C}_2) = \tilde{\mathbf{L}}$.

R4. *If* $|L(\mathbf{C}_2)| \neq |\tilde{\mathbf{L}}|$ *(suppose* $|\tilde{\mathbf{L}}| > |L(\mathbf{C}_2)|$*), and for any* $\tilde{\mathbf{C}} \subseteq \mathbf{C}_1$ *with* $|\tilde{\mathbf{C}}_1| = |\tilde{\mathbf{L}}|$ *and any* $V_i \in \mathbf{C}_2 \setminus \tilde{\mathbf{C}}$, $(\mathbf{A} \setminus \tilde{\mathbf{L}} \cup \{\mathbf{C}_1 \cup \mathbf{C}_2\} \setminus \{\tilde{\mathbf{C}}, V_i\}, \{\tilde{\mathbf{C}}, V_i\})$ *follows the GIN condition, then* $\tilde{\mathbf{L}}$ *contains the common parents of* $\mathbf{C}_2$*, i.e.,* $L(\mathbf{C}_2) \subseteq \tilde{\mathbf{L}}$.

C Additional Information on Experiments

C.1 Computing Infrastructure

The computing devices and platforms are listed as follows.

- OS: Microsoft Windows 11.
- CPU: AMD Ryzen 7 4800H with Radeon Graphics, 2900 Mhz.
- Memory: 16G.
- Python 3.8.18.

Algorithm 7 Finding Causal Clusters (multi factors)

Require: Data set $\mathbf{X} = \{X_1, \ldots, X_m\}$.
Ensure: The set of causal clusters $\mathbf{C}$ and its corresponding latent parent number set $\mathcal{L}$.
1: Initialize a cluster set ClusterList = $\emptyset$ and the group size GrLen = 2;
2: **while** $|\mathbf{A}| \geq 2 \times \text{GrLen} - 1$ **do**
3:     **repeat**
4:         Select a subset $\mathbf{Y}$ from $\mathbf{A}$ such that $|\mathbf{Y}| = \text{GrLen}$;
5:         **for** LaLen = 1 : GrLen - 1 **do**
6:             **if** $(\mathbf{A} \setminus \mathbf{Y}, \tilde{\mathbf{Y}})$ follows GIN condition for $\forall \tilde{\mathbf{Y}} \in \mathbf{Y}$ such that $\tilde{\mathbf{Y}} = \text{LaLen} + 1$ **then**
7:                 $\text{LPa}(\mathbf{Y}) = \text{LaLen}$;
8:                 Add $\mathbf{Y}$ into ClusterList;
9:             **end if**
10:        **end for**
11:    **until** All subsets with group length GrLen in $\mathbf{A}$ have been selected;
12: **end while**
13: Return $\mathbf{C}$ and $\mathcal{L}$;

Algorithm 8 Determine Latent Variables (multi factors)

Require: A cluster set $\mathbf{C}$, active variable set $\mathbf{A}$, and partial graph G
Ensure: Updated partial graph G
1: $\mathbf{C} \leftarrow$ Merge clusters from $\mathbf{C}$ according to Rules $R1$ and $R2$ of Proposition 2;
2: **for** each $C_i \in \mathbf{C}$ **do**
3:     $TagVar \leftarrow TRUE$;
4:     **for** each latent set L_j in G' **do**
5:         **if** L_j and C_i satisfy $R3$ of Corollary 1 **then**
6:             $G \leftarrow G \cup \{L_j \rightarrow V_i \mid V_i \in C_i\}$;
7:             $TagVar \leftarrow FALSE$;
8:             **break** the for loop of line 5;
9:         **else if** $|L_j| > \text{LPa}(C_i)$ and L_j and C_i satisfy $\mathcal{R}4$ of Corollary 3 **then**
10:            $G \leftarrow G \cup \{L'_j \rightarrow V_i \mid V_i \in C_i\}$, where $L'_j \subset L_j$ and $|L'_j| = \text{LPa}(C_i)$;
11:            $TagVar \leftarrow FALSE$;
12:            **break** the for loop of line 5;
13:        **else if** $|L_j| < \text{LPa}(C_i)$ and L_j and C_i satisfy $\mathcal{R}4$ of Corollary 3 **then**
14:            Introduce a new latent set L_k such that $|L_k| = |\,\text{LPa}(C_i)| - |L_j|$;
15:            $G \leftarrow G \cup \{\{L_j \cup L_k\} \rightarrow V_i \mid V_i \in C_i\}$;
16:            $TagVar \leftarrow FALSE$;
17:            **break** the for loop of line 5;
18:        **end if**
19:    **end for**
20:    **if** $TagVar = TRUE$ **then**
21:        Introduce a new latent set L_k with length $|\,\text{LPa}(C_i)|$ into G;
22:        $G \leftarrow G \cup \{L_k \rightarrow V_i \mid V_i \in C_i\}$;
23:    **end if**
24: **end for**

C.2 Real-world Experiments

C.2.1 Teacher's Burnout Study

Barbara Byrne conducted a study to investigate the impact of organizational (role ambiguity, role conflict, work overload, classroom climate, decision making, superior support, peer support) and personality (self-esteem, external locus of control) on three facets (emotional exhaustion, depersonalization, and personal accomplishment) of burnout in full-time elementary teachers (Byrne, 2016). The data set consists of 32 observed variables with 599 samples. The details of latent factors and their indicators are shown in Table 7 (See Chapter 6, Page 191 in (Byrne, 2016) for more details). As in practice, the ground-truth latent structure is usually hard to know, here we use the hypothesized model given in (Byrne, 2016) as a reference.

Latent Factors	Children (Indicators)
Role Ambiguity (RA)	RA_1, RA_2
Emotional Exhaustion (EE)	EE_1, EE_2, EE_3
Depersonalization (DP)	DP_1, DP_2
Role Conflict (RC)	RC_1, RC_2, WO_1, WO_2
Self-Esteem (SE)	SE_1, SE_2, SE_3
Personal Accomplishment (PA)	PA_1, PA_2, PA_3
Peer Support (PS)	PS_1, PS_2
Classroom (CC)	CC_1, CC_2, CC_3, CC_4
Decision Making (DM)	DM_1, DM_2
Superior Support (SS)	SS_1, SS_2
External Locus of Control (ELC)	$ELC_1, ELC_2, ELC_3, ELC_4, ELC_5$

Table 7: The latent factors and their indicators in teacher's burnout study.

Ours		**RLCD**	
$L_1 \sim \{RA_1, RA_2\}$	$\surd$	$L_1 \sim \{RA_1, RA_2, RC_1, EE_1\}$	$\times$
$L_2 \sim \{EE_1, EE_2, EE_3\}$	$\surd$	$L_2 \sim \{EE_2, EE_3\}$	$\times$
$L_3 \sim \{DP_1, DP_2\}$	$\surd$	$L_3 \sim \{DP_1, DP_2\}$	$\surd$
$L_4 \sim \{RC_1, RC_2, WO_1, WO_2\}$	$\surd$	$L_4 \sim \{RC_2, WO_1, WO_2\}$	$\times$
$L_5 \sim \{SE_1, SE_2, SE_3\}$	$\surd$	$L_5 \sim \{SE_1, SE_2, SE_3\}$	$\surd$
$L_6 \sim \{PA_1, PA_2, PA_3\}$	$\surd$	$L_6 \sim \{PA_1, PA_2, PA_3\}$	$\surd$
$L_7 \sim \{CC_1, CC_2, CC_3, CC_4\}$	$\surd$	$L_7 \sim \{CC_1, CC_2, CC_3, CC_4\}$	$\surd$
$L_8 \sim \{DM_1, DM_2, SS_1, SS_2\}$	$\times$	$L_8 \sim \{DM_1, DM_2, SS_1, SS_2\}$	$\times$
$L_9 \sim \{ELC_1, ELC_2, ELC_3, ELC_4, ELC_5\}$	$\surd$	$L_9 \sim \{ELC_1, ELC_2, ELC_3, ELC_4, ELC_5\}$	$\surd$

Table 8: The measurement model results of our method and RLCD (Dong et al., 2023).

Locating latent variables. We run our algorithm with the prior knowledge that the underlying graph contains only the one-factor cluster. The final output of the measurement model is shown above. Here we rename the name of the latent variables in RLCD's output for easier comparison. Compare to the reference model given in (Byrne, 2016), our method merges DM and SS into one latent factor and keeps other clusters correctly identified. Notice that (Dong et al., 2023) arises more errors in clustering step (L_1, L_2, L_4). A possible reason is that L_1 only have two measurement variables and are incapable of correctly locating by their method. These results further verify the efficacy of our algorithm. Besides, the structural model learning results (causal graph on latent variables) of our method and RLCD are:

Ours		**RLCD**	
$RA \to PA$	$\surd$	$RA \to DM/SS$	$\times$
$EE \to SE$	$\surd$	$SE \to DP$	$\surd$
$SE \to ELC$	$\surd$	$SE \to PA$	$\surd$
$DM/SS \to SE$	$\surd$	$DP \to PA$	$\surd$
$RC \to DP$	$\times$	$DP \to CC$	$\times$
$CC \to EE$	$\surd$	$RC \to DP$	$\times$
$ELC \to PA$	$\times$	$RC \to SE$	$\times$
$ELC \to DP$	$\times$	$RC \to ELC$	$\surd$
$RC \to EE$	$\surd$	$RC \to RA$	$\times$
$EE \to ELC$	$\times$		

Table 9: The structural model results of our method and RLCD (Dong et al., 2023).

Inferring latent variable structure. The F1 score of our results is 0.522. In contrast, RLCD obtains 0.364. In the output results of the RLCD, most of the edges connected to RC are incorrect. The possible reason is that some latent factors can not be discovered correctly, which further causes some unobserved confounding between latent variables. Note that previous method can not identify $SE \to ELC$ in principle, as they form an impure structure on latent variables. By solving CICA on SE and ELC using their observed descendants, our method can recover the causal direction $SE \to ELC$, which supports the necessitate of introducing two-sided projection.

C.2.2 BIG FIVE PERSONALITY

Dataset Description. The Big Five personality dataset is rooted in the Five-Factor Model (FFM), a seminal theoretical framework in personality psychology to characterize individual personality differences, proposed by American psychologists Paul Costa and Robert McCrae (Costa & McCrae, 1992). This dataset encompasses five core personality dimensions, namely **O**penness, **C**onscientiousness, **E**xtraversion, **A**greeableness, and **N**euroticism, abbreviated as the O-C-E-A-N model. Each dimension is operationally measured by 10 psychometric items, which are designed to capture the nuanced traits underlying each factor. For example, the Openness dimension includes items like "I am intrigued by abstract ideas", while the Conscientiousness dimension features items such as "I am diligent in fulfilling responsibilities".

The data were collected via the online interactive personality testing platform hosted on `https://openpsychometrics.org`, a widely recognized and ethically compliant public data acquisition channel in psychological research. The survey implementation adhered to established ethical norms in empirical psychology, including informed consent and anonymous participation. After data cleaning and validation, the final dataset utilized in this study comprises approximately 20,000 valid samples, covering 50 psychological measurement indicators (10 items per dimension across the five factors). Prior to subsequent analyses, we performed standardization on the data to ensure each variable follows a distribution with a mean of 0 and a variance of 1.

Measurement Model Learning. To determine the causal structure in the Big Five personality data, we first employed the GIN algorithm (Xie et al., 2022) to construct a measurement model. The core objective was to identify observed items that highly correspond to each personality dimension. During the clustering process, some items may reflect multiple personality dimensions: for instance, item O_9 ("I spend time reflecting on things") has dual connotations. On one hand, it reflects in-depth thinking about abstract and complex issues, which is consistent with the cognitive exploration traits of Openness; on the other hand, it involves reviewing and being prudent about one's own behaviors and tasks, aligning with the rigorous and self-disciplined traits of Conscientiousness. For item A_{10} ("I make people feel at ease."), on one hand, the sense of interpersonal security brought by empathy and friendliness is in line with the cognitive exploration traits of Agreeableness; from the perspective of Extraversion, the enthusiasm and talkativeness of extroverts can easily alleviate awkwardness. Such variables cannot correspond to a specific cluster and are therefore not included in the output of the measurement model. After screening via the GIN algorithm, the final output of the measurement model is as follows:

- **Openness**: $L_1\{O_2, O_4, O_7\}$, $L_2\{O_3, O_5, O_6, O_{10}\}$, $L_3\{O_1, O_8\}$;
- **Conscientiousness**: $L_4\{C_1, C_2, C_3, C_4, C_5, C_6, C_7, C_8, C_9, C_{10}\}$;
- **Extraversion**: $L_5\{E_1, E_2, E_4, E_5, E_6, E_7, E_8, E_9, E_{10}\}$;
- **Agreeableness**: $L_6\{A_1, A_2, A_3, A_4, A_5, A_6, A_7, A_8, A_9\}$;
- **Neuroticism**: $L_7\{N_1, N_2, N_3, N_4, N_5, N_6, N_7, N_8, N_9, N_{10}\}$.

The measurement model reveals that the latent variables L_4, L_5, L_6, and L_7 serve as unitary representations for Conscientiousness, Extraversion, Agreeableness, and Neuroticism, respectively, explaining the shared variance in their corresponding item responses. In contrast, the Openness dimension exhibits a more granular internal structure, decomposing into three distinct sub-clusters: L_1, L_2, and L_3. These sub-clusters correspond to the core components of "Cognitive exploration", namely abstract reasoning, creative imagination, and linguistic-cognitive complexity.

Causal Analysis Within Clusters. After obtaining the measurement model, we further applied our algorithm to uncover causal relationships within the clusters. We found several new conclusions that were not revealed by (Dong et al., 2023).

(i) Openness: In the Openness dimension, "difficulty in understanding" is the direct cause of "lack of interest"($O_2 \rightarrow O_4$) — when a person repeatedly fails to understand abstract content, it will directly weaken their willingness to explore this field, whereas if they can understand it easily, they will be more likely to develop interest. Imagination is the core source of creative output: on one hand, "vivid imagination" will directly give rise to "excellent and unique ideas"($O_3 \rightarrow O_5$), and conversely, a lack of imagination will directly restrict the quality of ideas; on the other hand, the breadth of imagination also directly determines the quantity of ideas, and "vivid imagination" will be transformed into "a constant stream of ideas"($O_3 \to O_{10}$). In addition, vocabulary reserve is the foundation of the complexity of language expression: "a rich vocabulary" will directly endow people with the ability to use complex and rare words($O_1 \to O_8$), while a poor vocabulary cannot support the use of difficult words.

(ii) Conscientiousness: In the Conscientiousness dimension, The intrinsic core trait of "liking order" directly drives individuals to maintain the orderly state of life and work through the behavior of "following a schedule"($C_7 \to C_9$); while the behavioral tendency of "paying attention to details" directly translates into the specific manifestation of "being exacting in work"($C_3 \to C_{10}$) — a high sensitivity to details directly acts on the control of omissions in work, thereby presenting a rigorous work state.

(iii) Extraversion: In the Extraversion dimension, on one hand, the intrinsic mindset of "feeling comfortable around people" serves as the core prerequisite for active social interaction — if an individual feels at ease in crowds, this mindset will directly prompt them to initiate conversations actively ($E_3 \to E_5$), and at the same time, it will directly drive them to interact with multiple people in social scenarios such as parties ($E_3 \to E_7$); on the other hand, the core tendency of "not liking to draw attention to oneself" is the direct trigger for social avoidance behaviors — the aversion to others' attention will directly guide the individual to choose a low - key position "keeping in the background" ($E_8 \to E_4$), and this sense of aversion will also directly suppress their desire to express themselves in front of strangers ($E_8 \to E_{10}$).

(iv) Agreeableness: In the Agreeableness dimension, in which A_4("I sympathize with others' feelings.") plays a key mediating role: "feeling others' emotions" is the prerequisite for generating "sympathizing with others' feelings"($A_9 \to A_4$) — only by accurately capturing others' emotional states can one further put oneself in others' shoes and generate emotional resonance, while the inability to perceive emotions will directly lead to a lack of empathy. On this basis, "sympathizing with others' feelings", as a mediating variable, becomes the direct driving force for altruistic behavior — a deep resonance with others' feelings will directly prompt individuals to take time out for others ($A_4 \to A_8$); conversely, if such empathy(A_4) is lacking, even if one can perceive others' emotions, it will directly reduce the willingness to engage in the altruistic behavior of active companionship.

(v) Neuroticism: In the Neuroticism dimension, on one hand, the core trait of "changing mood a lot" is directly externalized as the specific manifestation of "having frequent mood swings"($N_7 \to N_8$); on the other hand, the emotional tendency of "getting stressed out easily" exerts a direct impact through the accumulation of sustained states($N_1 \to N_{10}$) — being in a stressed state for a long time will directly lead to the continuous superposition of negative emotions, which in turn gives rise to the emotional outcome of "often feeling blue".

Structural Model Learning. Following the learning of the measurement model and cluster causal analysis, we further recovered the causal structure among latent variables. While some of our findings are generally consistent with (Dong et al., 2023), we present here only the newly discovered structural learning results.

Causal Relation: $\{L_1 \to L_2, L_1 \to L_3, L_4 \to L_6, L_6 \to L_5, L_4 \to L_1, L_1 \to L_5, L_7 \to L_5\}$.

(i)($L_1 \to L_2, L_1 \to L_3$): In the Openness dimension, "Abstract cognitive ability and interest orientation(L_1)" serve as the prerequisite for fostering "creative potential (L_2)" and "complexity of language expression (L_3)". Only by overcoming difficulties in understanding abstract concepts and maintaining interest in them can one provide cognitive support for the operation of imagination and the accumulation of vocabulary. On this basis, L_1 directly drives the manifestation of L_2 and L_3: strong abstract cognitive ability translates into rich imagination and excellent creative output, while a positive orientation toward abstract thinking enhances the depth of vocabulary reserves and the ability to use complex words; conversely, deficiencies in L_1regarding abstract cognition will directly restrict the development of creativity and the complexity of language expression.

(ii)($L_7 \to L_5$): "Emotional Instability (L_7)" exerts a negative regulatory effect on "social participation tendency (L_5)". Emotional fluctuations and feelings of anxiety directly suppress people's desire to interact, thereby leading to social avoidance behaviors such as staying in the background and being quiet around strangers.

D Related Work

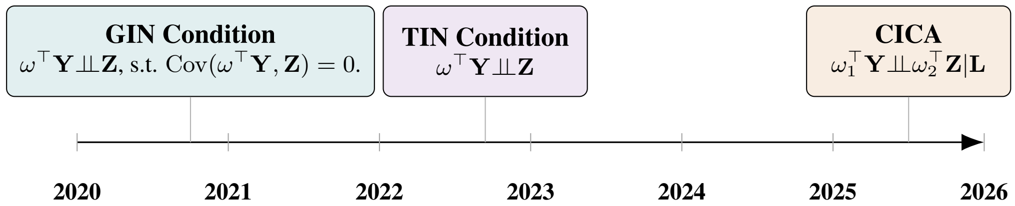


Figure 7: A timeline of tools to recover latent causal structure based on constructing independence.

Existing methods for handling causal discovery in the presence of latent confounders can be categorized into the following folds. Here we list the papers focusing on linear continuous variables,

- (i) Conditional independence constraints-based. This line of work uses conditional independence tests to infer causal graphs. The core idea is to find patterns of conditional independence among variables to reveal the underlying causal structure. By testing for independence among observed variables, these methods can discover the causal skeleton and orient some of the edges. These approaches can handle both linear and nonlinear causal relationships. Related work in this area include (Spirtes et al., 2000; Colombo et al., 2012; Akbari et al., 2021; Triantafillou & Tsamardinos, 2015).
- (ii) Rank deficiency-based. This line of work uses rank constraints of covariance matrices to locate latent variables and infer the causal skeleton. The core idea is that in linear causal models, the covariance matrix or its submatrices exhibit specific rank properties. By analyzing these rank deficiencies, it's possible to reveal the connection patterns between latent and observed variables. Related work in this area includes (Silva et al., 2002; 2006; Kummerfeld & Ramsey, 2016; Huang et al., 2022; Li et al., 2024).
- (iii) Matrix decomposition-based. This line of work proposes to identify the causal structure of latent variables by decomposing the covariance or precision matrix into matrices with specific structures, such as low-rank and sparse. Specifically, the low-rank matrix captures the causal relationships from latent variables to observed variables, while the sparse matrix represents the direct causal relationships among observed variables. Representatives include (Chandrasekaran et al., 2011; 2012; Anandkumar et al., 2013; Frot et al., 2019).
- (iv) Overcomplete independent component analysis (OICA)-based. This line of work leverages Overcomplete Independent Component Analysis (OICA) to handle problems with latent variables. OICA is a variant of Independent Component Analysis (ICA) which allows more source signals than observed signals, and thus can be used to learn the causal structure with latent variables. Related work in this area includes (Shimizu et al., 2009; Entner & Hoyer, 2010; Adams et al., 2021).
- (v) Generalized independent noise (GIN)-based. This line of work extends the independent noise condition to handle scenarios with latent variables. The core idea is that, for non-Gaussian linear causal mechanisms, higher-order statistics can be leveraged to identify latent structures. These methods typically use the non-Gaussianity of the latent variables to infer causal relationships, even in the presence of confounding. Related work in this area includes (Cai et al., 2019; Xie et al., 2020; Dai et al., 2022; Xie et al., 2023; Chen et al., 2022; 2023; Jin et al., 2023; Li et al., 2024; Xie et al., 2024).
- (vi) Higher-order cumulant-based. This line of work leverages higher-order cumulants to identify the causal structure when latent variables are present. For non-Gaussian distributions, cumulants can capture richer structural information than covariance alone. These studies show that the cumulant tensors of observed variables have specific rank constraints that can reveal the causal skeleton of latent variables. Related work in this area includes (Cai et al., 2023; Chen et al., 2024; Schkoda et al., 2024).
- (vii) Score-based. These methods frame the learning of latent variable causal models as a search problem, aiming to find the graph structure that best fits the data. They define a scoring function to measure a graph's goodness of fit, then use search algorithms (like

hill-climbing or beam search) to find the highest-scoring graph. Related work in this area includes (Agrawal et al., 2023; Ng et al., 2024).

D.1 Relation with (Li et al., 2024)

(Li et al., 2024) is an important contribution to the same problem. The primary contribution of (Li et al., 2024) is proving the identifiability of this full structure under milder assumptions than typically required. To achieve this, the authors formulate two identifiable cases. Case I: Arbitrary Distribution: This case allows for entirely arbitrary noise distributions. It relaxes the two-pure-children assumption but still requires each latent variable to have at least one pure child. It first uses tetrad constraints to find all "generalized pure pairs", then uses the guaranteed pure child as an auxiliary variable in further tetrad tests to successfully distinguish the pure pairs from the pseudo-pure pairs. Case II: Partial Non-Gaussianity: This requires no pure children but imposes a partial non-Gaussianity distribution requirement on the noise of specific variables. It constructs a specific linear combination of variables and checks for statistical independence. This condition holds for pseudo-pure pairs but fails for pure pairs due to the non-Gaussian noise. After identifying and grouping all latent variables using either Case I or Case II, the authors use a modified PC-MIMBuild algorithm to infer the final causal relationships between all variables.

While both our paper and (Li et al., 2024) both aim to recover causal structures with latent variables by relaxing strong assumptions like purity assumptions, we must respectfully clarify that our **CICA framework is fundamentally different and addresses a more general and challenging class of causal structures** that their method is not designed to solve.

1. Difference in methodological tools: the core technical approaches (one-sided vs. two-sided projection) are entirely different.

   In (Li et al., 2024)'s most relevant case (Case II, non-Gaussian), its identification theory is based on Lemma 3 to identify "pseudo-pure pairs". This involves finding a linear combination of variables that is independent of a single variable (e.g., $L(O_1, O_2, O_3) \perp\!\!\!\perp O_1$). This is a form of the "one-sided projection" ($\omega^\top Y \perp\!\!\!\perp Z$) discussed in our paper.

   Our paper's central motivation (Section 3.1) is that this entire class of "one-sided projection" tools (including GIN, TIN, and the one used by (Li et al., 2024)) is provably insufficient for the "fully impure" structures in our Figure 1. Our CICA principle is introduced specifically to overcome this, using a more powerful "two-sided projection" ($\omega_1^\top Y \perp\!\!\!\perp \omega_2^\top Z$) to find the additional identifiable traces that one-sided projection-based methods ignore.

2. Difference in structural limitations: this fundamental difference in tools leads to a critical difference in the types of graphs each method can solve.

   The identifiability results of (Li et al., 2024) are based on its Assumption 1, which requires that each latent variable has at least one generalized pure pair as children. While relaxing the full purity assumption, its framework still relies on searching for "generalized pure pairs" as anchors. In our motivating example (Figure 1(a), L confounds X_1, X_2, X_3 and $X_1 \to X_2 \to X_3$) is a "fully impure" structure. Here, L has no generalized pure pairs. As a result, the identification procedure of (Li et al., 2024) cannot be started.

   Our paper solves "fully impure" structures. Our key theoretical contribution (Lemma 8) proves that the true causal structure can still be identified from the sparsest CICA solution even in the absence of "generalized pure pairs". This further demonstrates that these challenging impure structures fall outside the scope of (Li et al., 2024), highlighting the distinct and necessary contribution of our CICA framework.

In summary, our work is fundamentally different from (Li et al., 2024) and is designed to solve a more general and challenging class of "fully impure" structures (like Figure 1) where no "generalized pure pair" exists, a problem that tetrad-based and one-sided-projection methods (like GIN, TIN, and (Li et al., 2024)) cannot address. We provide a novel theoretical foundation principle (conditional independence given latents) and a distinct technical solution (optimization via rank-proxies, identifiability via sparsity) to this challenging problem.

D.2 RELATION WITH CAUSAL COMPONENT ANALYSIS

Causal component analysis (CauCA) (Wendong et al., 2023) is a nice work which introduces an intermediate problem between independent component analysis and causal representation learning: recover causally related latent variables $\mathbf{Z}$ from non-linear mixtures $\mathbf{X} = f(\mathbf{Z})$ when the causal graph G among the latent variables $\mathbf{Z}$ is assumed to be known. The paper's primary contribution is providing identifiability proofs that the unmixing function f is identifiable up to element-wise scaling if one has access to a perfect stochastic intervention on every latent variable. It also proposes a likelihood-based estimation procedure using normalizing flows to learn the non-linear unmixing function and the causal mechanisms.

We would like to politely point out that, despite having similar names, our work and CauCA (Wendong et al., 2023) address fundamentally different questions:

	Ours	CauCA
Goal	Causal discovery based on the solution of proposed CICA	Learn the unknown unmixing function f and the causal mechanisms
Data	A single observational dataset	Multiple interventional datasets
Causal graph	Unknown	Known
Main contribution	1. A novel CICA principle that extracts components that are conditionally independent given latent variables. 2. A new identification theory and an estimation algorithm that recover the underlying causal structure based on the sparsest CICA solutions.	1. An identifiability proof that the unmixing function f is identifiable up to element-wise scaling if one has access to a perfect stochastic intervention on every latent variable. 2. A likelihood-based estimation procedure using normalizing flows to learn the non-linear unmixing function and causal mechanisms.

Table 10: Differences between our paper and CauCA.

E THE USE OF LARGE LANGUAGE MODELS (LLMS)

We used ChatGPT to refine writing only. The prompt was: "I am preparing a paper for submission to an international conference and would like your help to check for any grammatical issues and refine the wording or sentence structure where necessary to ensure conciseness and precision." Edits were applied paragraph-by-paragraph, and all outputs were verified and revised by the authors; no scientific content, analyses, or references were generated by the tool.