On the Representation of Causal Background Knowledge and its Applications in Causal Inference

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Abstract

Causal background knowledge about the existence or the absence of causal edges and paths is frequently encountered in observational studies. The shared directed edges and links of a subclass of Markov equivalent DAGs refined due to background knowledge can be represented by a causal maximally partially directed acyclic graph (MPDAG). In this paper, we first provide a sound and complete graphical characterization of causal MPDAGs and give a minimal representation of a causal MPDAG. Then, we introduce a novel representation called direct causal clause (DCC) to represent all types of causal background knowledge in a unified form. Using DCCs, we study the consistency and equivalency of causal background knowledge and show that any causal background knowledge set can be equivalently decomposed into a causal MPDAG plus a minimal residual set of DCCs. Polynomial-time algorithms are also provided for checking the consistency, equivalency, and finding the decomposed MPDAG and residual DCCs. Finally, with causal background knowledge, we prove a sufficient and necessary condition to identify causal effects and surprisingly find that the identifiability of causal effects only depends on the decomposed MPDAG. We also develop a local IDA-type algorithm to estimate the possible values of an unidentifiable effect. Simulations suggest that causal background knowledge can significantly improve the identifiability of causal effects.

1 Introduction

Causal background knowledge refers to the understanding or consensus of causal and non-causal relations in a system. Such information, as a supplement to data, may be obtained from domain knowledge or experts’ judgements (such as smoking causes lung cancer and eating betel nuts causes oral cancer), from common sense (such as a subsequent event is not a cause of a prior event), or even from previous experimental studies (such as double-blind experiments or A/B tests). Under the framework of causal graphical models, exploiting causal background knowledge may improve the identifiability of a causal effect in an observational study. For example, as shown in Figure 1, consider a simple causal chain with three binary variables: smoking, bronchitis and dyspnea. With observational data only, it is possible to consistently estimate a completed partially directed acyclic graph (CPDAG) shown in Figure 1a, representing a set of statistically equivalent DAGs called...
Figure 1: An CPDAG over three variables including smoking, bronchitis and dyspnea is given in Figure 1a, which represents the Markov equivalent class shown in Figures 1b.

Markov equivalent. In this case, the causal effect of smoking on bronchitis is not identifiable, as there are three Markov equivalent DAGs and the causal effects estimated based on each of them are not identical. However, if we have already known that smoking can cause dyspnea, then the causal effect of smoking on bronchitis is identifiable, since there is only one DAG in the Markov equivalence class satisfying this causal constraint.

This paper focuses on the representation of pairwise causal background knowledge and incorporating this knowledge into causal inference assuming no hidden variables or selection biases. We consider three types of pairwise causal background knowledge, including direct, ancestral and non-ancestral causal knowledge. A piece of direct causal knowledge is defined as the presence of a directed edge, and a piece of ancestral (non-ancestral) causal knowledge is defined as the presence (absence) of a directed path in a causal DAG.

Existing works on causal background knowledge mainly focus on direct causal knowledge (Dor and Tarsi, 1992; Meek, 1995; Perković et al., 2017; Henckel et al., 2022; Perković, 2020; Witte et al., 2020; Guo and Perković, 2021). Meek (1995) proved that the set of DAGs in a Markov equivalence class satisfying given direct causal knowledge is non-empty if and only if it can be represented by a causal maximally partially directed acyclic graph (MPDAG), which contains both directed and undirected edges. Benefiting from the compact graphical representation, many researchers discussed the identifiability and efficient estimation of a causal effect, or the estimation of all possible causal effects of a treatment on a response with direct causal knowledge (Perković et al., 2017; Henckel et al., 2022; Perković, 2020; Witte et al., 2020; Guo and Perković, 2021). Recently, Fang and He (2020) further studied non-ancestral causal knowledge and proved that non-ancestral causal knowledge can also be represented exactly by causal MPDAGs. However, causal MPDAGs may fail to represent ancestral causal knowledge. The DAGs in a Markov equivalence class satisfying given ancestral causal knowledge may satisfy some structural constraints that cannot be posed by any causal MPDAG. An example is provided in Example 1.

As a consequence, without a unified representation of all types of causal background knowledge, we have to regard causal background knowledge as path constraints, which puts global constraints on the possible DAG structures (Borboudakis and Tsamardinos, 2012). As a result, to use causal background knowledge one may need to explicitly or implicitly enumerate all equivalent DAGs in a given Markov equivalence class, and check the paths in each enumerated DAG (Borboudakis and Tsamardinos, 2012). This enumeration-based approach is infeasible in high dimensional settings as the number of Markov equivalent DAGs grows exponentially as the number of variables increases, which also limits the application of causal background knowledge in causal inference.

In this paper, we first give a sound and complete graphical characterization as well as a minimal representation of causal MPDAGs. The sufficient and necessary conditions are introduced under
In a graph $G$, we use $V$ and not a subset of such as $x$, variable sets or vectors. An instantiation of a variable or vector is denoted by a lowercase letter, $X$. The following three subsections devote to some preliminaries. Unless otherwise stated, we use on the study of local orientation rules for CPDAGs with direct causal clauses. Finally, we study the identifiability of causal effects when causal background knowledge is available, and surprisingly find that the identifiability of causal effects only depends on the decomposed MPDAG of the background knowledge. When a causal effect is not identifiable, its possible values depend on both the MPDAG and the residual set of direct causal clauses. For this case, we develop IDA-type algorithms to locally or semi-locally estimate the possible effects, based on the study of local orientation rules for CPDAGs with direct causal clauses.

The following three subsections devote to some preliminaries. Unless otherwise stated, we use capital letters such as $X$ to denote variables or vertices, and use boldface letters like $\mathbf{X}$ to denote variable sets or vectors. An instantiation of a variable or vector is denoted by a lowercase letter, such as $x$ and $x$. We use $\mathbf{X} \subseteq \mathbf{Y}$, $\mathbf{X} \subseteq \mathbf{Y}$ and $\mathbf{X} \not\subseteq \mathbf{Y}$ to denote that $\mathbf{X}$ is a subset, proper subset and not a subset of $\mathbf{Y}$, respectively.

### 1.1 Causal Graphical Models

In this paper, we use $\mathbf{V}(\mathcal{G})$, $\mathbf{E}(\mathcal{G})$, $\mathbf{E}_{d}(\mathcal{G})$ and $\mathbf{E}_{u}(\mathcal{G})$ to denote the vertex set, edge set, set of directed edges and set of undirected edges of a given graph $\mathcal{G}$, respectively, where $\mathcal{G}$ can be a directed, undirected or partially directed graph. The skeleton of $\mathcal{G}$ is the undirected graph obtained by removing all arrowheads from $\mathcal{G}$. For any $\mathbf{V}' \subseteq \mathbf{V}$, the induced subgraph of $\mathcal{G}$ over $\mathbf{V}'$, denoted by $\mathcal{G}(\mathbf{V}')$, is the graph with vertex set $\mathbf{V}'$ and edge set $\mathbf{E}' \subseteq \mathbf{E}$ containing all and only edges between vertices in $\mathbf{V}'$. The undirected subgraph and directed subgraph of $\mathcal{G}$ are denoted by $\mathcal{G}_u$ and $\mathcal{G}_d$, respectively. The former is defined as the undirected graph resulted by removing all directed edges and the latter is the directed graph obtained by removing undirected edges from $\mathcal{G}$. An undirected (or directed) induced subgraph of $\mathcal{G}$ over $\mathbf{V}' \subseteq \mathbf{V}$ is the induced subgraph of $\mathcal{G}_u$ (or $\mathcal{G}_d$) over $\mathbf{V}'$.

In a graph $\mathcal{G}$, $X_i$ is a parent of $X_j$ and $X_j$ is a child of $X_i$ if $X_i \rightarrow X_j$, and $X_i$ is a sibling of $X_j$ if $X_i - X_j$. Two vertices $X_i$ and $X_j$ are adjacent and called neighbors of each other if they are connected by an edge. We use $\text{pa}(X_i, \mathcal{G})$, $\text{ch}(X_i, \mathcal{G})$, $\text{si}(X_i, \mathcal{G})$, and $\text{adj}(X_i, \mathcal{G})$ to denote the sets of parents, children, siblings, and adjacent vertices of $X_i$ in $\mathcal{G}$, respectively. A graph is called complete if every two distinct vertices are adjacent. A vertex is simplicial if its neighbors induce a complete subgraph.

A path is a sequence of distinct vertices $(X_1, \cdots, X_n)$ such that any two consecutive vertices are adjacent. $X_1$ and $X_n$ are endpoints and the others are intermediate nodes. A path connecting $X \in \mathbf{X}$ and $Y \in \mathbf{Y}$ is proper if the intermediate nodes on the path are not in $\mathbf{X} \cup \mathbf{Y}$. If every two distinct vertices in a graph are connected by a path, then the graph is connected. A path from $X_1$ to $X_n$ is partially directed if $X_i \leftarrow X_{i+1}$ does not occur in $\mathcal{G}$ for any $i = 1, \ldots, n-1$. Moreover, a path from $X_1$ to $X_n$ is possibly causal if $X_i \leftarrow X_j$ does not occur in $\mathcal{G}$ for any $i, j = 1, \ldots, n$ and $i < j$, and is non-causal otherwise (Perković et al., 2017). A partially directed path is directed (undirected)
if every edge on it is directed (undirected). A (partially directed, directed, or undirected) cycle is a (partially directed, directed, or undirected) path from $X_i$ to $X_n$ together with a directed or an undirected edge from $X_n$ to $X_i$. A directed graph is acyclic (DAG) if there are no directed cycles. A partially directed acyclic graph (PDAG) is a partially directed graph without directed cycles. A chain graph is a partially directed graph in which partially directed cycles are all undirected. The length of a path (cycle) is the number of edges on the path (cycle). A vertex $X_j$ is a descendant of $X_i$ if there is a directed path from $X_i$ to $X_j$ or $X_i = X_j$; the sets of ancestors and descendants of $X_i$ in $\mathcal{G}$ are denoted by $an(X_i, \mathcal{G})$ and $de(X_i, \mathcal{G})$, respectively. A vertex $X_j$ is a possible descendant of $X_i$ if there is a possibly causal path from $X_i$ to $X_j$. A chord of a path (cycle) is an edge joining two nonconsecutive vertices on the path (cycle). An undirected graph is chordal if it has no chordless cycle with length greater than three.

Let $\pi = (X_1, \cdots, X_n)$ be a path in $\mathcal{G}$. $X_i \ (i \neq 1, n)$ is a collider on $\pi$ if $X_{i-1} \rightarrow X_i \leftarrow X_{i+1}$, and is a definite non-collider on $\pi$ if $X_{i-1} \leftarrow X_i$, or $X_i \rightarrow X_{i+1}$, or $X_{i-1} - X_i - X_{i+1}$ but $X_{i-1}$ is not adjacent to $X_{i+1}$. Moreover, $X_i$ is of definite status on $\pi$ if it is a collider, or a definite non-collider, or an endpoint on $\pi$ (Guo and Perković, 2021). A path $\pi$ is of definite status if its nodes are of definite status. For distinct vertices $X_i, X_j$ and $X_k$, if $X_i \rightarrow X_j \leftarrow X_k$ and $X_i$ is not adjacent to $X_k$ in $\mathcal{G}$, the triple $(X_i, X_j, X_k)$ is called a $v$-structure collided on $X_j$. A definite status path $\pi$ from $X$ to $Y$ is d-separated (blocked) by $Z \ (X, Y \notin Z)$ if $\pi$ has a definite non-collider in $Z$ or $\pi$ has no collider who has a descendant in $Z$, and is d-connected given $Z$ otherwise.

Two DAGs are Markov equivalent if they induce the same d-separation relations. Pearl et al. (1989) proved that two DAGs are equivalent if and only if they have the same skeleton and the same v-structures. A Markov equivalence class contains all DAGs equivalent to each other. A Markov equivalence class can be uniquely represented by a completed PDAG, or essential graph, defined as follows:

**Definition 1** (Completed PDAG (Andersson et al., 1997)). The completed PDAG (CPDAG) of a DAG $\mathcal{G}$, denoted by $\mathcal{G}^*$, is a PDAG that has the same skeleton as $\mathcal{G}$, and a directed edge occurs in $\mathcal{G}^*$ if and only if it appears in all equivalent DAGs of $\mathcal{G}$.

We assume that the CPDAG $\mathcal{G}^*$ of the Markov equivalence class containing the underlying DAG $\mathcal{G}$ is provided, and use $[\mathcal{G}]$ or $[\mathcal{G}^*]$ to represent the Markov equivalence class. Andersson et al. (1997) proved that a CPDAG is a chain graph, and its undirected subgraph is the union of disjoint connected chordal graphs, which are called chain components. A causal DAG model consists of a DAG $\mathcal{G}$ and a distribution $f$ over the same set $V$ such that $f(x_1, ..., x_n) = \prod_{i=1}^{n} f(x_i | pa(x_i, \mathcal{G}))$.

### 1.2 Causal Background Knowledge

In this paper, we mainly consider pairwise causal background knowledge, which can be formally defined in terms of constraints as follows.

**Definition 2** (Pairwise Causal Constraints). A direct causal constraint denoted by $X \rightarrow Y$ is a proposition saying that $X$ is a parent of $Y$, that is, $X$ is a direct cause of $Y$. An ancestral causal constraint denoted by $X \leftrightarrow Y$ is a proposition saying that $X$ is an ancestor of $Y$, that is, $X$ is a cause of $Y$. A non-ancestral causal constraint denoted by $X \rightarrowto Y$ is a proposition saying that $X$ is not an ancestor of $Y$, that is, $X$ is not a cause of $Y$. Moreover, $X$ is called the tail and $Y$ is called the head in the above notions.
Figure 2: A visualization of Meek’s rules. If the graph on the left-hand side of a rule is an induced subgraph of a PDAG, then orient the undirected edge such that the resulting subgraph is the one on the right-hand side of the rule.

Non-pairwise causal background knowledge will be discussed in Appendix B in the supplementary material. A pairwise causal constraint set is also called a (causal) background knowledge set for short. A pairwise causal constraint set over \( V \) consists of some of the constraints with heads and tails in \( V \). Given a DAG \( G \), a pairwise causal constraint set \( B \) over \( V(G) \) holds for \( G \) if and only if every proposition in \( B \) is true for \( G \). We define the restricted Markov equivalence class induced by \( G^* \) and \( B \) as follows.

**Definition 3** (Restricted Markov Equivalence Class). The restricted Markov equivalence class induced by a CPDAG \( G^* \) and a pairwise causal constraint set \( B \) over \( V(G^*) \), denoted by \([G^*, B] \), is composed of all equivalent DAGs in \([G^*] \) that satisfy \( B \).

A restricted Markov equivalence class \([G^*, B] \) is empty if none of the DAGs in \([G^*] \) satisfies \( B \). For example, if two exclusive constraints, say both \( X \rightarrowrightarrow Y \) and \( X \rightarrowrightarrow Y \), appear in \( B \), we have \([G^*, B] = \emptyset \). Otherwise, we say that \( B \) is consistent with \( G^* \) if \([G^*, B] \neq \emptyset \).

A PDAG is maximal (MPDAG) if it is closed under four Meek’s rules shown in Figure 2 (Meek, 1995). Given a CPDAG \( G^* \) and a pairwise causal constraint set \( B \) consistent with \( G^* \), the causal MPDAG of \([G^*, B] \) is defined as follows.

**Definition 4** (Causal MPDAG). The MPDAG \( H \) of a non-empty restricted Markov equivalence class \([G^*, B] \) induced by a CPDAG \( G^* \) and a pairwise causal constraint set \( B \) is a PDAG such that (1) \( H \) has the same skeleton and v-structures as \( G^* \), and (2) an edge is directed in \( H \) if and only if it appears in all DAGs in \([G^*, B] \). An MPDAG \( H \) is a causal MPDAG if there exists a CPDAG \( G^* \) and a pairwise causal constraint set \( B \) consistent with \( G^* \) such that \( H \) is the MPDAG of \([G^*, B] \).

It is easy to verify that Definition 4 indeed defines an MPDAG. Clearly, the MPDAG \( H \) of \([G^*, B] \) contains the common direct causal relations of all restricted Markov equivalence DAGs in \([G^*, B] \). Let \([H] \) be the set of DAGs which contain all directed edges of \( H \) and have the same skeleton and v-structures as \( H \). Following Definition 4, if \( H \) is the MPDAG of \([G^*, B] \), then every DAG in \([G^*, B] \) belongs to \([H] \), that is, \([G^*, B] \subseteq [H] \). An example illustrating that \([G^*, B] \) may be a proper subset of \([H] \) is shown by Example 1.

**Example 1.** Figure 3a shows a CPDAG \( G^* \), and \( G_1 \) to \( G_4 \) shown in Figures 3b to 3e are DAGs in \([G^*] \) satisfying the ancestral causal constraint \( B = \{X \rightarrowrightarrow Y\} \). That is, the restricted Markov equivalence class \([G^*, B] = \{G_1, G_2, G_3, G_4\} \). The causal MPDAG \( H \) of \([G^*, B] \) is shown in Figure 3f, which has two directed edges \( A \rightarrow Y \) and \( B \rightarrow Y \) as they are both in \( G_1 \) to \( G_4 \). On the other hand, \([H] \) consists of \( G_1 \) to \( G_6 \), meaning that \([G^*, B] \subseteq [H] \). In summary, \( B \) implies two direct causal relations, \( A \rightarrow Y \) and \( B \rightarrow Y \), as well as a constraint that \( X \) is a direct cause of \( A \) or \( B \). The MPDAG \( H \) does not imply the latter constraint.
Figure 3: An example of causal MPDAG. Let $\mathcal{B} = \{X \rightarrow Y\}$ and $\mathcal{H}$ be the MPDAG of $[\mathcal{G}^*, \mathcal{B}]$. $[\mathcal{G}^*, \mathcal{B}]$ is consisted of DAGs from $\mathcal{G}_1$ to $\mathcal{G}_4$ and $[\mathcal{H}]$ is consisted of DAGs from $\mathcal{G}_1$ to $\mathcal{G}_6$.

**Definition 5** (Fully Informative MPDAG). A causal MPDAG $\mathcal{H}$ is fully informative with respect to a restricted Markov equivalence class if the set $[\mathcal{H}]$ is identical to the restricted Markov equivalence class.

When $\mathcal{H}$ is fully informative with respect to $[\mathcal{G}^*, \mathcal{B}]$, $\mathcal{H}$ can represent $[\mathcal{G}^*, \mathcal{B}]$ exactly. When $\mathcal{B}$ only contains direct causal constraints, Meek (1995) proved that the MPDAG of $[\mathcal{G}^*, \mathcal{B}]$ is fully informative, and the MPDAG can be constructed in polynomial-time using Meek’s rules. Fang and He (2020) further showed that any non-ancestral causal constraint can be represented equivalently by some direct causal constraints and the corresponding fully informative $\mathcal{H}$ can be constructed from $\mathcal{G}^*$ and $\mathcal{B}$ in polynomial-time, too.

### 1.3 Intervention Calculus

In order to obtain the effect of an intervention on a response variable, Pearl (2009) employed the notion of **do-operator** to formulate the post-intervention distribution as follows: given a DAG $\mathcal{G}$ over vertex set $\mathbf{V} = \{X_1, ..., X_n\}$ and $\mathbf{X} \subseteq \mathbf{V}$,

$$f(\mathbf{v} \mid do(\mathbf{X} = \mathbf{x})) = \begin{cases} \prod_{x_i \in \mathbf{V} \setminus \mathbf{X}} f(x_i \mid pa(x_i, \mathcal{G}))|_{x_i = x_i}, & \text{if } \mathbf{v}|_{\mathbf{X} = \mathbf{x}}, \\ 0, & \text{otherwise}. \end{cases} \tag{1}$$

Here, $f(\mathbf{v} \mid do(\mathbf{X} = \mathbf{x}))$ (or $f(\mathbf{v} \mid do(\mathbf{x}))$ for short) is the post-intervention distribution over $\mathbf{V}$ after intervening on $\mathbf{X}$, by forcing $\mathbf{X}$ to equal $\mathbf{x}$; $\mathbf{v}$ is an instantiation of $\mathbf{V}$; $\mathbf{v}|_{\mathbf{X} = \mathbf{x}}$ means the value of $\mathbf{X}$ in the instantiation $\mathbf{v}$ equals $\mathbf{x}$. The post-intervention distribution $f(\mathbf{y} \mid do(\mathbf{x}))$ is defined by integrating out all variables other than $\mathbf{Y}$ in $f(\mathbf{v} \mid do(\mathbf{x}))$. Given a treatment set $\mathbf{X}$ and a response set $\mathbf{Y}$, if there exists an $\mathbf{x} \neq \mathbf{x}'$ such that $f(\mathbf{y} \mid do(\mathbf{x})) \neq f(\mathbf{y} \mid do(\mathbf{x}'))$, then $\mathbf{X}$ has a causal effect on $\mathbf{Y}$ (Pearl, 2009). Following the notion of Pearl (2009), we simply use $f(\mathbf{y} \mid do(\mathbf{x}))$ to represent the causal effect of $\mathbf{X}$ on $\mathbf{Y}$.

Given the underlying causal DAG, the post-intervention distribution can be calculated from observational distribution by using a number of criteria. For example, the post-intervention distribution
of a single response \( Y \notin pa(X, \mathcal{G}) \) after intervening on a single treatment \( X \) can be calculated by

\[
f(y \mid do(x)) = \int f(y \mid X = x, pa(X, \mathcal{G}) = u)f(u)du.
\]

If \( Y \in pa(X, \mathcal{G}) \), then \( f(y \mid do(x)) = f(y \mid do(x')) \) for any two instantiations \( x, x' \) of \( X \). Equation (2) is a special case of the back-door adjustment (Pearl, 1995, 2009), and \( pa(x, \mathcal{G}) \) is a back-door adjustment set. However, if the underlying DAG is not fully known, \( f(v \mid do(x)) \) may not be identifiable (Pearl, 2009). Recently, the identifiability of a causal effect given an MPDAG has been studied (Perković et al., 2017; Perković, 2020). Perković (2020) proved that \( f(v \mid do(x)) \) is identifiable if and only if every proper possibly causal path from \( X \) to \( Y \) starts with a directed edge in the given MPDAG.

If a causal effect is not identifiable, we can use the IDA framework to estimate all possible causal effects. The original IDA enumerates all possible causal effects of a single treatment \( X \) on a single response \( Y \) given a CPDAG by listing all possible parental sets of \( X \) and adjusting for each of them. To decide whether a set of variables is possible to be the parents of \( X \), Maathuis et al. (2009, Lemma 3.1) provided a locally valid orientation rule. Recently, Fang and He (2020, Theorem 1) extended the locally valid orientation rule to MPDAGs and proposed a fully local extension of IDA to deal with direct causal and non-ancestral causal constraints. For multiple interventions, Nandy et al. (2017) proposed the joint-IDA. Compared with IDA, this extension is semi-local, which uses Meek’s rules to check the validity of each candidate parental set. However, Meek’s rules are global in the sense that they require an entire PDAG as input. Perković et al. (2017) further extended joint-IDA to MPDAGs, and the algorithm is called semi-local IDA. The recent work on efficient adjustment (see, for example, Henckel et al., 2022) also motivates other extensions of IDA, such as the works of Witte et al. (2020); Liu et al. (2020a); Guo and Perković (2021).

In Section 2, we study the graphical characterization of causal MPDAGs and their minimal representation. Then, Section 3 introduces the direct causal clause and use it to represent pairwise causal constraints. Algorithms to check the consistency, equivalency of causal constraints, and to find the decomposed causal MPDAGs and residual direct causal clauses are given in Section 4. In Section 5, we focus on the identifiability of a causal effect and the methods to estimate all possible causal effects locally or semi-locally, and simulations are also given in this section. An additional algorithm, a short discussion on non-pairwise causal constraints, and detailed proofs are provided in the supplementary material.

## 2 A Graphical Characterization of Causal MPDAGs

In this section, we study the sufficient and necessary conditions for a partially directed graph to be a causal MPDAG as well as the minimal representation of a causal MPDAG. Before giving the main results in Theorem 1 and Theorem 2, we introduce two concepts related to partially directed graphs.

**Definition 6 (B-component).** Given a partially directed graph \( \mathcal{G} \), a B-component \( C^b \) of \( \mathcal{G} \) is an induced subgraph of \( \mathcal{G} \) over the vertices which are connected by an undirected path.

B-component generalizes the concept of chain component in a chain graph. In fact, a B-component of a chain graph is exactly one of its chain component. However, unlike chain components, a B-component may contain both directed and undirected edges. For example, the MPDAG \( \mathcal{H} \) shown
Definition 7 (Chain Skeleton). Given a partially directed graph $\mathcal{G}$, the chain skeleton of $\mathcal{G}$, denoted by $\mathcal{G}_c$, is the graph obtained from $\mathcal{G}$ by removing arrowheads of all directed edges in every B-component of $\mathcal{G}$.

According to the definition of B-component, all undirected edges of $\mathcal{G}$ appear in B-components of $\mathcal{G}$, so the undirected subgraph of $\mathcal{G}_c$ is union of the skeletons of the B-components of $\mathcal{G}$. Figure 4b displays the chain skeleton of $\mathcal{H}$ illustrated in Figure 4a. In Figure 4b, the induced subgraph of the chain skeleton $\mathcal{H}_c$ over $\{B, C, D\}$ is undirected.

Theorem 1 provides sufficient and necessary conditions for a partially directed graph $\mathcal{H} = (V, E)$ to be a causal MPDAG.

**Theorem 1.** A partially directed graph $\mathcal{H} = (V, E)$ is a causal MPDAG if and only if

(i) The chain skeleton $\mathcal{H}_c$ of $\mathcal{H}$ is a chain graph.

(ii) The skeleton of each B-component of $\mathcal{H}$ is chordal.

(iii) The vertices in the same B-component have the same parents in $\mathcal{H}_c$.

(iv) For any directed edge $X \rightarrow Y$ in any B-component $C^b$ of $\mathcal{H}$, $\text{pa}(X, \mathcal{H}) \subseteq \text{pa}(Y, \mathcal{H}) \setminus \{X\}$ and $\text{adj}(Y, C^b) \subseteq \text{adj}(X, C^b)$.

Comparing to the graphical characterizations of essential graphs (Andersson et al., 1997) and intervention essential graphs (Hauser and Bühlmann, 2012), the conditions in Theorem 1 are weaker since these two types of graphs are also causal MPDAGs. That is, these conditions are necessary but not sufficient for a graph to be an essential graph or an intervention essential graph.

In Theorem 1, condition (i) states a global characteristic of the partially directed graph $\mathcal{H}$, that is, all partially directed circles in the chain skeleton $\mathcal{H}_c$ of $\mathcal{H}$ are undirected. The last three conditions characterize the graphical structure related to B-components of $\mathcal{H}$. Condition (ii) states that the undirected induced subgraphs of $\mathcal{H}_c$ are chordal, and condition (iii) shows that a vertex out of a B-component is either a parent of all vertices in the B-component, or not a parent of any vertex in the B-component. Condition (iv) indicates that the neighbor/parental sets of two endpoints of a directed edge in a B-component should satisfy an inclusion relation.
In Section 1.2, a causal MPDAG is defined as an MPDAG that can represent a restricted Markov equivalence class induced by a CPDAG $G^*$ and a pairwise causal constraint set $B$. Below, we first show that such a CPDAG $G^*$ is unique.

**Proposition 1.** The restricted Markov equivalence class represented by any given causal MPDAG $H$ is induced by a unique CPDAG $G^*$ and some pairwise causal constraint set. Moreover, there exists a direct causal constraint set $B_d$ such that $[H] = [G^*, B_d]$.

Following Proposition 1, we introduce the definitions of generator and minimal generator.

**Definition 8 (Generator and Minimal Generator).** Let $H$ be a causal MPDAG and $G^*$ be the unique CPDAG of the restricted Markov equivalence classes represented by $H$. A direct causal constraint set (or equivalently, a set of directed edges) $A$ is called a generator of $H$ if $[H] = [G^*, A]$. A generator $A$ is called minimal if the number of direct causal constraints in $A$ is less or equal to other generators of $H$.

Proposition 1 shows that every causal MPDAG has a generator. Below we will show that the minimal generator is unique. A new concept called M-strongly protected is required.

**Definition 9 (M-Strongly Protected).** Let $H$ be a causal MPDAG. A directed edge $X \to Y$ in $H$ is M-strongly protected if $X \to Y$ occurs in at least one of five configurations in Figure 5 as an induced graph of $H$.

![Figure 5: Five configurations of M-strongly protected.](image)

The following proposition proves the uniqueness of minimal generator.

**Proposition 2.** Given a causal MPDAG $H$, a set of directed edges $A$ is a minimal generator of $H$ if and only if $A$ is the set of directed edges which are not M-strongly protected in $H$. Moreover, the minimal generator of $H$ is unique.

Proposition 2 also provides a method to find the minimal generator of a given causal MPDAG. For example, consider the causal MPDAG $H$ shown in Figure 4a, four directed edges $A \to B$, $A \to E$, $B \to E$ and $D \to E$ are M-strongly protected and the other three directed edges, $A \to C$, $A \to D$ and $C \to B$ are not, so $A = \{A \to C, A \to D, C \to B\}$ is the unique minimal generator of $H$. In summary, we have the following theorem.

**Theorem 2.** Let $H$ be a causal MPDAG, there is a unique CPDAG $G^*$ and a unique minimal generator $B_m$ such that $[H] = [G^*, B_m]$.

The first four configurations of M-strongly protected in Definition 9 are exactly the configurations of strongly protected defined for essential graphs. Andersson et al. (1997) proved that every directed edge in an essential graph is strongly protected. Therefore, strongly protected can be used to figure
out the directed edges that can be learned from observational data. In contrast, from Proposition 2 and Theorem 2, in a causal MPDAG, a directed edge can be learned from observational data, or can be inferred from the background knowledge in the minimal generator if the directed edge is M-strongly protected.

3 Representations of Causal Graphs with Pairwise Causal Constraints

Let $G^*$ be a CPDAG and $\mathcal{B}$ be a set of pairwise causal constraints consistent with $G^*$. As discussed in Section 1.2, a causal MPDAG $H$ of $[G^*, \mathcal{B}]$ may not be fully informative when $\mathcal{B}$ contains ancestral causal constraints. That is, $[G^*, \mathcal{B}]$ can not be represented by any causal MPDAG exactly. In this section, we will first introduce a new representation called direct causal clauses that can be used to represent all types of pairwise causal constraints, and discuss the consistency and equivalency of direct causal clauses. Then, in Section 3.2, we show that any causal background knowledge set can be equivalently decomposed into a causal MPDAG plus a minimal residual set of direct causal clauses, and prove sufficient and necessary conditions for a causal MPDAG $H$ of $[G^*, \mathcal{B}]$ to be fully informative.

3.1 Direct Causal Clauses

In this section, we develop a non-graphical tool called direct causal clause to uniformly represent direct, ancestral and non-ancestral causal constraints.

**Definition 10 (Direct Causal Clause).** A direct causal clause (DCC for short) $\kappa$, also denoted by $\kappa_t \rightarrow \kappa_h$, over a variable set $V$ is a proposition saying that $\kappa_t$ is a direct cause of at least one variable in $\kappa_h$, where $\kappa_t \in V$ is called the tail of $\kappa$, and $\kappa_h \subseteq V$ satisfying $\kappa_t \not\in \kappa_h$ is a head set whose elements are called the heads of $\kappa$.

When the head set $\kappa_h$ of a DCC $\kappa$ is a singleton set, say $\kappa_h = \{D\}$, $\kappa_t \rightarrow \kappa_h$ is equivalent to the proposition that $\kappa_t$ is a direct cause of $D$, denoted by $\kappa_t \rightarrow D$. For ease of presentation, we will use $\kappa_t \rightarrow D$ or $\kappa_t \rightarrow D$ to replace $\kappa_t \rightarrow \{D\}$ and use them interchangeably in the following paper. Given a DAG $G$ and a DCC $\kappa$ over the same variable set $V$, we say that $\kappa$ holds for $G$ if $\kappa_h \cap ch(\kappa_t, G) \neq \emptyset$.

**Proposition 3.** For any DAG $G$ over $V$, we have that (i) a DCC $\kappa$ over $V$ with $\kappa_h = \emptyset$ never holds for $G$, and (ii) for any DCC $\kappa$ over $V$, $\kappa \iff \bigvee_{D \in \kappa_h} (\kappa_t \rightarrow D)$ for $G$.

The first statement of Proposition 3 naturally holds since for any $\kappa$ with $\kappa_h = \emptyset$, $\kappa_h \cap ch(\kappa_t, G) = \emptyset$, no matter whether $ch(\kappa_t, G) = \emptyset$ or not. Even if for a singleton graph $G = (\kappa_t, \emptyset)$ containing $\kappa_t$ only, $\kappa_t \rightarrow \emptyset$ does not hold for $G$. Proposition 3 also shows that a DCC $\kappa$ holds for $G$ if and only if there exists at least one variable $D \in \kappa_h$ such that $\kappa_t \rightarrow D$ holds for $G$. It implies that a DCC is a disjunction of direct causal constraints.

To show that DCCs can be used to represent pairwise causal constraints, we introduce a concept of critical set as follows.
Figure 6: An illustration of critical set and Theorem 3. Figure 6a shows a CPDAG. Figures 6b and 6c show the equivalent DCCs to the causal background knowledge $A \rightarrow Y$ and $D \rightarrow Y$, respectively. Figures 6d to 6f enumerate three possible orientations of the edges $D \rightarrow A$ and $D \rightarrow X$ in $G^*$ with the constraint $D \rightarrow \{A, X\}$.

**Definition 11 (Critical Set).** Let $G^*$ be a causal MPDAG, $X, Y$ be two distinct vertices in $G^*$. The critical set of $X$ with respect to $Y$ in $G^*$, denoted by $C_{XY}(G^*)$, consists of all neighbors of $X$ lying on at least one chordless partially directed path from $X$ to $Y$.

This concept was first introduced for CPDAGs by Fang and He (2020). As an example, consider the CPDAG shown in Figure 6a. The critical set of $A$ with respect to $Y$ consists of $B$ and $C$, as $A \rightarrow B \rightarrow Y$ and $A \rightarrow C \rightarrow Y$ are two chordless partially directed path from $A$ to $Y$. On the other hand, variable $X$ is not in $C_{AY}(G^*)$, since $A \rightarrow X \rightarrow C \rightarrow Y$ has a chord $A \rightarrow C$ and $A \rightarrow X \rightarrow B \rightarrow Y$ has a chord $A \rightarrow B$. Similarly, the critical set of $D$ with respect to $Y$ is $\{A, X\}$, for $D \rightarrow A \rightarrow B \rightarrow Y$ and $D \rightarrow X \rightarrow C \rightarrow Y$ are chordless.

**Theorem 3.** Let $G^*$ be a CPDAG, $X, Y \in V(G^*)$ and $G \in [G^*]$, and $C_{XY}(G^*)$ be the critical set of $X$ with respect to $Y$ in $G^*$. We have,

- (i) $X$ is a direct cause of $Y$ in $G$ if and only if $X \rightarrow Y$ holds for $G$;
- (ii) $X$ is a cause of $Y$ in $G$ if and only if $X \rightarrow C_{XY}(G^*)$ holds for $G$;
- (iii) $X$ is not a cause of $Y$ in $G$ if and only if $C \rightarrow X$ holds for $G$ for any $C \in C_{XY}(G^*)$.

Theorem 3 is an extension of Lemma 2 in Fang and He (2020) for all pairwise causal constraints. Analogue to Definition 3, we can define the restricted Markov equivalence class $[G^*, \mathcal{K}]$ induced by a CPDAG $G^*$ and a set $\mathcal{K}$ of DCCs over $V(G^*)$, as the subset of $[G^*]$ in which every DAG satisfies all DCCs in $\mathcal{K}$. Likewise, the MPDAG of a non-empty $[G^*, \mathcal{K}]$ can also be defined analogously to Definition 4. Given a CPDAG and a set of pairwise causal constraints, Theorem 3 proves that there is a set of DCCs which induces the same restricted Markov equivalence class as the set of pairwise causal constraints induces.

From Theorem 3, the global path constraints are transformed to the local ones that only put constraints on the edges between $X$ and its neighbors. An polynomial time algorithm proposed by Fang et al. (2022, Algorithm 2) can be used to find critical sets, so we can efficiently obtain the equivalent DCCs from a given CPDAG and pairwise causal constraints.
Example 2. Consider the CPDAG $G^*$ shown in Figure 6a. Recall that $C_{AY}(G^*) = \{B, C\}$ and $C_{DY}(G^*) = \{A, X\}$. Suppose that $A \rightarrow Y$ holds for the underlying DAG, then by Theorem 3, $B \rightarrow A$ and $C \rightarrow A$ holds. Since $B \rightarrow A$ if $A \rightarrow Y$, we equivalently have $D \rightarrow Y$. Furthermore, if $D \rightarrow Y$ holds, then by Theorem 3 we equivalently have $D \rightarrow \{A, X\}$, meaning that $D$ is a direct cause of $A$ or $X$ in the underlying DAG. Figures 6d to 6f enumerate three possible orientations of the edges $D - A$ and $D - X$ in $G^*$ with the constraint $D \rightarrow \{A, X\}$. For any DAG in $[G^*, D \rightarrow Y]$, the edge orientations of $D - A$ and $D - X$ must be one of the three possibilities shown in Figures 6d to 6f. Conversely, every DAG in $[G^*, D \rightarrow Y]$ whose edges between $D$ and $\{A, X\}$ are identical to one of the configurations shown in Figures 6d to 6f must satisfy the constraint $D \rightarrow Y$.

Below, we discuss the consistency of a DCC set and the equivalency of two DCC sets with respect to a given CPDAG. We first introduce the definition of consistency as follow.

**Definition 12** (Consistency). Given a CPDAG $G^*$ and a set $K$ of DCCs over $V(G^*)$, $K$ is consistent with $G^*$ if $[G^*, K] \neq \varnothing$.

Following Definition 12, a set $K$ of DCCs over $V(G^*)$ is consistent with $G^*$ if and only if there exists at least one equivalent DAG $G \in [G^*]$ which satisfies all clauses in $K$. Below, we give a definition of equivalency of two sets of DCCs such that we can discuss the consistency of a set of DCCs via its consistent reduced form.

**Definition 13** (Equivalency). Given a CPDAG $G^*$, two sets $K_1$ and $K_2$ of DCCs over $V(G^*)$ are equivalent with respect to $G^*$ if $[G^*, K_1] = [G^*, K_2]$.

Let $\kappa := \kappa_t \rightarrow \kappa_h$ be a DCC. Denoting $[G^*, \{\kappa\}]$ by $[G^*, \kappa]$ for convenience and assuming that $\kappa$ is over $V(G^*)$, the following propositions give several equivalent reduced forms of $\kappa$.

**Proposition 4**. For any given CPDAG $G^*$ and a direct causal clause $\kappa := \kappa_t \rightarrow \kappa_h$, we have that (i) $[G^*, \kappa] = [G^*]$ if $ch(\kappa_t, G^*) \cap \kappa_h \neq \varnothing$, (ii) $[G^*, \kappa] = [G^*, \kappa_t \rightarrow (\kappa_h \cap adj(\kappa_t, G^*))]$ and (iii) $[G^*, \kappa_t \rightarrow (\kappa_h \cap pa(\kappa_t, G^*))]$.

In Proposition 4, the first result holds since every $G \in [G^*]$ satisfies $\kappa$ when $ch(\kappa_t, G^*) \cap \kappa_h \neq \varnothing$. Therefore, a DCC with $ch(\kappa_t, G^*) \cap \kappa_h \neq \varnothing$ is redundant for $G^*$. For any $G \in [G^*]$, $G$ satisfies $\kappa$ if and only if there exists at least a variable $D \in \kappa_h$ such that $\kappa_t \rightarrow D$ appears in $G$. If such a variable $D$ exists, it must be adjacent to $\kappa_t$, so the second equation holds. Similarly, the third equation holds since $D$ must not a direct cause of $\kappa_t$. Consequently, we give a reduce form of a set of DCCs $K$ in Definition 14.

**Definition 14** (Reduced Form). Given a CPDAG $G^*$ and a set of DCCs $K$ over $V(G^*)$, a reduced form of $K$ with respect to $G^*$, denoted by $K(G^*)$, is defined as follows.

$$K(G^*) := \{\kappa_t \rightarrow (\kappa_h \cap sib(\kappa_t, G^*)) \mid \kappa \in K \text{ and } \kappa_h \cap ch(\kappa_t, G^*) = \varnothing\}.$$ (3)

**Proposition 5** (Equivalent Reduced Form). Given a CPDAG $G^*$ and a set of DCCs $K$ over $V(G^*)$, we have that $K$ is equivalent to $K(G^*)$ defined in Equation (3).

Proposition 5 shows that the reduced form of $K$ is equivalent to $K$ with respect to $G^*$. Below, we define a subset of $K$ restricted on an undirected induced subgraph of $G^*$.
Definition 15 (Restriction Subset). Given an undirected induced subgraph $U$ of a CPDAG $G^*$ over $V(U) \subseteq V(G^*)$, and a set of DCCs $K$ over $V(G^*)$, the restriction subset of $K$ on $U$ is defined by

$$K(U) := \{ \kappa \in K(G^*) \mid \{ \kappa_t \} \cup \kappa_h \subseteq V(U) \}. \quad (4)$$

It can be seen that $K(G^*) = K(G^*_U)$. Basically, $K(U)$ consists of all clauses in $K(G^*)$ whose tail and heads are all in $U$. The following concept of potential leaf nodes are of the key importance in checking consistency of a set of DCCs.

Definition 16 (Potential Leaf Node). Let $G^*$ be a CPDAG and $K$ be a set of DCCs over $V(G^*)$. Given an undirected induced subgraph $U$ of $G^*$ and a vertex $X$ in $U$, $X$ is called a potential leaf node in $U$ with respect to $K$ and $G^*$, if $X$ is a simplicial vertex in $U$ and $X$ is not the tail of any clause in $K(U)$.

We note that, if $U = (\{ X \}, \emptyset)$ only contains a singleton $X$, then $X$ is trivially a potential leaf node in $U$ with respect to any $K$ that does not contain any DCC of the form $X \rightarrow \emptyset$. A leaf node of a directed graph is a vertex who has no child. Analogously, a potential leaf node defined above is a vertex who may have no child in at least one $G$ in $[G^*, K]$ (see Lemma 9 in the supplementary material for more details). Now, we give the sufficient and necessary condition for a set of DCCs $K$ to be consistent with $G^*$.

**Theorem 4.** Let $G^*$ be a CPDAG and $K$ be a set of DCCs over $V(G^*)$. Then, the following two statements are equivalent.

(i) $K$ is consistent with $G^*$.

(ii) (Potential-leaf-node condition) Any connected undirected induced subgraph of $G^*$ has a potential leaf node with respect to $K$ and $G^*$.

The proof of Theorem 4 also motivates a polynomial-time algorithm to check the consistency of DCCs. The details are given in Section 4.1. The potential-leaf-node condition given in Theorem 4 is similar to the fact that any induced subgraph of a DAG has a leaf node. Below we give an example to demonstrate this result.

**Example 3.** Recall that in Example 2 we show that, with respect to the CPDAG $G^*$ (Figure 6a), $A \rightarrow Y$ is equivalent to $C \xrightarrow{\text{or}} A$ and $B \xrightarrow{\text{or}} A$, and $D \rightarrow Y$ is equivalent to $D \xrightarrow{\text{or}} \{ A, X \}$. Suppose we have both $A \rightarrow Y$ and $D \rightarrow Y$, then the equivalent DCCs $K$ consists of $C \xrightarrow{\text{or}} A$, $B \xrightarrow{\text{or}} A$ and $D \xrightarrow{\text{or}} \{ A, X \}$. However, since $\{ D, A, X, B \}$ induces an undirected subgraph where none of the vertices is a potential leaf node with respect to $K$ and $G^*$, $K$ is inconsistent by Theorem 4.

To end this section, we give sufficient and necessary conditions that two DCC sets, $K_1$ and $K_2$ are equivalent with respect to a CPDAG $G^*$. We will show that, these conditions can be expressed either in terms of consistency or in terms of redundancy defined as follows.

**Definition 17** (Redundancy). Given a restricted Markov equivalence class $[G^*, K]$ induced by a CPDAG $G^*$ and a set $K$ of DCCs over $V(G^*)$, a DCC $\kappa$ over $V(G^*)$ is redundant with respect to $[G^*, K]$ if $[G^*, K] = [G^*, K \cup \{ \kappa \}]$. 

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According to Definition 17, a DCC $\kappa$ is redundant with respect to $[G^*, K]$ if and only if $\kappa$ holds for all DAGs in $[G^*, K]$. With this concept, the following Theorem 5 discusses the equivalency of two sets of consistent DCCs.

**Theorem 5.** Given a CPDAG $G^*$, and two sets of DCCs $K_1$ and $K_2$ over $V(G^*)$, the following statements are equivalent.

(i) $K_1$ and $K_2$ are equivalent given $G^*$.

(ii) Every DCC in $K_1$ is redundant with respect to $[G^*, K_2]$, and every DCC in $K_2$ is redundant with respect to $[G^*, K_1]$.

(iii) For every $\kappa \in K_1$, $\cup_{D \in K_2} \{D \rightarrow \kappa_1\} \cup K_2$ is not consistent with $G^*$, and for every $\kappa \in K_2$, $\cup_{D \in K_1} \{D \rightarrow \kappa_1\} \cup K_1$ is not consistent with $G^*$,

Theorem 5 builds the relations among equivalency, redundancy and consistency. Moreover, using the third statement of Theorem 5, we can check whether two sets of DCCs are equivalent through checking the consistency of a series of DCC sets.

### 3.2 Equivalent Decomposition of Pairwise Causal Constraints

Theorem 3 proves that any set of pairwise causal constraints can be equivalently represented by a set of DCCs. Recall that in Definition 4 we construct an MPDAG which represents all common direct causal relations shared by all DAGs in a restricted Markov equivalence class. Combining Theorem 3 and Definition 4, we have an equivalent decomposition of pairwise causal constraints.

**Proposition 6 (Equivalent Decomposition).** Let $G^*$ be a CPDAG, $B$ be a set of consistent pairwise causal constraints, and $H$ be the MPDAG of $[G^*, B]$. Then, there exists a set of DCCs $R$ such that $[G^*, B] = [H, R]$, where $[H, R]$ denotes the subset of $[H]$ consisting of DAGs satisfying all clauses in $R$, and $R$ is minimal in the sense that $[G^*, B] \subseteq [H, R']$ for any $R' \subseteq R$.

Given a CPDAG, Proposition 6 indicates that any set of pairwise causal constraints can be equivalently decomposed into the MPDAG of the induced restricted Markov equivalence class plus a minimal residual set of DCCs. Moreover, since the MPDAG $H$ contains all direct causal edges that appear in all DAGs in $[G^*, B]$, any directed edge in the MPDAG of $[G^*, R]$ is also in $H$. That is, $R$ cannot bring more directed causal edges other than those in $H$.

When the residual set of DCCs is empty, the MPDAG of the induced restricted Markov equivalence class is fully informative. As mentioned in Section 1.2, a sufficient condition that guarantees the emptiness of a residual set is when $B$ only contains direct and non-ancestral causal constraints. Yet, this condition is not necessary, as shown in the following example.

**Example 4.** Figure 7a shows a CPDAG $G^*$. Consider two ancestral causal constraints $B \rightarrow E$ and $D \rightarrow A$. By Proposition 6, $B \rightarrow E$ and $D \rightarrow A$ are equivalent to $D \rightarrow \{C, D\}$ and $D \rightarrow \{B, C\}$, respectively, which are visualized by arcs in Figure 7b. Let $K = \{B \rightarrow \{C, D\}, D \rightarrow \{B, C\}\}$. We first find the MPDAG $H$ of $[G^*, K]$. If there is a DAG $G \in [G^*, K]$ where $C \rightarrow B$ is in $G$, then by the constraint $B \rightarrow \{C, D\}$, $B \rightarrow D$ is in $G$. Likewise, by the constraint $D \rightarrow \{B, C\}$, $D \rightarrow C$ is in $G$. However, $C \rightarrow B \rightarrow D \rightarrow C$ is a directed cycle. Therefore, every DAG in $[G^*, K]$ should have $B \rightarrow C$, implying that $B \rightarrow C$ is in $H$. Similarly, $D \rightarrow C$ is in $H$. Finally, by Meek’s...
A sufficient and necessary condition for an MPDAG to be fully informative is given below.

Theorem 6. Suppose that $G^*$ is a CPDAG, $K$ is a set of consistent DCCs, and $H$ is the MPDAG of $[G^*, K]$. Then, the following statements are equivalent.

(i) $H$ is fully informative with respect to $K$ and $G^*$, and

(ii) for any $\kappa \in K$, either $\kappa_h \cap \text{sib}(\kappa_t, H)$ induces an incomplete subgraph of $H$, or $\kappa_h \cap \text{ch}(\kappa_t, H) \neq \emptyset$.

We note that, in Section 4.2, we give a polynomial-time algorithm to find the MPDAG given a CPDAG $G^*$ and a set $K$ of DCCs. With the found MPDAG, the condition in statement (ii) can also be verified in polynomial time.

Example 5. Figure 8a shows a CPDAG $G^*$ and a set of DCCs $K$ consisting of $D \rightarrow \{B, E\}$, $E \rightarrow \{A, C\}$, $E \rightarrow \{B, F\}$ and $G \rightarrow \{B, H\}$, and Figure 8b shows the MPDAG of $[G^*, K]$. (How to find this MPDAG is left to Example 8, Section 4.2). Since $E \rightarrow A$, $E \rightarrow F$ and $G \rightarrow H$ are in the MPDAG, $E \rightarrow \{A, C\}$, $E \rightarrow \{B, F\}$ and $G \rightarrow \{B, H\}$ are redundant given $H$. However, $D \rightarrow \{B, E\}$ is not redundant, as $\{B, E\}$ induces a complete subgraph of $H$. Therefore, in this example, the MPDAG $H$ is not fully informative.

Notice that, given a DCC $\kappa$, if $\kappa_h \cap \text{sib}(\kappa_t, H)$ induces an incomplete subgraph of $H$, then $\kappa_h \cap \text{sib}(\kappa_t, G^*)$ induces an incomplete subgraph of $G^*$. Conversely, if $\kappa_h \cap \text{sib}(\kappa_t, G^*)$ induces an incomplete subgraph of $G^*$, then by Rule 1 of Meek’s rules, $\kappa$ holds for all DAGs in $[G^*]$, and thus $\kappa$
is redundant. For a given DCC set $K$, removing the above redundant DCCs from the equivalent reduced form $K(G^*)$, we define a subset of $K(G^*)$ as follows.

$$K^c(G^*_u) := \{ \kappa \mid \kappa \in K(G^*_u) \text{ and the induced subgraph } G^*(\kappa_h) \text{ is complete} \}. \quad (5)$$

Based on the above argument, we have the following corollary.

**Corollary 1.** Let $H$ be an MPDAG representing the restricted Markov equivalence class induced by a CPDAG $G^*$ and a set $K$ of consistent DCCs, then $[H] = [G^*, K]$ if and only if for any $\kappa \in K^c(G^*_u)$, $\kappa_h \cap ch(\kappa_t, H) \neq \emptyset$ holds.

### 4 Polynomial-Time Algorithms

This section devotes to the algorithms for checking consistency and equivalency of DCCs, and for finding the MPDAG and the minimal residual sets of DCCs given a CPDAG and a set of pairwise causal constraints. As we will show, all the proposed algorithms are of polynomial-time.

#### 4.1 Algorithms for Checking Consistency and Equivalency

Recall that Theorem 4 provides a sufficient and necessary condition for consistency. The proof of Theorem 4 also motivates an algorithm for checking consistency. Algorithm 1 shows the schema. The inputs of Algorithm 1 are a CPDAG $G^*$ and a set $K$ of DCCs over $V(G^*)$. It first initializes $U$ by $G^*_u$, and then sequentially removes potential leaf nodes from $U$ in lines 2-6, until no more potential leaf node can be found.

Algorithm 1 runs the while-loop at most $|V(G^*)|$ times. Every time it runs the while-loop, it checks whether all vertices in $U$ are simplicial and are not the tails of the clauses in $K(U)$. The complexity of the former is bounded by $O(|V(G^*)|)$, and the complexity of the later is also bounded by $O(|V(G^*)|)$ if we build an index of the tails of the clauses in $K(U)$. Therefore, the complexity of Algorithm 1 is upper bounded by $O(|V(G^*)|^3)$.

Algorithm 1 is highly related to the perfect elimination ordering (PEO) of a chordal graph (Blair and Peyton, 1993; Maathuis et al., 2009). In fact, when $K$ is consistent, the ordering of the removal

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**Algorithm 1** Checking the consistency of a DCC set.

**Require:** A CPDAG $G^*$ and a set $K$ of DCCs over $V(G^*)$.

**Ensure:** A Boolean value indicating whether $K$ is consistent with $G^*$.

1. Set $U = G^*_u$ and compute $K(U)$ according to Equation (3) and Equation (4),
2. while $U$ has a potential leaf node with respect to $K$ and $G^*$, do
3. find a potential leaf node in $U$ respect to $K$ and $G^*$ and denote it by $Y$,
4. update $U$ by removing $Y$ and the edges connected to $Y$,
5. update $K(U)$ by removing all clauses whose heads contain $Y$,
6. end while
7. if $U$ is an empty graph, then
8. return True.
9. end if
10. return False.
potential leaf nodes is a PEO of the chordal graph $G_\ast^u$. PEOs are important to construct Markov equivalent DAGs. We refer the interested readers to Appendix C.1 in the supplementary material for more details. We also remark that, when causal background knowledge set contains only direct causal constraints, Algorithm 1 degenerates to the algorithm proposed by Dor and Tarsi (1992).

Example 6 (continued). We next use Algorithm 1 to check the consistency of $K = \{C \overset{\rightarrow}{\to} A, B \overset{\leftarrow}{\to} A, D \overset{\rightarrow}{\to} \{A, X\}\}$ with respect to $G^\ast$ illustrated in Figure 6a. We first set $U = G_\ast^u$, which is the induced subgraph of $G^\ast$ over $\{A, B, C, D, X\}$. With respect to $K$, however, $U$ has no potential leaf node, meaning that the while-loop (lines 2-6) is not triggered. As $U$ is not empty, Algorithm 1 returns False.

In some circumstances, causal background knowledge is not obtained all at once. Therefore, we also need an approach to sequentially check consistency. That is, given a CPDAG $G^\ast$ and a consistent pairwise causal constraint set $B$, we would like to know whether a newly obtained pairwise causal constraint set is consistent with $G^\ast$, together with $B$. This issue will be investigated in Appendix A in the supplementary material.

Finally, with Algorithm 1 and Theorem 5, we can check the equivalency of two DCC sets, as shown in Algorithm 2. Note that, to accelerate the procedure, we first check the consistency of $K_1$ and $K_2$ separately. If neither $K_1$ nor $K_2$ is consistent with $G^\ast$ then they are equivalent; if one of them is consistent with $G^\ast$ but the other is not, then they are not equivalent.

### 4.2 Algorithms for Finding MPDAGs and Minimal DCC Sets

We first discuss how to find the MPDAG of $[G^\ast, K]$ induced by a CPDAG $G^\ast$ and a set $K$ of DCCs consistent with $G^\ast$. By the definition of MPDAG, it suffices to find all common direct causal

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**Algorithm 2** Checking the equivalency of two DCC sets.

**Require:** A CPDAG $G^\ast$ and two sets $K_1$ and $K_2$ of DCCs over $V(G^\ast)$.

**Ensure:** A Boolean value indicating whether $K_1$ is equivalent to $K_2$ given $G^\ast$.

1: if both $K_1$ and $K_2$ are consistent with $G^\ast$, then  
2: for $\kappa \in K_1$, do  
3: if $\bigcup_{D \in \kappa_t} \{D \to \kappa_t\} \cup K_2$ is consistent with $G^\ast$, then  
4: return False.  
5: end if  
6: end for  
7: for $\kappa \in K_2$, do  
8: if $\bigcup_{D \in \kappa_t} \{D \to \kappa_t\} \cup K_1$ is consistent with $G^\ast$, then  
9: return False.  
10: end if  
11: end for  
12: return True.

13: else if neither $K_1$ nor $K_2$ is consistent with $G^\ast$, then  
14: return True.  
15: else  
16: return False.  
17: end if
relations shared by all DAGs in \([G^*, K]\). A new concept is needed before proceeding.

**Definition 18 (Orientation Component).** Given a CPDAG \(G^*\) and a DCC set \(K\) consistent with \(G^*\), with respect to \(K\) and \(G^*\), a connected undirected induced subgraph \(U\) of \(G^*\) is called an orientation component for a vertex \(X\) if \(X\) is the only potential leaf node in \(U\).

**Example 7.** We illustrate the concept of orientation component in this example. Figure 9a shows a CPDAG \(G^*\). Consider \(K = \{A \leftarrow \{X, B, D\}, B \leftarrow \{X, A\}, B \leftarrow \{X, C, Y\}, X \leftarrow \{B, C\}\}\). Since \(\{X, B, D\}\) \(\cap\) \(sib(A, G^*) = \{X, B\}\) and \(\{X, C, Y\}\) \(\cap\) \(ch(B, G^*) \neq \emptyset\), by Equation (3), \(K(G^*_{u})\) consists of \(A \leftarrow \{X, B\}\), \(B \leftarrow \{X, A\}\), \(B \leftarrow \{X, C, Y\}\), \(X \leftarrow \{B, C\}\), which are visualized by arcs in Figure 9b. First, consider the undirected induced subgraph \(U\) over \(\{A, B, X\}\). By definition, \(K(U)\) consists of \(A \leftarrow \{X, B\}\) and \(B \leftarrow \{X, A\}\). Therefore, there is only one potential leaf node in \(U\), namely \(X\), and thus \(U\) is an orientation component for \(X\). Next, consider the undirected induced subgraph \(U\) over \(\{X, B, C\}\). \(K(U)\) has only one constraint \(X \leftarrow \{B, C\}\), hence \(U\) has two potential leaf nodes \(B\) and \(C\). Finally, consider the entire undirected subgraph \(G^*_{u}\). \(G^*_{u}\) has only one potential leaf node \(C\), thus \(G^*_{u}\) is an orientation component for \(C\).

![Figure 9: An example to demonstrate the concept of orientation component.](image)

The following proposition shows that an orientation component can be used to identify some direct causal relations.

**Proposition 7.** Let \(G^*\) be a CPDAG and \(K\) be a set of DCCs consistent with \(G^*\). For any orientation component \(U\) for \(X\) with respect to \(K\) and \(G^*\) with \(\text{adj}(X, U) \neq \emptyset\), all variables in \(\text{adj}(X, U)\) are direct causes of \(X\) in every DAG in \([G^*, K]\).

Together with the directed edges in the CPDAG, the orientation components can completely characterize the common direct causal relations given a CPDAG and a set of DCCs.

**Theorem 7.** Let \(G^*\) be a CPDAG and \(K\) be a set of DCCs consistent with \(G^*\), then \(X \rightarrow Y\) is in every DAG in \([G^*, K]\) if and only if \(X \rightarrow Y\) appears in \(G^*\) or there exists an orientation component for \(Y\) containing \(X\) with respect to \(K\) and \(G^*\).

Graphically, Theorem 7 shows all possible sources of the directed edges in an MPDAG. Consider Figure 9b as an example. As discussed in Example 7, the undirected induced subgraph over \(\{A, B, X\}\) and \(\{A, B, X, C\}\) are orientation components for \(X\) and \(C\) respectively. If \(X \rightarrow B\) is in
The maximal orientation component for

Proposition 8. Let \( G^* \) be a CPDAG and \( K \) be a set of DCCs consistent with \( G^* \). Suppose that with respect to \( K \) and \( G^* \), \( U_1 \) and \( U_2 \) are two orientation components for the same vertex \( X \), then the undirected induced subgraph of \( G^* \) over \( V(U_1) \cup V(U_2) \) is also an orientation component for \( X \).

In some literature, the undirected induced subgraph of \( G^* \) over \( V(U_1) \cup V(U_2) \) is called the union of \( U_1 \) and \( U_2 \). Thus, Proposition 8 indicates that the union of two orientation components for \( X \) is still an orientation component for \( X \). This result motivates the definition of maximal orientation component.

Definition 19 (Maximal Orientation Component, MOC). Given a CPDAG \( G^* \) and a set \( K \) of DCCs consistent with \( G^* \), with respect to \( K \) and \( G^* \), an orientation component for a variable \( X \) is called maximal if every orientation component for \( X \) is its induced subgraph.

Based on Definition 19 and Theorem 7, we have the following corollary.

Corollary 2. Let \( G^* \) be a CPDAG and \( K \) be a set of DCCs consistent with \( G^* \), then \( X \rightarrow Y \) is in every DAG in \( [G^*, K] \) if and only if \( X \rightarrow Y \) is in \( G^* \) or the maximal orientation component for \( Y \) with respect to \( K \) and \( G^* \) contains \( X \).

Corollary 2 yields a method to find the MPDAG of a restricted Markov equivalence class. The key step is to find the maximal orientation component of a variable, whose procedure is given in Algorithm 3. Algorithm 3 is a generalization of Algorithm 1. The first step of Algorithm 3 is to set \( U_m \) to be the chain component containing \( X \), and compute \( K_m = K(U_m) \). This is because the maximal orientation component for \( X \) is an induced subgraph of the chain component to \( X \) belongs. If \( U_m \) is an orientation component for \( X \), then it is definitely maximal. Otherwise, the

Algorithm 3 Finding the maximal orientation component for a vertex.

Require: A CPDAG \( G^* \), a set \( K \) of DCCs consistent with \( G^* \), and a vertex \( X \) in \( G^* \).
Ensure: The maximal orientation component for \( X \) with respect to \( K \) and \( G^* \).
1: Set \( U_m \) to be the chain component containing \( X \), and compute \( K_m = K(U_m) \);
2: while \( U_m \) is not an orientation component for \( X \), do
3: find a potential leaf node in \( U_m \) and denote it by \( Y \);
4: update \( U_m \) by removing \( Y \) and the edges connected to \( Y \);
5: update \( K_m \) by removing all clauses whose heads contain \( Y \);
6: end while
7: return \( U_m \).
while-loop begins. Since $X$ is not the only potential leaf node in $U_m$, based on Theorem 4, there must be another potential leaf node $Y$ in $U_m$. We then remove $Y$ and the edges connected to $Y$. The resulting graph is the induced subgraph of $U_m$ over $V(U_m) \setminus \{Y\}$, and we still denote it by $U_m$. Finally, we remove from $K_m$ those clauses whose heads include $Y$. This is equivalent to setting $K_m = K_m(U_m)$. The while-loop ends when $U_m$ is an orientation component for $X$. Note that, since in each loop we remove one vertex, $U_m$ will eventually become an orientation component for $X$ in the finite number of loops. The correctness of Algorithm 3 is guaranteed by the following theorem.

**Theorem 8.** The outputted undirected graph of Algorithm 3 is identical to the maximal orientation component for $X$ with respect to $K$ and $G^*$. 

Similar to Algorithm 1, the complexity of Algorithm 3 is upper bounded by $O(|V(G^*)|^3)$. Applying Algorithm 3 to each vertex separately, we can find the MPDAG of a restricted Markov equivalence class based on Corollary 2, as shown by the following example.

**Example 8.** Figure 10a shows a CPDAG $G^*$ and a set of DCCs $K$ consisting of $D \rightarrow \{E, B\}$, $E \rightarrow \{A, C\}$, $E \rightarrow \{B, F\}$ and $G \rightarrow \{B, H\}$. We first show how to use Algorithm 3 to find the maximal orientation component for $A$. Note that, since $G^*$ is undirected, $G^* = G^*$ and $K(G^*) = K$. As $C, A, H$ are potential leaf nodes in $G^*$, $G^*$ is not an orientation component for $A$, which triggers the while-loop. In the first loop, we remove $C$ and the edges connected to $C$ first, resulting the undirected graph $U_m$ shown in Figure 10b, and then remove $E \rightarrow \{A, C\}$ from $K$ as it has a head not in $U_m$. The remaining clauses are $D \rightarrow \{E, B\}$, $E \rightarrow \{B, F\}$ and $G \rightarrow \{B, H\}$, which are visualized by arcs in Figure 10b. Since $H$ is still a potential leaf node in $U_m$, we remove $H$ and the edges connected to $H$ from the current graph, and remove $G \rightarrow \{B, H\}$ from the current graph.

![Figure 10: An illustrative example to show how to use Algorithm 3 to find the MPDAG.](image-url)
set of clauses. The result is shown in Figure 10c. In the next two loops, we sequentially remove G (Figure 10d) and F (Figure 10e). Finally, we have the undirected graph shown in Figure 10e, which is the maximal orientation component for A. Similarly, using Algorithm 3 we can find the maximal orientation components for F, G and H separately, which are shown in Figures 10f to 10h, respectively. Note that, The maximal orientation components for the remaining variables are all empty graphs. Therefore, by Corollary 2, E → A, B → A, E → F, B → F, F → G, B → G, B → H, F → H, and G → H are all and only directed edges in the MPDAG. The resulted MPDAG is given in Figure 10i.

Algorithm 4 Finding MPDAG and minimal residual set.

Require: A CPDAG $G^*$, a consistent causal constraint set $B$.
Ensure: The MPDAG of $[G^*, B]$ and a minimal residual set of DCCs.

1: Construct the equivalent DCCs $K$ based on Theorem 3,
2: Let $H = G^*$,
3: for $X \in V(G^*)$, do
4: find the maximal orientation component for $X$ according to Algorithm 3 and denote it by $U$,
5: for $Y \in \text{adj}(X, U)$, do
6: Replace $Y - X$ by $Y \rightarrow X$ in $H$,
7: end for
8: end for
9: while $K \neq \varnothing$, do
10: if there exists a $\kappa \in K$ such that $\cup \{D \rightarrow \kappa_t\} \cup K$ is inconsistent with $G^*$, then
11: set $K = K \setminus \{\kappa\}$,
12: else
13: break
14: end if
15: end while
16: return $H$ and $K$.

Algorithm 4 summarizes the procedure of decomposing pairwise causal constraints, where lines 2 to 9 show how to use Algorithm 3 to find the MPDAG. To find a minimal residual set of DCCs, we can sequentially remove from $K$ a redundant DCC $\kappa$. By Theorem 5, $\kappa$ is redundant in $[G^*, K]$ if and only if $\cup_{D \in \kappa} \{D \rightarrow \kappa_t\} \cup K$ is inconsistent with $G^*$. Here, Algorithm 1 can be applied to check consistency. Note that, such a minimal subset may not be unique, and their sizes may also different. Thus, the above decomposition is order-dependent.

5 Causal Inference with Background Knowledge

In this section, we study the causal inference problem when causal background knowledge is available. It is well-known that the causal effect of a treatment (or multiple treatments) on a response (or multiple responses) may not be identifiable given a CPDAG, while additional information in background knowledge could make the causal effect identifiable or less uncertain. In Section 5.1, we study the identification condition of a causal effect under restricted Markov equivalence represented by a CPDAG and a set of DCCs, and in Section 5.2, when a causal effect is unidentifiable, we further extend the IDA framework to estimate all possible causal effects.
5.1 Identifiability

We first present the definition of causal effect identifiability. This definition is a generalization of Pearl (2009) and Perković et al. (2017) to restricted Markov equivalence class induced by a CPDAG and background knowledge.

**Definition 20** (Causal Effect Identifiability). Let \( G^* \) be a CPDAG over vertex set \( V \) and \( B \) be a consistent causal constraint set (or a consistent DCC set). Suppose that \( X, Y \subseteq V \) are two disjoint vertex sets. The causal effect of \( X \) on \( Y \) is identifiable from \( G^* \) and \( B \) (or in \( [G^*, B] \)), if for any two distinct DAGs \( G_1, G_2 \in [G^*, B] \) and observational distribution \( f \) Markovian to \( G_1 \) and \( G_2 \), the interventional distributions \( f_1(y \mid do(x)) \) and \( f_2(y \mid do(x)) \) computed from two causal models \( (G_1, f(V)) \) and \( (G_2, f(V)) \), respectively, are equivalent.

Our main result of identifiability is given below.

**Theorem 9.** Let \( G^* \) be a CPDAG and \( B \) be a consistent pairwise causal constraint set (or a consistent DCC set). Denote by \( \mathcal{H} \) the MPDAG of \( [G^*, B] \). For any two disjoint vertex sets \( X, Y \subseteq V(G^*) \), the causal effect of \( X \) on \( Y \) is identifiable from \( G^* \) and \( B \) if and only if every proper possibly causal path from \( X \) to \( Y \) starts with a directed edge in \( \mathcal{H} \).

Interestingly, the identification condition provided in Theorem 9 is identical to the one for MPDAG proposed by Perković (2020). That is, the causal effect of \( X \) on \( Y \) is identifiable in \([G^*, B]\) if and only if it is identifiable in \([\mathcal{H}]\), where \( \mathcal{H} \) is the MPDAG representing \([G^*, B]\). Recall that in Section 3.2 we represent an arbitrary causal constraint set by an MPDAG plus a residual, minimal set of DCCs. Thus, Theorem 9 implies that only the MPDAG determines the identifiability, and the additional information carried by the residual set contributes nothing to the identifiability.

**Example 9.** Consider the MPDAG \( \mathcal{H} \) with two DCCs \( A \rightarrow\leftarrow \{B, C\} \) and \( C \rightarrow\leftarrow \{A, X\} \) shown in Figure 11a. By Theorem 9, the causal effect of \( X \) on \( Y \) is not identifiable, as \( X - A \rightarrow Y \) and \( X - C \rightarrow Y \) are possibly causal paths on which the first edges are undirected. To verify this result, we enumerate all possible parental sets of \( X \) in Figures 11b to 11e. It can be seen that the causal effect of \( X \) on \( Y \) is definitely zero in Figure 11b, while the causal effects of \( X \) on \( Y \) are possibly non-zero in Figures 11c to 11e.

Since the causal effect identification condition for \( G^* \) and \( B \) is the same as that for an MPDAG, the method of estimating identifiable effects with an MPDAG can be directly applied in our setting. We refer the readers to Perković (2020) for the detailed algorithm.
The following corollary of Theorem 9 provides conditions under which a causal background knowledge set can definitely increase the number of identifiable effects.

**Corollary 3.** Suppose that $G^*$ is a CPDAG over vertex set $V$ and $K$ is a set of DCCs consistent with $G^*$, then the following two statements are equivalent.

(i) At least one unidentifiable effect in $[G^*]$ becomes identifiable in $[G^*, K]$.

(ii) The DAGs in $[G^*, K]$ have at least one common direct causal relation that is not encoded by a directed edge in $G^*$.

In particular, if $K$ is derived from a consistent causal background knowledge set $B$ and there is a direct or non-ancestral causal constraint in $B$ which does not hold for all DAGs in $[G^*]$, or there is an ancestral causal constraint $X \rightarrow Y$ in $B$ such that $Y \rightarrow X$ does not hold for all DAGs in $G^*$, then at least one unidentifiable effect in $[G^*]$ becomes identifiable in $[G^*, K]$.

Among the identifiable effects, some can be calculated by adjustment criterion. The following theorem gives a sound and complete adjustment criterion.

**Theorem 10.** Let $G^*$ be a CPDAG over vertex set $V$ and $B$ be a consistent pairwise causal constraint set (or a consistent DCC set). Denote by $H$ the MPDAG of $[G^*, B]$. For any pairwise disjoint vertex sets $X, Y, Z \subseteq V$, $Z$ is an adjustment set for $(X, Y)$ with respect to $G^*$ and $B$ if and only if $Z$ satisfies the b-adjustment criterion relative to $(X, Y)$ in $H$.

The definitions of adjustment set and b-adjustment criterion in Theorem 10 is given below.

**Definition 21 (Adjustment Set).** Let $G^*$ be a CPDAG over vertex set $V$ and $B$ be a consistent pairwise causal constraint set (or a consistent DCC set). Suppose that $X, Y, Z \subseteq V$ are pairwise disjoint vertex sets. Then, $Z$ is called an adjustment set for $(X, Y)$ with respect to $G^*$ and $B$ if for any DAG $G \in [G^*, B]$ and observational distribution $f$ Markovian to $G$, the interventional distribution $f(y \mid do(x))$ can be calculated by

$$f(y \mid do(x)) = \begin{cases} \int f(y \mid x, z)f(z)dz, & \text{if } Z \neq \emptyset, \\ f(y \mid x), & \text{otherwise.} \end{cases}$$

**Definition 22 (b-AdjustmentCriterion (Perković et al., 2017)).** Let $X, Y, Z \subseteq V$ be pairwise disjoint vertex sets in an MPDAG $H$, and $\text{Forb}(X, Y, H)$ be the set of variables which are possible descendants of some $W \notin X$ lying on a proper possibly causal path from $X$ to $Y$. Then, $Z$ satisfies the b-adjustment criterion relative to $(X, Y)$ in $H$ if: (i) all proper possibly causal paths from $X$ to $Y$ start with a directed edge in $H$, (ii) $Z \cap \text{Forb}(X, Y, H) = \emptyset$, and (iii) all proper definite status non-causal paths from $X$ to $Y$ are blocked by $Z$ in $H$.

Notice that adjustment criterion in Theorem 10 is the same as that in Perković et al. (2017, Theorem 4.4) for a restricted Markov equivalence class $[H]$ induced by an MPDAG $H$. Thanks for Theorem 10, the results on optimal adjustment sets for MPDAGs can be naturally extended to general causal background knowledge. The details can be found in Henckel et al. (2022); Rotnitzky and Snucler (2020).
5.2 Estimating Possible Causal Effects

When a causal effect is not identifiable, we can estimate its bound by enumerating all possible causal effects. Based on the proposed Algorithm 1 for checking consistency, it is straightforward to extend the semi-local IDA (Perković et al., 2017, Algorithm 2) to estimating all possible causal effects of multiple treatments on multiple responses. Moreover, by Theorem 10, the optimal IDA (Witte et al., 2020) and minimal IDA (Guo and Perković, 2021) can similarly extended. Thus, in the following, we mainly focus on extending the IDA framework to fully-locally estimate all possible causal effects of a single treatment on a single target. The key result is the following local orientation rules for CPDAGs with DCCs.

**Theorem 11.** Let $\mathcal{K}$ be a DCC set consistent with a CPDAG $\mathcal{G}^*$, and $\mathcal{H}$ be the MPDAG of $[\mathcal{G}^*, \mathcal{K}]$. For any vertex $X$ and $S \subseteq \text{sib}(X, \mathcal{H})$, the following statements are equivalent.

(i) There is a DAG $\mathcal{G}$ in $[\mathcal{G}^*, \mathcal{K}]$ such that $\text{pa}(X, \mathcal{G}) = S \cup \text{pa}(X, \mathcal{H})$ and $\text{ch}(X, \mathcal{G}) = \text{sib}(X, \mathcal{H}) \cup \text{ch}(X, \mathcal{H}) \setminus S$.

(ii) The restriction subset of $\mathcal{K} \cup D_X$ on $\mathcal{G}^*(\text{sib}(X, \mathcal{G}^*))$ is consistent with $\mathcal{G}^*(\text{sib}(X, \mathcal{G}^*))$, where $D_X := \{u \rightarrow X \mid u \in \text{pa}(X, \mathcal{H}) \cup S\} \cup \{X \rightarrow v \mid v \in \text{sib}(X, \mathcal{H}) \cup \text{ch}(X, \mathcal{H}) \setminus S\}$.

We remark that $\mathcal{G}^*(\text{sib}(X, \mathcal{G}^*))$ is a chordal graph, which itself is a CPDAG (Andersson et al., 1997), and thus the consistency in statement (ii) is well-defined. Theorem 11 provides a method to locally enumerate all possible parental sets of a given $X$, which are then used to estimate all possible causal effects. Algorithm 5 shows the procedure.

**Algorithm 5** The bgk-IDA algorithm

**Require:** A CPDAG $\mathcal{G}^*$, a consistent pairwise causal constraint set $\mathcal{B}$, a treatment $X$, and a response $Y$.

**Ensure:** $\Theta_X$ which stores all possible causal effects of $X$ on $Y$.

1: derive the DCC set $\mathcal{K}$ from $\mathcal{G}^*$ and $\mathcal{B}$ based on Theorem 3,
2: construct the MPDAG $\mathcal{H}$ of $[\mathcal{G}^*, \mathcal{K}]$,
3: for each $S \subseteq \text{sib}(X, \mathcal{H})$ such that the restriction subset of $\mathcal{K} \cup D_X$ on $\mathcal{G}^*(\text{sib}(X, \mathcal{G}^*))$ is consistent with $\mathcal{G}^*(\text{sib}(X, \mathcal{G}^*))$, where $D_X$ is defined in Theorem 11, do
4: estimate the causal effect of $X$ on $Y$ by adjusting for $S \cup \text{pa}(X, \mathcal{H})$, and add the causal effect to $\Theta_X$,
5: end for
6: return $\Theta_X$.

To illustrate Theorem 11, Figure 12 shows the four impossible parental sets of $X$ in the MPDAG shown in Figure 11a. Recall that $X$ has 3 siblings, meaning that there are totally 8 candidate parental sets of $X$. For example, if we let $B \rightarrow X$ and $X \rightarrow \{A, C\}$ (Figure 12a) then $C \rightarrow \{X, A\}$ indicates that $C \rightarrow A$, and further causes $A \rightarrow B$ by the constraint $A \rightarrow \{B, C\}$. Hence, $\mathcal{K} \cup \{B \rightarrow X, X \rightarrow A, X \rightarrow C\}$ on $\mathcal{G}^*(\text{sib}(X, \mathcal{G}^*))$ is inconsistent with $\mathcal{G}^*(\text{sib}(X, \mathcal{G}^*))$, as $X \rightarrow A \rightarrow B \rightarrow X$ is a directed cycle.
5.3 Simulations

We empirically study how causal background knowledge improves the identifiability of a causal effect in this subsection. We use randomly sampled chordal graphs instead of CPDAGs in our simulations since the impact of the clauses can be separately considered for each chain component of the CPDAG after transforming causal background knowledge into DCCs (please refer to Lemma 10 in the supplementary material for details).

For each combination of \( n \in \{10, 30\} \) and \( e \), where \( e \in \{10, 15, 20, 25\} \) if \( n = 10 \) and \( e \in \{30, 45, 60, 75\} \) if \( n = 30 \), we first sampled 500 chordal graphs with \( n \) vertices and \( e \) edges. Next, for each chordal graph \( G^* \), we treated it as a CPDAG and sampled a DAG \( G \) from \( [G^*] \), and assigned each edge in \( G \) with a weight sampled from Uniform(0.5, 2). \( G \) was regarded as the underlying true DAG. Then, we sampled a treatment \( X \) as well as a response \( Y \). Finally, we used the bgk-IDA to compute the possible causal effects of \( X \) on \( Y \), with \( b \) direct, ancestral, or non-ancestral causal constraints randomly generated according to \( G \), where \( b \in \{0, 1, 2, 3, 4, 5\} \) for \( n = 10 \) and \( b \in \{0, 3, 6, 9, 12, 15\} \) for \( n = 30 \). Here, we assumed the data generating mechanism is linear-Gaussian with equal variances, and the causal effects were estimated from the true covariance matrix computed from \( G \).

We used the causal mean square error (CMSE) to measure the discrepancy between an estimated multi-set of possible effects and the true effect computed with \( G \) (Tsirlis et al., 2018; Liu et al., 2020b). Denote by \( \hat{\Theta}_{XY} \) and \( \theta_{XY} \) the estimated multi-set of possible causal effects and the true causal effect, respectively. Then, the CMSE is defined as

\[
\text{CMSE}(\hat{\Theta}_{XY}, \theta_{XY}) = \frac{1}{m} \sum_{i=1}^{m} \left( \hat{\theta}_i - \theta_{XY} \right)^2,
\]

where \( m = |\hat{\Theta}_{XY}| \) and \( \hat{\theta}_i \in \hat{\Theta}_{XY} \) is an estimated possible causal effect. The CMSE can be viewed as the averaged square distance between each possible effect and the true effect. Therefore, CMSE equals zero indicates that the true causal effect is identifiable, and the lower the CMSE, the higher the identifiability of a causal effect.

For each sampled DAG and \( X,Y \), we computed three sequences of CMSEs, which correspond to three types of background knowledge. Each sequence of CMSEs has 6 elements, corresponding to 6 possible values of \( b \). For each sequence, we divided all CMSEs by the one corresponding to \( b = 0 \), and the ratio is called a rescaled CMSE.

Figure 13 shows the rescaled CMSE sequences. It can be seen that the rescaled CMSE drops quickly as the number of constraints increases. Moreover, given the same number of constraints,
the rescaled CMSE of providing ancestral causal constraints is much less than that of providing
direct causal constraints, and the latter is also much less than that of providing non-ancestral
constraints in general. The reason of this phenomena is because ancestral causal constraints are
more informative than non-ancestral causal constraints in the sense that $X$ is a cause of $Y$ implies
that $Y$ is not a cause of $X$ but not vice versa.

We also examined other metrics including the number of possible causal effects and the interval
determined by the minimum and maximum values of a set of possible effects, and the results are
similar to those shown in Figure 13.

6 Discussion

Causal background knowledge is frequently encountered in real-world problems. Assuming both
causal background knowledge and a sufficiently large observational data set are available, this paper
systematically studies the representation of causal background knowledge, and demonstrates the
potential of exploiting causal background knowledge in causal inference. The main contribution of
the paper is three-fold.

Firstly, we investigate the graphical characterization of causal MPDAGs. We present sufficient and
necessary graphical conditions for a partially directed graph to be a causal MPDAG. MPDAGs
are important in representing common direct causal relations in a restricted Markov equivalent
class. Our graphical characterization provides an opportunity to better understand the graphical
properties of causal MPDAGs.

Despite the wide use of causal MPDAGs, they may fail to represent ancestral causal knowledge
exactly. Therefore, we develop direct causal clauses to represent all types of causal background
knowledge in a unified form. Because of the local nature of the direct causal clauses, our new
representation brings a lot of convenience. As a result, we can now check the consistency of causal
background knowledge or the equivalency of two causal background knowledge sets in polynomial-time. Moreover, we prove that any causal background knowledge set can be decomposed into a causal MPDAG and a minimal residual set of direct causal clauses, and the decomposed causal MPDAG can be found in polynomial-time, too.

The decomposition of causal background knowledge plays an important role in causal inference. The third contribution of our work is that, we show that the decomposed causal MPDAG entirely determines the identifiability of a causal effect, and the residual direct causal clauses alone contributes nothing to the identifiability, but may reduce the possible values of an unidentifiable effect. We also develop IDA-type algorithms to locally or semi-locally estimate possible causal effects. With the proved sufficient and necessary identification condition, adjustment criterion and the IDA-type algorithms, we can not only identify causal effects, but also estimate their values or bounds.

In this paper, we assumed that a CPDAG is learned before exploiting causal background knowledge. In fact, causal background knowledge is also useful for causal discovery. We expect that the proposed representation could motivate new learning algorithms of causal structures. Besides, our exploitation of causal background knowledge in causal inference relies on the assumption that causal background knowledge is consistent with the true CPDAG (or the learned CPDAG). How to generalize these results to inconsistent background knowledge is also important. Finally, studying the representation of causal background knowledge in a system with hidden variables and selection biases is also an interesting future work.

Appendix

A A Sequential Method for Checking Consistency

In this section, we present an approach to sequentially check consistency. Suppose that \( \mathcal{G}^* \) is a CPDAG and \( \mathcal{K} \) is a set of consistent DCCs, and \( \mathcal{H} \) is the MPDAG representing \( [\mathcal{G}^*, \mathcal{K}] \). A set of DCCs \( \mathcal{K}' \) is called consistent with \( \mathcal{G}^* \) given \( \mathcal{K} \), if \( \mathcal{K}' \cup \mathcal{K} \) is consistent with \( \mathcal{G}^* \). For any DCC \( (X \overset{\text{or}}{\rightarrow} D) \in \mathcal{K}' \), it holds that,

\[
K \cup \{ X \overset{\text{or}}{\rightarrow} D \} \text{ is inconsistent} \iff X \overset{\text{or}}{\rightarrow} D \text{ does not hold for any DAG in } [\mathcal{G}^*, \mathcal{K}] \\
\iff \forall \mathcal{G} \in [\mathcal{G}^*, \mathcal{K}], \text{ch}(X, \mathcal{G}) \cap D = \emptyset \\
\iff \forall \mathcal{G} \in [\mathcal{G}^*, \mathcal{K}], \ D \subseteq \text{pa}(X, \mathcal{G}) \\
\iff \forall \mathcal{G} \in [\mathcal{G}^*, \mathcal{K}], \ D \rightarrow X \\
\iff D \subseteq \text{pa}(X, \mathcal{H}).
\]

Therefore, the consistency of \( \mathcal{K}' \) with \( \mathcal{G}^* \) given \( \mathcal{K} \) can be checked sequentially: picking one DCC from the current \( \mathcal{K}' \) per time; if the clause is consistent with \( \mathcal{G}^* \) given \( \mathcal{K} \), then adding it to the current \( \mathcal{K} \) and updating the current MPDAG based on \( \mathcal{K} \).

**Example 10.** Following Example 6, we now use the sequential method to check the consistency of \( \mathcal{K} = \{ G \overset{\text{or}}{\rightarrow} A, B \overset{\text{or}}{\rightarrow} A, D \overset{\text{or}}{\rightarrow} \{ A, X \} \} \) with respect to \( \mathcal{G}^* \) shown in Figure 6a. If the first DCC chosen from \( \mathcal{K} \) is \( D \overset{\text{or}}{\rightarrow} \{ A, X \} \), then the updated MPDAG, denoted by \( \mathcal{H} \), is the one shown in
B Non-Pairwise Causal Background Knowledge

In this section, we present some discussions on non-pairwise causal background knowledge. Non-pairwise causal background knowledge is also common in practice. For example, tiered background knowledge is non-pairwise. Given a disjoint partition \( T := \{ V_1, V_2, \ldots, V_n \} \) of the variable set \( V \), tiered background knowledge is a proposition saying that for all \( X_i \in V_i \) and \( X_j \in V_j \) such that \( 1 \leq i \leq j \leq n \), either \( X_i \rightarrow X_j \) or \( X_i \not\rightarrow X_j \) (Andrews et al., 2020). Nonetheless, most non-pairwise causal background knowledge can be viewed as Boolean combinations of pairwise causal background knowledge. For instance, tiered background knowledge can be interpreted and denoted by

\[
\text{tbk}^T := \bigwedge_{X_i \in V_i, X_j \in V_j} \left( X_i \rightarrow X_j \lor (X_i \not\rightarrow X_j \land X_j \not\rightarrow X_i) \right).
\]

Moreover, given a CPDAG \( G^* \), as \( X_i \rightarrow X_j \land X_j \rightarrow X_i \) holds for all DAGs in \( \mathcal{G}^* \) if and only if \( X_i \not\in \text{adj}(X_j, G^*) \), we have

\[
\text{tbk}^T \iff \bigwedge_{X_i \in V_i, X_j \in V_j, X_i \in \text{adj}(X_j, G^*), 1 \leq i \leq j \leq n} X_i \rightarrow X_j.
\]

Thus, the results in the main text can be extended to tiered background knowledge.

Unfortunately, directly extend our results to an arbitrary Boolean combination of causal background knowledge is difficult. Nevertheless, a possible solution exists. Let \( \mathcal{B} \) be a set of Boolean combinations of causal background knowledge. It is clear that a DAG satisfies all constraints in \( \mathcal{B} \) if and only if \( \land_{b \in \mathcal{B}} b \) holds for the DAG. Since for any \( b \in \mathcal{B} \), \( b \) is a Boolean combination of causal background knowledge, \( \land_{b \in \mathcal{B}} b \) can be reformulated into its disjunctive normal form,

\[
\bigwedge_{b \in \mathcal{B}} b = \bigvee_I \left( \bigwedge_{j \in J} c_{ij} \right),
\]

where \( I, J \) are finite indicator sets, and each \( c_{ij} \) is a direct, non-ancestral or ancestral causal constraint. For each \( i \in I \), let \( \mathcal{B}_i = \{ c_{ij} \mid j \in J \} \), we can then extend our results to each \( \mathcal{B}_i \) and combine them together. For example, to check the consistency of \( \land_{b \in \mathcal{B}} b \), it suffices to show that there exists a consistent \( \mathcal{B}_i \); to construct the MPDAG representing \( \mathcal{G}^*, \mathcal{B} \), one need first construct the MPDAG for each \( \mathcal{B}_i \), then subtract all common direct causal relations from those MPDAGs.
We remark that, the bottleneck of the above solution is the computation of Equation (7). Generally, the disjunctive normal form is not unique, and the reformulation may be exponentially difficult. How to efficiently represent Boolean combinations of causal background knowledge is regarded as future work.

C Proofs

Before presenting all detailed proofs of the theorems, propositions and corollaries of the main text, we introduce some helpful concepts and results in Appendix C.1. In the following paper, for a variable $X$ and a non-empty variable set $Y$, we will use the notion $Y \rightarrow X$ to represent $Y \rightarrow X$ for all $Y \in Y$, and use the notion $X \rightarrow Y$ to represent $X \rightarrow Y$ for all $Y \in Y$.

C.1 Preliminaries

We briefly review some graphical properties of chordal graphs and CPDAGs. In a graph, a cycle with length three is called a triangle. A path is called unshielded if none of its three consecutive vertices forms a triangle. For a graph $G$ over vertex set $V$, $M \subseteq V$ is called a clique if $M$ induces a complete subgraph. A clique is called maximal if it is not a proper subset of any other cliques.

Let $C$ be a chordal graph over vertex set $V(C)$. Any induced subgraph of $C$ is chordal. It can be proved that any chordal graph has a simplicial vertex, and moreover, any non-complete chordal graph has two non-adjacent simplicial vertices (Blair and Peyton, 1993). A perfect elimination ordering (PEO) of $C$ is a total ordering of the vertices in $V(C)$, denoted by $\beta = (V_1, V_2, \cdots, V_n)$, such that for any $V_i, i = 1, 2, \cdots, n$, $adj(V_i, C) \cap \{V_i, V_{i+1}, \cdots, V_n\}$ induces a complete subgraph of $V(C)$. An undirected graph is chordal if and only if it has a PEO.

Given a PEO $\beta = (V_1, V_2, \cdots, V_n)$ of $C$, if we orient the edges in $C$ such that $adj(V_i, C) \cap \{V_i, V_{i+1}, \cdots, V_n\}$ are parents of $V_i$, then the resulting directed graph is acyclic and v-structure-free. Conversely, any v-structure-free DAG who has the same skeleton as $C$ can be oriented from $C$ according to some PEO of $C$.

Let $G^*$ be a CPDAG. It was pointed by Maathuis et al. (2009) that (i) no orientation of the edges not oriented in $G^*$ will create a directed cycle which includes an edge or edges that were oriented in $G^*$, and (ii) no orientation of an edge not directed in $G^*$ can create a new v-structure with an edge that was oriented in $G^*$. As any orientation of the edges in $G^*$ which does not create directed cycles or v-structures corresponds to a DAG in $[G^*]$, we can separately orient the undirected edges in each chain component such that every resulting directed graph is a DAG without v-structure.

C.2 Proof of Proposition 1

We first prove Proposition 1 as it is required in proving Theorem 1.

Proof. The first claim holds because the definition of causal MPDAG implies that for any restricted Markov equivalence class $[G^*, B]$ that can be represented by $\mathcal{H}$, $G^*$ and $\mathcal{H}$ have the same skeleton and v-structures.
To prove the second claim, let $[G^*, B]$ be a restricted Markov equivalence class that can be represented by $H$, and let $B_d = E_d(H) \setminus E_d(G^*)$. It is easy to verify that orienting undirected edges in $G^*$ according to $B_d$ does not introduce any v-structure or directed cycle and the resulting PDAG is closed under Meek’s rules, as the resulting PDAG is exactly $H$. Therefore, $[H] = [G^*, B_d]$.

C.3 Proof of Theorem 1

We first introduce two properties of chordal graphs. For the completeness of the paper, the proofs of these results are also provided.

Lemma 1. Let $C$ be a connected chordal graph, then the following claims hold for $C$.

1. For any simplicial vertex $X$ in $C$, there is a unique maximal clique containing $X$.

2. If $C$ is not complete, then for any non-simplicial vertex $Y$ in $C$ that is adjacent to some simplicial vertex $X$, $Y$ has a neighbor $Z \neq X$ which is not adjacent to $X$.

Proof of Lemma 1. For any simplicial vertex $X$ in $C$, if there are two distinct maximal cliques $M_i, M_j$ containing $X$, then there exist $X_i \in M_i$ and $X_j \in M_j$ such that $X_i$ and $X_j$ are not adjacent, since otherwise $M_i \cup M_j$ is also a maximal clique. Note that both $X_i$ and $X_j$ are adjacent to $X$, hence $X$ is not simplicial, which is contrary to the assumption. This completes the proof of the first claim.

We next prove the second claim. Let $M_i$ be the maximal clique containing $X$. Since $X$ is simplicial, $Y$ is adjacent to $X$ implies that $Y \in M_i$. Assume, for the sake of contradiction, that every neighbor of $Y$ other than $X$ is adjacent to $X$, then $\text{adj}(Y, C) \subseteq M_i$, which means $\text{adj}(Y, C)$ induces a complete subgraph of $C$. This is contradicted to the assumption that $Y$ is non-simplicial. Therefore, the second claim holds true.

Next, we present Lemmas 2-8 in the following. These lemmas contribute to the proof of the necessity of Theorem 1.

Lemma 2 (Necessity of Condition (ii)). For each B-component $C^b$ of a causal MPDAG $H$, the skeleton of $C^b$ is a chordal graph.

Proof of Lemma 2. According to Proposition 1, the skeleton of each B-component of a causal MPDAG is an induced subgraph of a chain component of a CPDAG. The result comes from the fact that any induced subgraph of a chordal graph is still chordal.

Lemma 3 (Necessity of Condition (iii)). Let $H$ be a causal MPDAG and $C^b$ be a B-component of $H$. For any vertex $X \notin V(C^b)$, if $X \rightarrow Y$ for some vertex $Y \in V(C^b)$, then $X \rightarrow Y$ for every vertex $Y \in V(C^b)$.

Proof of Lemma 3. If $|V(C^b)| = 1$, then Lemma 3 naturally holds. Assume that $|V(C^b)| > 1$, then $\text{sib}(Y, C^b) \neq \emptyset$ by the definition of B-component. Since every B-component is a connected graph, to prove Lemma 3 it suffices to show that $X \rightarrow Z$ for every $Z \in \text{sib}(Y, C^b)$. This is because every
vertex in $C^b$ other than $Y$ is connected to $Y$ by an undirected path. If the conclusion holds for every $Z \in sib(Y, C^b)$, then the same argument can be successively applied to every vertex along the path.

For any vertex $Z \in sib(Y, C^b)$, it is clear that $X$ and $Z$ are adjacent, since otherwise, by Rule 1 of Meek’s rules, it holds that $Y \rightarrow Z$ is in $\mathcal{H}$, which is contradicted to $Z \in sib(Y, C^b)$. As $X \notin V(C^b)$, $X$ and $Z$ must be connected by a directed edge. If $Z \rightarrow X$, then $Z \rightarrow Y$ can be oriented as $Z \rightarrow Y$ by Rule 2 of Meek’s rules, which is also contradicted to $Z \in sib(Y, C^b)$. Thus, we have $X \rightarrow Z$.

**Lemma 4** (Necessity of Condition (i)). Given a causal MPDAG $\mathcal{H}$, the chain skeleton $\mathcal{H}_c$ of $\mathcal{H}$ is a chain graph. Furthermore, $\mathcal{H}_c$ is also an MPDAG.

**Proof of Lemma 4.** We first prove that the graph $\mathcal{H}_c$ is a chain graph, which suffices to show that every partially directed cycle in $\mathcal{H}_c$ is an undirected cycle. Assume that there is a partially directed cycle in $\mathcal{H}_c$ which has at least one directed edge, and the cycle is of the following form: $X_{11} \rightarrow X_{21} \cdot \cdot \cdot X_{2n} \rightarrow \cdot \cdot \cdot \rightarrow X_{k1} \cdot \cdot \cdot X_{kn} \rightarrow X_{1n} \cdot \cdot \cdot X_{11}$. Based on the definitions of $\mathcal{H}_c$ and B-component, $X_{21}, \cdot \cdot \cdot ,X_{2n}$ are in the same B-component while $X_{11}$ is not in this B-component. By Lemma 3, it holds that $X_{11} \rightarrow X_{2n}$. Similarly, $X_{2n} \rightarrow X_{3n} \rightarrow \cdot \cdot \cdot \rightarrow X_{kn} \rightarrow X_{11}$, which together with $X_{11} \rightarrow X_{2n}$ gives a directed cycle. Since all directed edges in $\mathcal{H}_c$ are also in $\mathcal{H}$, we have constructed a directed cycle in $\mathcal{H}$, which is contradicted to the definition of causal MPDAG.

We then show that $\mathcal{H}_c$ is an MPDAG. Since we have already proved that there is no (partially) directed cycle in $\mathcal{H}_c$ except undirected ones, $\mathcal{H}_c$ is a PDAG. What remains is to show that $\mathcal{H}_c$ is closed under four Meek’s rules.

(i) If $\mathcal{H}_c$ is not closed under the first Meek’s rule, then $\mathcal{H}_c$ has an induced subgraph $X \rightarrow Y \rightarrow Z$, in which $X \notin \text{adj}(Z, \mathcal{H}_c)$. By the construction of $\mathcal{H}_c$, $Y$ and $Z$ are in the same B-component of $\mathcal{H}$ while $X$ is not in that B-component. According to Lemma 3, $X \rightarrow Z$ must be in $\mathcal{H}_c$, which is contradicted to the assumption that $X \notin \text{adj}(Z, \mathcal{H}_c)$.

(ii) If $\mathcal{H}_c$ is not closed under the second Meek’s rule, then $\mathcal{H}_c$ has an induced subgraph consisting of $X \rightarrow Y \rightarrow Z$ and $X \rightarrow Z$. By the similar argument for (i), $Y \rightarrow X$ must be in $\mathcal{H}_c$, which leads to a contradiction.

(iii) If $\mathcal{H}_c$ is not closed under the third Meek’s rule, then $\mathcal{H}_c$ has an induced subgraph with the configuration shown in Figure 15a. In this case, $X, Y, Z_1, Z_2$ are in the same B-component. Again, by the construction of $\mathcal{H}_c$, $Y \rightarrow Z_2, Z_1 \rightarrow Z_2$ should not be in $\mathcal{H}_c$, which leads to a contradiction.

(iv) If $\mathcal{H}_c$ is not closed under the forth Meek’s rule, then one of the configurations shown in Figures 15b-15d must appear in $\mathcal{H}_c$ as an induced subgraph. In the following, we will prove that none

![Figure 15: The cases discussed in the proof of Lemma 4](image-url)
of the configurations is in $\mathcal{H}_c$. In fact, if $\mathcal{H}_c$ has an induced subgraph with the configuration shown in Figure 15b, then by the similar argument for (iii), $Z_1 \rightarrow Z_2 \rightarrow Y$ should not be in $\mathcal{H}_c$ as $X, Y, Z_1, Z_2$ are in the same B-component of $\mathcal{H}$. If $\mathcal{H}_c$ has an induced subgraph with the configuration shown in Figure 15c, then the induced subgraph of $\mathcal{H}_c$ over $X, Z_2, Y$ is not closed under the second Meek’s rule. Similarly, in Figure 15d, the induced subgraph of $\mathcal{H}_c$ over $Z_1, Z_2, X$ is not closed under the second Meek’s rule either. This completes the proof.

Lemma 5. Given a causal MPDAG $\mathcal{H}$, if a directed edge in $\mathcal{H}$ can be oriented by Rule 1 or Rule 4 of Meek’s rules, then the involved vertices of the corresponding Meek’s rule are not in the same B-component.

We remark that, a directed edge $Y \rightarrow Z$ can be oriented by Rule 1 means that there is an $X /\notin \text{adj}(Z, \mathcal{H})$ such that $X \rightarrow Y$ is in $\mathcal{H}$. In this case, $X,Y,Z$ are the involved vertices of Rule 1. The meaning of the expression that “a directed edge can be oriented by Rule 4” is similar. We also note that, the condition of Lemma 5 does not rule out the possibility that the edge can also be oriented by Rules 1, 3 or be from the background knowledge set.

Proof of Lemma 5. If a directed edge $Y \rightarrow Z$ can be oriented by Rule 1 of Meek’s rules, then there exists a vertex $X \in V(\mathcal{H})$ such that $X \rightarrow Y$ and $X /\notin \text{adj}(Z, \mathcal{H})$. We need to prove that $X,Y,Z$ are not in the same B-component of $\mathcal{H}$. Assume, for the sake of contradiction, that $X,Y,Z$ are in the same B-component $C_b$, then there is an undirected path $Y - W_1 - \cdots - W_n - Z$ connecting $Y$ and $Z$ where $n \geq 1$ and $W_i \in C_b$ for $i = 1, 2, \cdots, n$. Since $Y-W_1$ is undirected, we have $X \in \text{adj}(W_1, \mathcal{H})$, otherwise we would have $Y \rightarrow W_1$ due to Rule 1 of Meek’s rules. Similarly, $Y \in \text{adj}(W_n, \mathcal{H})$ since $Y \rightarrow Z - W_n$ is in $\mathcal{H}$.

Figure 16: An illustration of the graph structure discussed in the proof of Lemma 5. A dashed undirected edge connecting two vertices indicates they are adjacent, but the direction of the edge is not relevant to the proof.

If $n = 1$ or $X \in \text{adj}(W_n, \mathcal{H})$, then $W_n \rightarrow Z$ should be in $\mathcal{H}$ by Rule 4 of Meek’s rules (Figure 16), which is contradicted to our assumption. Now consider the case where $n > 1$ and $X /\notin \text{adj}(W_n, \mathcal{H})$. Since $X \rightarrow Y$, by the first Meek’s rule we have $Y \rightarrow W_n$. Moreover, since $W_{n-1} - W_n$, it holds that $Y \in \text{adj}(W_{n-1}, \mathcal{H})$. Let $k := \text{arg max}_{1 \leq j \leq n-1} X \in \text{adj}(W_j, \mathcal{H})$ denote the largest subscript of the vertex on the path which is adjacent to $X$, then by the same argument we can show that $Y \rightarrow W_i$ for $i = k + 1, \cdots, n$ and $Y \in \text{adj}(W_k, \mathcal{H})$. Note that, the induced subgraph of $\mathcal{H}$ over $X, Y, W_k$ and $W_k$ is the same as the left-hand side of the forth Meek’s rule, $W_k \rightarrow W_{k+1}$ is in $\mathcal{H}$, which is contrary to our assumption.

If a directed edge $X \rightarrow Y$ can be oriented by Rule 4 of Meek’s rules, then there exist vertices $Z_1, Z_2 \in \mathcal{H}$ such that $\mathcal{H}$ has an induced subgraph shown in Figures 15b-15d. Note that, $Z_2 \rightarrow Y$
can be oriented by Rule 1 of Meek’s rules since \( Z_1 \rightarrow Z_2 \) and \( Z_1 \) is not adjacent to \( Y \), \( Z_1, Z_2 \) and \( Y \) are not in the same B-component by the first part of the proof. Thus, \( X, Z_1, Z_2 \) and \( Y \) are not in the same B-component, which completes the proof.

Lemma 6. Let \( \mathcal{H} \) be a causal MPDAG and \( C^b \) be a B-component of \( \mathcal{H} \). If a directed edge in \( C^b \) can be oriented by Meek’s rules, then it can only be oriented by Rule 2 of Meek’s Rules, and the directed edges in the configuration on the left-hand side of Rule 2 are all in \( C^b \).

Proof of Lemma 6. Let \( X \rightarrow Y \) be a directed edge in \( C^b \) that can be oriented by Meek’s rules. If \( X \rightarrow Y \) can be oriented by the first Meek’s rule, then there is a \( Z \notin \text{adj}(Y, \mathcal{H}) \) such that \( Z \rightarrow X \) is in \( \mathcal{H} \). By Lemma 3, \( Z \in \mathcal{V}(C^b) \). However, this is impossible based on Lemma 5. Therefore, \( X \rightarrow Y \) cannot be oriented by the first Meek’s rule.

If \( X \rightarrow Y \) can be oriented by the third Meek’s rule, then there are \( Z_1, Z_2 \in \text{sib}(X, \mathcal{H}) \) such that \( Z_1 \rightarrow Y \leftarrow Z_2 \) is a v-structure in \( \mathcal{H} \). This means that \( X, Y, Z_1 \) and \( Z_2 \) are in the same B-component of \( \mathcal{H} \). However, as implied by Proposition 1, any B-component is an induced subgraph of some chain component of a CPDAG, and thus the v-structure \( Z_1 \rightarrow Y \leftarrow Z_2 \) is not allowed in \( C^b \), leading to a contradiction.

If \( X \rightarrow Y \) can be oriented by the forth Meek’s rule, then there are \( Z_1 \in \text{sib}(X, \mathcal{H}) \) and \( Z_2 \in \text{adj}(X, \mathcal{H}) \) such that \( X - Z_1 \rightarrow Z_2 \rightarrow Y \) and \( Z_1 \notin \text{adj}(Y, \mathcal{H}) \). Since \( Z_1 - X \), we have that \( Z_1, X \) and \( Y \) are in the same B-component \( C^b \). By Lemma 5, \( Z_2 \) is not in \( C^b \). However, Lemma 3 implies that if \( Z_2 \rightarrow Y \), then \( Z_2 \rightarrow Z_1 \) should also be in \( \mathcal{H} \). This is contrary to the assumption that \( X \rightarrow Y \) can be oriented by the forth Meek’s rule.

Finally, if \( X \rightarrow Y \) can be oriented by the second Meek’s rule, then there is a \( Z \) such that \( X \rightarrow Z \rightarrow Y \) is in \( \mathcal{H} \). By Lemma 3, \( Z \) is in \( C^b \). Thus, \( X \rightarrow Z \) and \( Z \rightarrow Y \) are all in \( C^b \).

Lemma 7. Given a causal MPDAG \( \mathcal{H} \) and a B-component \( C^b \) of \( \mathcal{H} \), let \( M_i \) and \( M_j \) be two distinct maximal cliques of \( C^b \) such that \( M_{ij} := M_i \cap M_j \neq \emptyset \). For any vertex \( X \in M_i \setminus M_{ij} \) and \( Y \in M_{ij} \), the directed edge \( X \rightarrow Y \) does not exist in \( C^b \).

Proof of Lemma 7. \( X \in M_i \setminus M_{ij} \) implies that there must be a \( Z \in M_j \setminus M_{ij} \) such that \( Z \) is not adjacent to \( X \), since otherwise, \( X \) is adjacent to every vertex in \( M_j \) and consequently \( X \in M_j \). Assume that such a directed edge \( X \rightarrow Y \) exists in \( \mathcal{H} \), then such a \( Z \) must be a child of \( Y \) in \( \mathcal{H} \) based on the first Meek’s rule. This is contradicted to Lemma 6.

Lemma 8 (Necessity of Condition (iv)). Given a causal MPDAG \( \mathcal{H} \) and a B-component \( C^b \) of \( \mathcal{H} \), for any directed edge \( X \rightarrow Y \) in \( C^b \), we have that (i) \( \text{adj}(Y, C^b) \subseteq \text{adj}(X, C^b) \), and (ii) \( \text{pa}(X, \mathcal{H}) \subseteq \text{pa}(Y, \mathcal{H}) \setminus \{X\} \).

Proof of Lemma 8. We first prove the correctness of statement (i). For any directed edge \( X \rightarrow Y \) in a B-component \( C^b \) of \( \mathcal{H} \), there is a maximal clique \( M_i \) of \( C^b \) containing both \( X \) and \( Y \). If \( \text{adj}(Y, C^b) \not\subseteq \text{adj}(X, C^b) \), then there exists a vertex \( Z \) satisfying \( Z \in \text{adj}(Y, C^b) \) but \( Z \notin \text{adj}(X, C^b) \), implying that \( Y \) and \( Z \) also belong to another maximal clique \( M_j \) of \( C^b \) which does not contain \( X \). Hence, we have that \( X \in M_i \setminus M_{ij} \) and \( Y \in M_{ij} \), which is contradicted to Lemma 7.

We next show that statement (ii) holds. When \( \text{pa}(X, \mathcal{H}) = \emptyset \), the result is trivial, so we assume that \( \text{pa}(X, \mathcal{H}) \neq \emptyset \). For any vertex \( Z \in \text{pa}(X, \mathcal{H}) \), if \( Z \notin C^b \), then \( Z \rightarrow Y \) by Lemma 3. If \( Z \in C^b \), then we have \( Z \in \text{adj}(Y, \mathcal{H}) \), since otherwise, \( Z \rightarrow X \rightarrow Y \) implies that \( X \rightarrow Y \) can be oriented by
the first Meek’s rule, contradicted to Lemma 6. Therefore, \( Z \rightarrow Y \) appears in \( \mathcal{H} \) by applying Rule 2 of Meek’s rules.

Finally, we present the proof of Theorem 1.

**Proof of Theorem 1.** The necessity of conditions (i)-(iv) follow from Lemma 4, Lemma 2, Lemma 3, and Lemma 8, respectively. In the following, we will prove the sufficiency of conditions (i) to (iv). Let \( \mathcal{H} = (V, E) \) be a partially directed graph which satisfies conditions (i)-(iv). Our goal is to show that \( \mathcal{H} \) is an MPDAG and \( \mathcal{H} \) is causal.

We first show that \( \mathcal{H} \) is acyclic. That is, there is no directed cycle in \( \mathcal{H} \). Assume, for the sake of contradiction, that there exist directed cycles in \( \mathcal{H} \) and let \( \rho = (X_1, X_2, \ldots, X_n, X_1) \) be the shortest one. By condition (i), all the vertices on \( \rho \) are in the same B-component, since otherwise, the corresponding cycle of \( \rho \) in \( \mathcal{H}_c \) is a partially directed cycle that has at least one directed edge, which is contradicted to condition (i). If \( n = 3 \), then \( X_3 \in \text{pa}(X_1, \mathcal{H}) \) while \( X_3 \notin \text{pa}(X_2, \mathcal{H}) \), meaning that \( \text{pa}(X_1, \mathcal{H}) \not\subseteq \text{pa}(X_2, \mathcal{H}) \), which is contradicted to condition (iv). If \( n > 3 \), however, condition (iv) implies that \( X_n \rightarrow X_2 \), and thus \( X_n \rightarrow X_2 \rightarrow X_3 \rightarrow \cdots \rightarrow X_n \) is a directed cycle of length \( n - 1 \), contrary to the assumption that \( \rho \) is the shortest. Therefore, \( \mathcal{H} \) is acyclic.

To prove that \( \mathcal{H} \) is an MPDAG, it suffices to show that \( \mathcal{H} \) is closed under Meek’s rules. We will consider each rule separately in below.

(i) If \( \mathcal{H} \) is not closed under Rule 1 of Meek’s rules, then \( \mathcal{H} \) has an induced subgraph \( X \rightarrow Y \rightarrow Z \), in which \( X \notin \text{adj}(Z, \mathcal{H}) \). Since \( Y \) and \( Z \) are connected by an undirected edge, there exists a B-component \( C^b \) of \( \mathcal{H} \) such that \( Y, Z \in C^b \). According to condition (iii), \( X \in C^b \), otherwise \( X \rightarrow Z \) should be in \( \mathcal{H} \). However, if \( X \in C^b \), then \( Z \in \text{adj}(Y, C^b) \) but \( Z \notin \text{adj}(X, C^b) \), which is contradicted to condition (iv). Thus, \( \mathcal{H} \) is closed under the first Meek’s rule.

(ii) If \( \mathcal{H} \) is not closed under Rule 2 of Meek’s rules, then \( \mathcal{H} \) has an induced subgraph consists of \( X \rightarrow Y \rightarrow Z \) as well as \( X \rightarrow Z \). By condition (iii), \( X, Y, Z \) are in the same B-component. However, for the directed edge \( Y \rightarrow Z \), \( X \in \text{pa}(Y, \mathcal{H}) \) but \( X \notin \text{pa}(Z, \mathcal{H}) \setminus \{Y\} \), which is contradicted to condition (iv). Thus, \( \mathcal{H} \) is closed under the second Meek’s rule.

(iii) If \( \mathcal{H} \) is not closed under Rule 3 of Meek’s rules, then \( \mathcal{H} \) has an induced subgraph shown in Figure 15a. The vertices \( X, Y, Z_1, Z_2 \) are in the same B-component \( C^b \). However, this is impossible as \( Y \in \text{adj}(Z_2, C^b) \) but \( Y \notin \text{adj}(Z_1, C^b) \).

(iv) If \( \mathcal{H} \) is not closed under Rule 4 of Meek’s rules, then \( \mathcal{H} \) has an induced subgraph shown in one of Figures 15b-15d. By the similar argument for (ii), no matter which induced subgraph \( \mathcal{H} \) has, the vertices \( X, Y, Z_1, Z_2 \) are in the same B-component \( C^b \). However, for the directed edge \( Z_1 \rightarrow Z_2 \), we have \( Y \in \text{adj}(Z_2, C^b) \) but \( Y \notin \text{adj}(Z_1, C^b) \), contrary to condition (iv). Hence, \( \mathcal{H} \) is closed under the forth Meek’s rule.

So far, we have proved that \( \mathcal{H} \) is an MPDAG. It remains to show that \( \mathcal{H} \) is causal. By the definition of causal MPDAG, it suffices to show that there is a DAG that has the same skeleton and the same v-structures as \( \mathcal{H} \), or equivalently, there exists an orientation of all undirected edges in \( \mathcal{H} \) that does not create a new v-structure or a directed cycle.

We first claim that (1) no orientation of the undirected edges in \( \mathcal{H} \) will create a directed cycle which includes a directed edge or edges in \( \mathcal{H}_c \) and (2) no orientation of an undirected edge in \( \mathcal{H} \)
can create a new v-structure with an edge that was oriented in \( \mathcal{H}_c \). In fact, the first claim holds because of condition (i), and the second claim holds because of condition (iii).

Based on the above two claims, to prove that \( \mathcal{H} \) is causal, it suffices to show that the skeleton of each B-component of \( \mathcal{H} \) has a perfect elimination ordering whose corresponding DAG contains the existing directed edges in that B-component.

Let \( \mathcal{C}^b \) be a B-component of \( \mathcal{H} \). If \( \mathcal{C}^b \) is a complete graph with \( n \) vertices, then every vertex is simplicial in \( \mathcal{C}^b \). We claim that, there exists a vertex \( V_1 \) in \( \mathcal{C}^b \) which has no child in \( \mathcal{C}^b \). In fact, if every vertex in \( \mathcal{C}^b \) has a child in \( \mathcal{C}^b \), then there will be a directed cycle in \( \mathcal{C}^b \), which is impossible. Note that, the induced subgraph of \( \mathcal{C}^b \) over \( V(\mathcal{C}^b) \setminus \{ V_1 \} \) is still complete. Hence, repeat the above procedure we can find a sequence of vertices \( V_1, V_2, \ldots, V_n \). It can be easily verified that the ordering of the vertices forms a PEO of \( \mathcal{C}^b \), and the corresponding DAG contains all directed edges in \( \mathcal{C}^b \).

We then consider the case where \( \mathcal{C}^b \) is not a complete graph. Assume that every simplicial vertex has a child in \( \mathcal{C}^b \). Let \( X \) be a simplicial vertex and \( \mathbf{M}_i \) be the (unique) maximal clique that contains \( X \) (Lemma 1). Denote by \( \mathbf{S} \) the set of simplicial vertices of \( \mathcal{C}^b \) contained in \( \mathbf{M}_i \). Since \( \mathbf{M}_i \) induces a complete subgraph of \( \mathcal{C}^b \), \( \mathbf{S} \subseteq \mathbf{M}_i \) also induces a complete subgraph of \( \mathcal{C}^b \). If every simplicial vertex in \( \mathbf{S} \) has a child which is also in \( \mathbf{S} \), then we can construct a directed cycle. Thus, there must be a simplicial vertex in \( \mathbf{S} \) whose child is not in \( \mathbf{S} \). Without loss of generality, we can assume that such a vertex is \( X \). Notice that, \( \mathcal{C}^b \) is an incomplete connected chordal graph, \( \mathbf{M}_i \setminus \mathbf{S} \neq \emptyset \), and thus \( X \rightarrow Y \) is in \( \mathcal{C}^b \) for some \( Y \in \mathbf{M}_i \setminus \mathbf{S} \). As \( \mathbf{S} \) consists of all simplicial vertices contained in \( \mathbf{M}_i \), \( Y \) is not simplicial, and thus there is a \( Z \in \text{adj}(Y, \mathcal{C}^b) \) that is not adjacent to \( X \) (Lemma 1). This means that \( \text{adj}(Y, \mathcal{C}^b) \nsubseteq \text{adj}(X, \mathcal{C}^b) \), which violates condition (iv).

Therefore, we can find a simplicial vertex, denoted by \( V_1 \), that does not have any child in \( \mathcal{C}^b \). Since the induced subgraph of \( \mathcal{C}^b \) over \( V(\mathcal{C}^b) \setminus \{ V_1 \} \) is still chordal, we can repeat the above procedure and find a sequence vertices \( V_1, V_2, \ldots, V_n \). Again, it can be checked that the ordering of the vertices forms a PEO of \( \mathcal{C}^b \), and the corresponding DAG contains all directed edges in \( \mathcal{C}^b \). This completes the proof.

\( \Box \)

C.4 Proof of Proposition 2

**Proof.** To prove the sufficiency, we first show that \( A \) is a generator of \( \mathcal{H} \), and then prove its minimality.

Denote by \( \mathcal{G}^* \) the CPDAG with the same skeleton and v-structures as \( \mathcal{H} \). To prove that \( A \) is a generator of \( \mathcal{H} \), or equivalently, to prove that \( \mathcal{H} \) is the MPDAG of \( [\mathcal{G}^*, A] \), by Corollary 2 it suffices to show that for every directed edge \( X \rightarrow Y \) in \( E_d(\mathcal{H}) \setminus (E_d(\mathcal{G}^*) \cup A) \), an orientation component for \( Y \) with respect to \( A \) and \( \mathcal{G}^* \) contains \( X \).

By construction of \( A \), the edges in \( E_d(\mathcal{H}) \setminus (E_d(\mathcal{G}^*) \cup A) \) are all M-strongly protected. On the other hand, as \( \mathcal{H} \) can be viewed as the MPDAG of \( [\mathcal{G}^*, E_d(\mathcal{H})] \), the maximal orientation component for \( Y \) with respect to \( E_d(\mathcal{H}) \) and \( \mathcal{G}^* \), denoted by \( U \), contains \( X \). In the following, we will show that \( U \) is an orientation component for \( Y \) with respect to \( A \) and \( \mathcal{G}^* \).

Suppose that, with respect to \( A \) and \( \mathcal{G}^* \), \( U \) is not an orientation component for \( Y \), then by the definition of orientation component, there exists another potential leaf node \( Z \) in \( U \) with respect to \( A \) and \( \mathcal{G}^* \). Such a variable \( Z \) must have the following properties.
(P1) $Z$ is simplicial in $U$.

(P2) If an undirected edge connected to $Z$ in $U$ is directed in $A$, $Z$ is not the tail of that directed edge.

(P3) For every sibling $W$ of $Z$ in $U$ such that $Z \rightarrow W$ is in $H$ (such a $W$ definitely exists), $Z \rightarrow W$ is not in $A$. (Note that, since every directed edge in $A$ is also in $H$, $Z \rightarrow W$ is in $H$ implies that $W \rightarrow Z$ is not in $A$ either).

The third property comes from that fact that, with respect to $E_d(H)$ and $G^*$, $U$ is the maximal orientation component for $Y$.

Since $Z \rightarrow W$ is not in $A$, $Z \rightarrow W$ is $M$-strongly protected in $H$. Note that, $Z$ and $W$ are adjacent in $U$, they are in the same chain component of $G^*$. We first prove that $Z \rightarrow W$ can only occur in the configurations (a), (c) and (e), and the involved vertices in those configurations are all in the same chain component of $G^*$.

(i) If $Z \rightarrow W$ occurs in the configuration (a), then there exists a vertex $W_2 \notin adj(W, H)$ such that $W_2 \rightarrow Z \rightarrow W$ is in $H$. If $W_2$ is not in the same chain component as $Z$ and $W$, then $W_2 \rightarrow Z$ implies that $W_2 \rightarrow W$ is also in $H$, which is contradicted to the configuration (a).

(ii) If $Z \rightarrow W$ occurs in the configuration (b), then there is a vertex $W_2 \notin adj(Z, H)$ such that $Z \rightarrow W \leftarrow W_2$, which is a $v$-structure collided in $W$, is in $H$. This means that $W_2$ is not in the same chain component as $Z$, and thus, $W_2 \rightarrow Z$ should be in $H$, leading to a contradiction.

(iii) If $Z \rightarrow W$ occurs in the configuration (c), then there is a vertex $W_2$ such that $Z \rightarrow W_2 \rightarrow W$ is in $H$. If $W_2$ is not in the same chain component as $Z$ and $W$, then $W_2 \rightarrow W$ implies that $W_2 \rightarrow Z$ is also in $H$, which is contradicted to the configuration (e).

(iv) If $Z \rightarrow W$ occurs in the configuration (d), then there are vertices $W_2, W_3 \in sib(Z, H)$ such that $W_2$ is not adjacent to $W_3$ in $H$ and $W_2 \rightarrow W \leftarrow W_3$ is in $H$. It is easy to see that $W_2$, $W_3$ and $\{Z, W\}$ are in different chain components, and thus, $W_2 \rightarrow Z \leftarrow W_3$ should be in $H$. This is contradicted to the configuration (d).

(v) If $Z \rightarrow W$ occurs in the configuration (e), then there are vertices $W_2, W_3 \in sib(Z, H)$ such that $W_2 \rightarrow W_3 \rightarrow W$ and $W_2$ is not adjacent to $W$ in $H$. If $W_3$ is not in the same chain component as $Z$ and $W$, then $W_3 \rightarrow Z$ should be in $H$, contradicted to the configuration. If $W_2$ not in the same chain component as $Z$, $W$ and $W_3$, then $W_2 \rightarrow Z$ should also be in $H$, contradicted to the configuration.

Below, we will consider the configurations (a), (c) and (e) separately and show that although $Z \rightarrow W$ is $M$-strongly protected in $H$, $Z \rightarrow W$ cannot occur in any of these configurations.

(i) If $Z \rightarrow W$ occurs in the configuration (a), then there exists a vertex $W_2 \notin adj(W, H)$ such that $W_2$, $Z$ and $W$ are in the same chain component and $W_2 \rightarrow Z$ is in $H$. If $W_2 \in V(U)$, then $Z$ is not simplicial in $U$, which is contradicted to (P1). Thus, $W_2 \notin V(U)$. We claim that the induced subgraph of $G^*$ over $V(U) \cup \{W_2\}$, denoted by $U'$, is also an orientation component for $Y$ with respect to $E_d(H)$ and $G^*$. In fact, with respect to $E_d(H)$ and $G^*$, since none of the vertices except for $Y$ is a potential leaf node in $U$, the vertices in $V(U) \setminus \{Y\}$
are definitely not potential leaf nodes in $U'$ either. On the other hand, $W_2$ is not a potential leaf node in $U'$, as $W_2 \to Z$ is in $E_d(H)$, the consistency of $E_d(H)$ with $G^*$ implies that the only potential leaf node in $U'$ must be $Y$ (Theorem 4). Therefore, $U'$ is also an orientation component for $Y$ with respect to $E_d(H)$ and $G^*$. This is contradicted to the maximality of $U$.

(ii) If $Z \to W$ occurs in the configuration (e), then there are vertices $W_2, W_3 \in \text{sib}(Z, H)$ such that $W_2 \to W_3 \to W$ and $W_2$ is not adjacent to $W$ in $H$. If both $W_2$ and $W_3$ are in $V(U)$, then $Z$ is not a simplicial vertex in $U$, which is again contradicted to (P1). On the other hand, if either $W_2$ or $W_3$ is not in $V(U)$, then by the similar argument given in (i), the induced subgraph of $G^*$ over $V(U) \cup \{W_2, W_3\}$ is also an orientation component for $Y$ with respect to $E_d(H)$ and $G^*$. This is again contradicted to the maximality of $U$.

(iii) If $Z \to W$ occurs in the configuration (c), then there is a vertex $W_2$ such that $Z \to W_2 \to W$ is in $H$. If $W_2 \notin V(U)$, then by the similar argument given in (i), the induced subgraph of $G^*$ over $V(U) \cup \{W_2\}$ is also an orientation component for $Y$ with respect to $E_d(H)$ and $G^*$, contradicted to the maximality of $U$. Hence, $W_2 \in V(U)$, and by (P3), $Z \to W_2$ is also $M$-strongly protected in $H$. By the same argument given in (i) and (ii), $Z \to W_2$ can only occur in the configuration (c). Repeat the above procedure we can find a sequence of vertices $W_2, W_3, \cdots W_n, \cdots$ in $adj(Z, U)$, such that $Z \to W_i$ for $i = 2, 3, \cdots$ and $W \leftarrow W_2 \leftarrow W_3 \leftarrow \cdots \leftarrow W_n \leftarrow \cdots$. Note that, since the above procedure never ends, but there are only a finite number of vertices in $adj(Z, U)$, a subpath of $W \leftarrow W_2 \leftarrow W_3 \leftarrow \cdots$ must be a directed cycle, leading to a contradiction.

Therefore, although $Z \to W$ is $M$-strongly protected in $H$, $Z \to W$ cannot occur in any of the configurations (a) to (e). This is impossible. Thus, $U$ is an orientation component for $Y$ with respect to $A$ and $G^*$. Consequently, $A$ is a generator of $H$.

We then show that $A$ is minimal. If there is another generator $A^-$ of $H$ such that $|A^-| < |A|$, then there is a directed edge $X \to Y$ in $A$ which is not in $A^-$. Since $A^-$ is a generator of $H$ and $X \to Y$ is in $H$, $X \to Y$ is either in a $v$-structure of the form $X \to Y \leftarrow Z$, or can be oriented by Meek’s rules. This means that $X \to Y$ occurs in at least one configurations labeled by (a) to (e) as an induced subgraph of $H$. Hence, $X \to Y$ is $M$-strongly protected in $H$, which is contrary to the assumption that $X \to Y$ is in $A$. This completes the proof of sufficiency.

Next, we prove the necessity. Let $A$ be a minimal generator of $H$. We first show that $A$ contains all directed edges in $H$ that are not $M$-strongly protected. Suppose that there is a directed edge $X \to Y \notin A$ which is in $H$ but not $M$-strongly protected. Then, since $A$ generates $H$, $X \to Y$ is either in a $v$-structure of the form $X \to Y \leftarrow Z$, or can be oriented by Meek’s rules. This means that $X \to Y$ occurs in at least one configurations labeled by (a) to (e) as an induced subgraph of $H$. That is, $X \to Y$ is $M$-strongly protected. This is contradicted to our assumption. We next show that $A$ only contains the directed edges in $H$ that are not $M$-strongly protected. In fact, if this is not the case, then the proper subset of $A$ which consisted of the directed edges that are not $M$-strongly protected in $H$ is a generator of $H$, meaning that $A$ is not minimal, which is a contradiction.

Finally, the uniqueness follows from the fact that the set of directed edges in $H$ that are not $M$-strongly protected in $H$ is unique.

□

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C.5 Proof of Theorem 2

Proof. The conclusion follows directly from Propositions 1 and 2.

C.6 Proof of Proposition 3

Proof. Both claims hold by the definition of DCC, and thus we omit the proof.

C.7 Proof of Theorem 3

Proof. The first statement is clearly true and the third statement can be derived from Fang and He (2020, Lemma 2). Since the second statement is the inverse of the third statement, the proof is completed.

C.8 Proof of Proposition 4

Proof. The proof follows directly from the definition of DCC.

C.9 Proof of Proposition 5

Proof. The proof follows from Proposition 4.

C.10 Proof of Theorem 4

We first prove two lemmas.

Lemma 9. Let $G^*$ be a CPDAG, $K$ be a set of consistent DCCs, and $\mathcal{U}$ be a connected undirected induced subgraph of $G^*$. For any DAG $G \in [G^*, K]$, every leaf node in the induced subgraph of $G$ over $V(\mathcal{U})$ is a potential leaf node in $\mathcal{U}$ with respect to $K$ and $G^*$.

Proof. Denote by $G_{\text{sub}}$ the induced subgraph of $G$ over $V(\mathcal{U})$. By the definition of undirected induced subgraph and the fact that every partially directed cycle in $G^*$ is an undirected cycle (Andersson et al., 1997), $\mathcal{U}$ is the induced subgraph of $G^*$ over $V(\mathcal{U})$. Thus, two vertices are adjacent in $\mathcal{U}$ if and only if they are adjacent in $G_{\text{sub}}$. Let $V_{\text{leaf}}$ be a leaf node in $G_{\text{sub}}$. By the definition of potential leaf node, to prove the lemma it suffices to show that, (1) $\text{adj}(V_{\text{leaf}}, \mathcal{U})$ induces a complete subgraph of $\mathcal{U}$, and (2) $V_{\text{leaf}}$ is not the tail of any DCC in $K(\mathcal{U})$.

As $V_{\text{leaf}}$ is a leaf node in $G_{\text{sub}}$, $\text{adj}(V_{\text{leaf}}, G_{\text{sub}}) \rightarrow V_{\text{leaf}}$ are in $G_{\text{sub}}$. Since $\text{adj}(V_{\text{leaf}}, G_{\text{sub}}) \subseteq \text{sib}(V_{\text{leaf}}, G^*)$, the configuration $\text{adj}(V_{\text{leaf}}, G_{\text{sub}}) \rightarrow V_{\text{leaf}}$ contains no v-structure collided on $V_{\text{leaf}}$. Thus, $\text{adj}(V_{\text{leaf}}, G_{\text{sub}})$ induces a complete subgraph of $G_{\text{sub}}$, meaning that $\text{adj}(V_{\text{leaf}}, \mathcal{U})$ induces a complete subgraph of $\mathcal{U}$. This completes the proof of statement (1). On the other hand, if there is a $V_{\text{leaf}} \rightarrow \kappa_h$ in $K(\mathcal{U})$, then by Equation (4), $\kappa_h \subseteq \text{adj}(V_{\text{leaf}}, \mathcal{U}) = \text{adj}(V_{\text{leaf}}, G_{\text{sub}})$ and $V_{\text{leaf}} \rightarrow \kappa_h$ is in $K(G^*)$. Notice that $K$ is equivalent to $K(G^*)$, $V_{\text{leaf}} \rightarrow \kappa_h$ must hold for $G$. Consequently, $V_{\text{leaf}} \rightarrow \kappa_h$ holds for $G_{\text{sub}}$. However, $V_{\text{leaf}}$ is a leaf node in $G_{\text{sub}}$, which leads to a contradiction.
Lemma 9 suggests that if a vertex is not a potential leaf node in some connected undirected induced subgraph \( U \), then it cannot be a leaf node in the induced subgraph over \( V(U) \) of any restricted Markov equivalent DAG.

**Lemma 10.** Let \( G^* \) be a CPDAG and \( \mathcal{K} \) be a set of DCCs. Then, \( \mathcal{K} \) is consistent with \( G^* \) if and only if \( \mathcal{K}(C) \) is consistent with \( C \) for any chain component \( C \).

**Proof.** Suppose that \([G^*, \mathcal{K}(G^*_u)] \neq \emptyset \) and let \( G \in [G^*, \mathcal{K}(G^*_u)] \). For any chain component \( C \), let \( G_{\text{sub}} \) denote the induced subgraph of \( G \) over \( V(C) \). It is easy to verify that \( G_{\text{sub}} \in [C, \mathcal{K}(C)] \). Conversely, if \([C, \mathcal{K}(C)] \neq \emptyset \) for any chain component \( C \), then choose \( G_C \in [C, \mathcal{K}(C)] \) arbitrarily for each chain component and orient undirected edges in \( G^* \) according to \( \{G_C\} \). That is, orient \( X \rightarrow Y \) in \( G^* \) as \( X \rightarrow Y \) if \( X \) is a parent of \( Y \) in the DAG \( G_C \), where \( C \) is the chain component containing \( X \) and \( Y \). Notice that \( G_u^* \) is a union of (disjoint) chain components, we have

\[
\mathcal{K}(G_u^*) = \bigcup C \mathcal{K}(C),
\]

where \( C \) is a chain component. It is straightforward to show that the resulting DAG with the orientations defined above is in \([G^*, \mathcal{K}(G_u^*)]\), according to Appendix C.1 as well as Equation (8).

Finally, we present the proof of Theorem 4.

**Proof of Theorem 4.** We first prove the necessity. If \( \mathcal{K} \) is consistent, then there is a DAG \( G \) in \([G^*, \mathcal{K}]\). Let \( U \) be an arbitrary connected undirected induced subgraph of \( G^* \), and denote the induced subgraph of \( G \) over \( V(U) \) by \( G_{\text{sub}} \). Since any induced subgraph of a DAG is still a DAG, \( G_{\text{sub}} \) is a DAG, and thus it must have a leaf node \( V_{\text{leaf}} \). By Lemma 9, we can conclude that \( V_{\text{leaf}} \) is a potential leaf node in \( U \) with respect to \( \mathcal{K} \) and \( G^* \).

We next prove the sufficiency. By Lemma 10, \( \mathcal{K} \) is consistent with \( G^* \) if and only if \( \mathcal{K}(C) \) is consistent with \( C \) for any chain component \( C \). Therefore, given a chain component \( C \), our goal is to prove that \( \mathcal{K}(C) \) is consistent with \( C \), providing that the potential-leaf-node condition holds. Based on the analysis in Appendix C.1, we need to construct a PEO of \( C \) such that the corresponding DAG satisfies all DCCs in \( \mathcal{K}(C) \). By assumption, \( C \) has a potential leaf node with respect to \( \mathcal{K} \) and \( G^* \), denoted by \( V_1 \). By the definition of potential leaf node, \( V_1 \) is simplicial in \( C \). Next, consider the induced subgraph of \( C \) over \( V(C) \setminus \{V_1\} \), denoted by \( C_2 \). \( C_2 \) is clearly connected. Hence, by assumption \( C_2 \) has a potential leaf node, denoted by \( V_2 \). Following the above procedure, we have a sequence of undirected graphs \( \mathcal{C} = C_1, C_2, \ldots, C_m \) and a sequence of vertices \( (V_1, V_2, \ldots, V_m) \), where \( m = |V(C)| \). By the construction, the ordering of the vertices in this sequence forms a PEO of \( C \). Denote by \( G_C \) the corresponding DAG of this PEO. If there is a \( V_i \xrightarrow{\alpha} \kappa_h \in \mathcal{K}(C) \) which does not hold for \( G_C \), then \( \kappa_h \rightarrow V_i \) are in \( G_C \). This means \( \kappa_h \subseteq \{V_{i+1}, V_{i+1}, \ldots, V_m\} \), which contradicts the construction of the vertex sequence as \( V_i \) is definitely not a potential leaf node in the induced subgraph \( C_i \). Therefore, \( G_C \in [C, \mathcal{K}(C)] \). This completes the proof of Theorem 4. \( \square \)
C.11 Proof of Theorem 5

Proof. The equivalency of statements (i) and (ii) follows from the definition of equivalency and redundancy. Observed that when \( \mathcal{K} \) is consistent with \( \mathcal{G}^* \),

\[
\kappa_t \xrightarrow{\text{or}} \kappa_h \text{ is redundant with respect to } \mathcal{G}^*, \mathcal{K} \iff \forall \mathcal{G} \in [\mathcal{G}^*, \mathcal{K}], \kappa_t \xrightarrow{\text{or}} \kappa_h \text{ holds for } \mathcal{G}
\]

\[
\iff \forall \mathcal{G} \in [\mathcal{G}^*, \mathcal{K}], \text{ch}(\kappa_t, \mathcal{G}) \cap \kappa_h \neq \emptyset
\]

\[
\iff \forall \mathcal{G} \in [\mathcal{G}^*, \mathcal{K}], \kappa_h \notin \text{pa}(\kappa_t, \mathcal{G})
\]

\[
\iff \{ \kappa_h \to \kappa_t \} \cup \mathcal{K} \text{ is inconsistent with } \mathcal{G}^*.
\]

Therefore, statement (ii) is equivalent to statement (iii) if both \( \mathcal{K}_1 \) and \( \mathcal{K}_2 \) are consistent with \( \mathcal{G}^* \). If neither \( \mathcal{K}_1 \) nor \( \mathcal{K}_2 \) is consistent with \( \mathcal{G}^* \), then statements (i) and (iii) hold simultaneously. Finally, if \( \mathcal{K}_1 \) is consistent with \( \mathcal{G}^* \) but \( \mathcal{K}_2 \) is not, then statements (i) does not hold. Thus, we need only to show that statements (iii) does not hold either. In fact, by Equation 9, if \( \cup_{D \in \mathcal{K}_2} \{ D \to \kappa_t \} \cup \mathcal{K}_1 \) is not consistent with \( \mathcal{G}^* \) for every \( \kappa \in \mathcal{K}_2 \), then every \( \kappa \in \mathcal{K}_2 \) is redundant with respect to \( [\mathcal{G}^*, \mathcal{K}] \). Consequently, \( \mathcal{K}_2 \cup \mathcal{K}_1 \) is equivalent to \( \mathcal{K}_1 \) given \( \mathcal{G}^* \) and thus is consistent. However, this is impossible, as the union of an inconsistent DCC and a consistent DCC is definitely inconsistent. \( \square \)

C.12 Proof of Proposition 6

Proof. Proposition 6 follows from Theorem 3. \( \square \)

C.13 Proof of Theorem 6

The proof of Theorem 6 requires the following lemma.

Lemma 11. Let \( \mathcal{H} \) be a causal MPDAG. For any vertex \( X \) and \( S \subseteq \text{sib}(X, \mathcal{H}) \), if \( S \) induces a complete subgraph of \( \mathcal{H} \), then there is a DAG \( \mathcal{G} \in [\mathcal{H}] \) in which \( S \subseteq \text{pa}(X, \mathcal{G}) \).

Proof. Without loss of generality, we assume that the skeleton of \( \mathcal{H} \), denoted by \( \mathcal{C} \), is a connected chordal graph, and \( \mathcal{H} \) is the MPDAG representing \([\mathcal{C}, \mathcal{B}_d]\) for some direct causal constraints \( \mathcal{B}_d \) (Proposition 1). That is, \([\mathcal{H}] = [\mathcal{C}, \mathcal{B}_d]\). We first show that \( \text{pa}(X, \mathcal{H}) \cup S \cup \{ X \} \) induces a complete subgraph of \( \mathcal{H} \). In fact, if \( \text{pa}(X, \mathcal{H}) = \emptyset \), then \( \text{pa}(X, \mathcal{H}) \cup S \cup \{ X \} \) is complete. If \( \text{pa}(X, \mathcal{H}) \neq \emptyset \), then for any \( p \in \text{pa}(X, \mathcal{H}) \) and \( S \in S \), \( p \) and \( S \) are adjacent in \( \mathcal{H} \), since otherwise, \( X \to S \) should appear in \( \mathcal{H} \) due to the maximality of \( \mathcal{H} \). Thus, \( \text{pa}(X, \mathcal{H}) \cup S \cup \{ X \} \) is also complete.

Fang and He (2020, Theorem 1) proved that for any vertex \( X \) and \( S \subseteq \text{sib}(X, \mathcal{H}) \), the following three statements are equivalent.

(i) There is a DAG \( \mathcal{G} \) in \([\mathcal{H}]\) such that \( \text{pa}(X, \mathcal{G}) = S \cup \text{pa}(X, \mathcal{H}) \) and \( \text{ch}(X, \mathcal{G}) = \text{sib}(X, \mathcal{H}) \cup \text{ch}(X, \mathcal{H}) \setminus S \).

(ii) Orienting \( S \to X \) and \( X \to \text{sib}(X, \mathcal{H}) \setminus S \) in \( \mathcal{H} \) does not introduce any new v-structure collided on \( X \) or any directed triangle containing \( X \).

(iii) The induced subgraph of \( \mathcal{H} \) over \( S \) is complete, and there does not exist an \( S \in S \) and a \( C \in \text{sib}(X, \mathcal{H}) \setminus S \) such that \( C \to S \) is in \( \mathcal{H} \).
Denote by $M$ a maximal clique containing $pa(X, H) \cup S \cup \{X\}$ (which definitely exists but may not be unique) and let $M_0 = M \cap pa(X, H) = pa(X, H)$, $M_1 = M \cap ch(X, H)$ and $M_2 = M \cap sib(X, H)$. We first show that if $M_1 = \emptyset$, then there is a DAG $G \in [H]$ such that $pa(X, G) = M_3 \cup pa(X, H)$ and $ch(X, G) = sib(X, H) \cup ch(X, H) \setminus M_3$. As $M_1 \subset M$, $M_3$ induces a complete subgraph of $H$. Suppose that there is a $P \in M_3$ and a $C \in sib(X, H) \setminus M_3$ such that $C \rightarrow P$, then $C$ is adjacent to every vertex in $pa(X, H) \cup M_3$, since otherwise, $X \rightarrow P'$ is in $H$ for any $P' \in pa(X, H) \cup M_3$ which is not adjacent to $C$, and is contradicted to the assumption that $pa(X, H) \cup M_3 \subseteq pa(X, H) \cup sib(X, H)$. However, $C$ is adjacent to every vertex in $pa(X, H) \cup M_3$ implies that $C$ is adjacent to every vertex in $M = M_3 \cup M_0$, meaning that $M$ is not a maximal clique. This leads to a contradiction. The desired result then follows from Fang and He (2020, Theorem 1).

On the other hand, assume that $M_1 \neq \emptyset$ for any maximal clique $M$ containing $pa(X, H) \cup S \cup \{X\}$. In the following, we will construct a maximal clique $M$ containing $pa(X, H) \cup S \cup \{X\}$, such that orienting $M_3 \rightarrow X$ and $X \rightarrow sib(X, H) \setminus M_3$ does not violate statement (iii) of Fang and He (2020, Theorem 1).

Let $M^0$ be an arbitrary maximal clique containing $pa(X, H) \cup S \cup \{X\}$. If orienting $M^0_3 \rightarrow X$ and $X \rightarrow sib(X, H) \setminus M^0$ does not violate statement (iii) of Fang and He (2020, Theorem 1), then the proof is completed. If otherwise, let $C^0 \subseteq sib(X, H) \setminus M^0_3$ be the set of vertices such that for any $C \in C^0$, $C \rightarrow P$ for some $P \in M^0$. Using the same argument given in the last paragraph, we can prove that $C$ is adjacent to every vertex in $pa(X, H) \cup M_3^0$ for any $C \in C^0$. Likewise, it can be shown that any two distinct vertices in $C^0$, if exist, are adjacent. Hence, $C^0 \cup M_3^0 \cup pa(X, H)$ is a clique.

Let $M^1$ be a maximal clique containing $\{X\} \cup C^0 \cup M^0 \cup pa(X, H)$. By assumption, $M_1^1 \neq \emptyset$ and $S \subseteq M^0 \subseteq M^1$. If orienting $M^1_3 \rightarrow X$ and $X \rightarrow sib(X, H) \setminus M^1$ does not violate statement (iii) of Fang and He (2020, Theorem 1), then the proof is completed. Otherwise, following the above procedure we can find a new maximal clique $M^2$ containing $\{X\} \cup C^1 \cup M^1 \cup pa(X, H)$, where $C^1 \subseteq sib(X, H) \setminus M^1_3$ be the set of vertices such that for any $C \in C^1$, $C \rightarrow P$ for some $P \in M^1$. Note that, $S \subseteq M^0 \subseteq M^1 \subseteq \cdots \subseteq M^1 \subseteq \cdots \subseteq sib(X, H)$ implies that the above construction will eventually stop as $sib(X, H)$ is a finite set. That is, we will finally find an $M = M^1_3$ containing $pa(X, H) \cup S \cup \{X\}$ such that orienting $M_3 \rightarrow X$ and $X \rightarrow sib(X, H) \setminus M_3$ does not violate statement (iii) of Fang and He (2020, Theorem 1), which completes the proof.

**Proof of Theorem 6.** By definition, $H$ is fully informative with respect to $K$ and $G^*$ if and only if $\kappa_t \xrightarrow{or} \kappa_h$ holds for all DAGs in $[H]$ for any $\kappa \in K$, where $\kappa := \kappa_t \xrightarrow{or} \kappa_h$.

If $\kappa_h \cap ch(\kappa_t, H) \neq \emptyset$, then $\kappa_t \xrightarrow{or} \kappa_h$ holds for all DAGs in $[H]$. If $\kappa_h \cap sib(\kappa_t, H)$ induces an incomplete subgraph of $H$, then there exist $V_1, V_2 \in \kappa_h \cap sib(\kappa_t, H)$ such that $V_1, V_2$ are not adjacent. By the first rule of Meek’s rules, for any DAG in $[H]$, either $V_1$ or $V_2$ is a child of $\kappa_t$. Thus, $\kappa_t \xrightarrow{or} \kappa_h \cap sib(\kappa_t, H)$ holds for all DAGs in $[H]$.

Conversely, if $\kappa_h \cap ch(\kappa_t, H) = \emptyset$ and the induced subgraph of $H$ over $\kappa_h \cap sib(\kappa_t, H)$ is complete, then by Lemma 11, there is a DAG $G \in [H]$ in which $\kappa_h \cap sib(\kappa_t, H) \subseteq pa(\kappa_t, G)$. Therefore, $\kappa_t \xrightarrow{or} \kappa_h$ does not hold for $G$.

**C.14 Proof of Corollary 1**

*Proof.* Corollary 1 follows from Theorem 6 and Equation 5. □
C.15 Proof of Proposition 7

Proof. By Lemma 9, for any DAG $G \in [G^*, K]$, the leaf node in the induced subgraph of $G$ over $V(U)$, denoted by $G_{\text{sub}}$, must be $X$, as $X$ is the unique potential leaf node in $U$ with respect to $K$ and $G^*$. The desired result comes from the fact that $\text{adj}(X, G_{\text{sub}}) = \text{adj}(X, U)$. \qed

C.16 Proof of Theorem 7

Proof. The sufficiency follows from Proposition 7, and below we prove the necessity. Since $H$ has the same skeleton as $G^*$, it suffices to prove that, for two adjacent variables $X$ and $Y$, if $X \rightarrow Y$ is not in $G^*$ and there is no orientation component for $Y$ containing $X$ with respect to $K$ and $G^*$, then $X \rightarrow Y$ is not in $H$.

As $X \rightarrow Y$ is not in $G^*$ but $X$ and $Y$ are adjacent, $Y$ is either a parent or a sibling of $X$ in $G^*$. If $Y \rightarrow X$ is in $G^*$, then $Y \rightarrow X$ is in $H$, which completes the proof. Now consider the case where $X \rightarrow Y$ is in $G^*$. According to our assumption, with respect to $K$ and $G^*$, every connected undirected induced subgraph containing $X$ and $Y$ is not an orientation component for $Y$. If there is a such subgraph which is an orientation component for $X$, then by Proposition 7 and the definition of MPDAG, $Y \rightarrow X$ is in $H$.

On the other hand, with respect to $K$ and $G^*$, if every connected undirected induced subgraph containing $X$ and $Y$ is neither an orientation component for $X$ nor an orientation component for $Y$, then by Theorem 4, it either have a potential leaf node which is neither $X$ nor $Y$, or have exactly two potential leaf nodes which are $X$ and $Y$. In the following, we will prove that there is a DAG $G_1 \in [G^*, K]$ in which $X \rightarrow Y$ and there is also a DAG $G_2 \in [G^*, K]$ in which $Y \rightarrow X$. According to symmetry, we need only to prove that there is a DAG $G \in [G^*, K]$ in which $X \rightarrow Y$.

To prove this claim, it suffices to show that $K \cup \{X \rightarrow Y\}$ is consistent with $G^*$. By Theorem 4, any connected undirected induced subgraph $U$ has a potential leaf node with respect to $K$ and $G^*$. If $U$ does not contain $X$ or $Y$, then it can be easily verify that the potential leaf node of $U$ with respect to $K$ and $G^*$ is still a potential lead node with respect to $K \cup \{X \rightarrow Y\}$ and $G^*$. If $U$ contains both $X$ and $Y$, then we have that,

(i) if $U$ has a potential leaf node with respect to $K$ and $G^*$ which is neither $X$ nor $Y$, then by the definition of potential leaf node, such a vertex is still a potential leaf node with respect to $K \cup \{X \rightarrow Y\}$ and $G^*$;

(ii) if $U$ had exactly two potential leaf nodes which are $X$ and $Y$, then with respect to $K \cup \{X \rightarrow Y\}$ and $G^*$, $Y$ is still a potential leaf node in $U$.

Therefore, any connected undirected induced subgraph of $G^*$ has a potential leaf node with respect to $K \cup \{X \rightarrow Y\}$ and $G^*$. The desired result follows from Theorem 4. \qed

C.17 Proof of Proposition 8

Proof. Since $U_1$ is an orientation components for $X$ with respect to $K$ and $G^*$, for any $Y_1 \in V(U_1)$ such that $Y_1 \neq X$, either $Y_1$ is a non-simplicial node in $U_1$, or there is a $\kappa \in K(U_1)$ such that
\( \kappa_t = Y_1 \). Denote by \( \mathcal{U}_1 \) the undirected induced subgraph of \( \mathcal{G}^* \) over \( V(\mathcal{U}_1) \cup V(\mathcal{U}_2) \). If \( Y_1 \) is a non-simplicial node in \( \mathcal{U}_1 \), then it is a non-simplicial node in \( \mathcal{U}_1 \), as two non-adjacent vertices in \( \mathcal{U}_1 \) remains non-adjacent in \( \mathcal{U}_2 \). Moreover, if there exists a \( \kappa \in \mathcal{K}(\mathcal{U}_1) \) such that \( \kappa_t = Y_1 \), then \( \kappa \in \mathcal{K}(\mathcal{U}_2) \). Hence, \( Y_1 \) is not a potential leaf node in \( \mathcal{U}_2 \) with respect to \( \mathcal{K} \) and \( \mathcal{G}^* \). Following the same argument, none of the vertices in \( V(\mathcal{U}_2) \setminus \{X\} \) is a potential leaf node of \( \mathcal{U}_2 \) with respect to \( \mathcal{K} \) and \( \mathcal{G}^* \). However, due to the consistency, \( \mathcal{U}_2 \) should have at least one potential leaf node. Therefore, \( X \) is the only potential leaf node of \( \mathcal{U}_2 \) with respect to \( \mathcal{K} \) and \( \mathcal{G}^* \), which completes the proof.

\[ \square \]

C.18 Proof of Corollary 2

**Proof.** The conclusion follows directly from Proposition 8 and Theorem 7.

\[ \square \]

C.19 Proof of Theorem 8

**Proof.** It is easy to see that the outputted graph of Algorithm 3, denoted by \( \mathcal{U}_{out} \), is an orientation component for \( X \) with respect to \( \mathcal{K} \) and \( \mathcal{G}^* \). Assuming that \( \mathcal{U}_{out} \) is not maximal, then the true maximal orientation component for \( X \) with respect to \( \mathcal{K} \) and \( \mathcal{G}^* \), denoted by \( \mathcal{U}_{true} \), is a proper super graph of \( \mathcal{U}_{out} \). Recall that Algorithm 3 removes one vertex from the current graph in each while loop until the current graph is \( \mathcal{U}_{out} \). Since \( V(\mathcal{U}_{out}) \subseteq V(\mathcal{U}_{true}) \), let \( \{Y_{i_1}, Y_{i_2}, \ldots, Y_{i_k}\} = V(\mathcal{U}_{true}) \setminus V(\mathcal{U}_{out}) \), where the subscript of each \( Y_i \) indicates the number of loops when it is removed. Without loss of generality we can assume that \( i_1 < i_2 < \cdots < i_k \). Based on Algorithm 3, the vertices that are removed before \( Y_{i_1} \), if exist, are not in \( V(\mathcal{U}_{out}) \), since otherwise, the while loop ends before considering \( Y_{i_1} \). Let \( \mathcal{U}_1 \) be the undirected graph right before removing \( Y_{i_1} \). By Algorithm 3, with respect to \( \mathcal{K} \) and \( \mathcal{G}^* \), \( \mathcal{U}_1 \) is not an orientation component for \( X \) and \( Y_{i_1} \) is a potential lead node in \( \mathcal{U}_1 \). This means \( Y_{i_1} \) is a simplicial node in \( \mathcal{U}_1 \) and there is no DCC in \( \mathcal{K}(\mathcal{U}_1) \) in which \( Y_{i_1} \) is the tail. Note that \( \mathcal{U}_{true} \) is the true subgraph of \( \mathcal{U}_1 \) over \( V(\mathcal{U}_{true}) \) and \( Y_{i_1} \in V(\mathcal{U}_{true}) \), \( Y_{i_1} \) is also a simplicial node in \( V(\mathcal{U}_{true}) \). Moreover, there is no DCC in \( \mathcal{K}(\mathcal{U}_{true}) \) in which \( Y_{i_1} \) is the tail, as \( \mathcal{K}(\mathcal{U}_{true}) \subseteq \mathcal{K}(\mathcal{U}_1) \). Thus, \( Y_{i_1} \) is a potential leaf node in \( \mathcal{U}_{true} \) with respect to \( \mathcal{K} \) and \( \mathcal{G}^* \), meaning that \( \mathcal{U}_{true} \) is not an orientation component for \( X \). This leads to a contradiction, and hence \( \mathcal{U}_{out} \) is maximal.

\[ \square \]

C.20 Proof of Theorem 9

The key ingredient for proving the identifiability is the following lemma.

**Lemma 12.** Let \( \mathcal{H} \) be an MPDAG representing \([\mathcal{G}^*, \mathcal{K}]\) induced by a CPDAG \( \mathcal{G}^* \) and a set of consistent DCCs \( \mathcal{K} \). Then, for any vertex \( X \), there is a DAG \( \mathcal{G} \) in \([\mathcal{G}^*, \mathcal{K}]\) such that \( \text{ch}(X, \mathcal{G}) = \text{sib}(X, \mathcal{H}) \cup \text{ch}(X, \mathcal{H}) \).

**Proof.** It suffices to show that \( \mathcal{K} \cup \{X \rightarrow W \mid W \in \text{sib}(X, \mathcal{H})\} \) is consistent with \( \mathcal{G}^* \). For any connected undirected induced subgraph \( \mathcal{U} \) of \( \mathcal{G}^* \), a potential leaf node in \( \mathcal{U} \) with respect to \( \mathcal{K} \) and \( \mathcal{G}^* \), if it is not \( X \), is still a potential leaf node in \( \mathcal{U} \) with respect to \( \mathcal{K} \cup \{X \rightarrow W \mid W \in \text{sib}(X, \mathcal{H})\} \) and \( \mathcal{G}^* \). On the other hand, if \( X \) is the only potential leaf node in \( \mathcal{U} \) with respect to \( \mathcal{K} \) and \( \mathcal{G}^* \), then \( \text{adj}(X, \mathcal{U}) \rightarrow X \) are in \( \mathcal{H} \). Consequently, \( W \) is not in \( \mathcal{U} \) since \( W \in \text{sib}(X, \mathcal{H}) \), and hence \( X \) is
exists a multivariate Gaussian density \( f \).

Perković (2020, Proposition 3.2) showed that,

**Lemma 13** (Perković (2020), Proposition 3.2). Let \( \mathcal{H} \) be a causal MPDAG. If there is a proper possibly causal path \( \pi = (X, W, U, ..., Y) \) from \( X \in \mathbf{X} \) to \( Y \in \mathbf{Y} \) such that \( X \to W \to U \to \cdots \to Y \) is in one DAG \( \mathcal{G}_1 \in [\mathcal{H}] \) and \( X \leftarrow W \to U \to \cdots \to Y \) is in another DAG \( \mathcal{G}_2 \in [\mathcal{H}] \), then there exists a multivariate Gaussian density \( f \) over \( \mathbf{E}(\mathcal{G}^*) \) such that \( f_1(y \mid do(x)) \neq f_2(y \mid do(x)) \), where \( f_1(y \mid do(x)) \) and \( f_2(y \mid do(x)) \) are interventional distributions computed from two causal models \((\mathcal{G}_1, f(\mathbf{V})) \) and \((\mathcal{G}_2, f(\mathbf{V})) \), respectively.

Lemma 13 results the following corollary.

**Corollary 4.** Let \( \mathcal{H} \) be an MPDAG representing \([\mathcal{G}^*, \mathcal{K}] \) for a CPDAG \( \mathcal{G}^* \) and a set of consistent DCCs \( \mathcal{K} \). If there is a proper possibly causal path \( \pi = (X, W, U, ..., Y) \) from \( X \in \mathbf{X} \) to \( Y \in \mathbf{Y} \) such that \( X \to W \to U \to \cdots \to Y \) is in one DAG \( \mathcal{G}_1 \in [\mathcal{G}^*, \mathcal{K}] \) and \( X \leftarrow W \to U \to \cdots \to Y \) is in another DAG \( \mathcal{G}_2 \in [\mathcal{G}^*, \mathcal{K}] \), then there exists a multivariate Gaussian density \( f \over \mathbf{E}(\mathcal{G}^*) \) such that \( f_1(y \mid do(x)) \neq f_2(y \mid do(x)) \), where \( f_1(y \mid do(x)) \) and \( f_2(y \mid do(x)) \) are interventional distributions computed from two causal models \((\mathcal{G}_1, f(\mathbf{V})) \) and \((\mathcal{G}_2, f(\mathbf{V})) \), respectively.

Corollary 4 holds because \([\mathcal{G}^*, \mathcal{K}] \subseteq [\mathcal{H}] \), Thus, we omit the proof. Analogue to Corollary 4, we have,

**Lemma 14.** Let \( \mathcal{H} \) be an MPDAG representing \([\mathcal{G}^*, \mathcal{K}] \) for a CPDAG \( \mathcal{G}^* \) and a set of consistent DCCs \( \mathcal{K} \). If there is a proper possibly causal path \( \pi = (X, W, U, ..., Y) \) from \( X \in \mathbf{X} \) to \( Y \in \mathbf{Y} \) such that \( X \to W \to U \to \cdots \to Y \) and \( X \leftarrow W \to U \to \cdots \to Y \) are in one DAG \( \mathcal{G}_1 \in [\mathcal{G}^*, \mathcal{K}] \), and \( X \to W \to U \to \cdots \to Y \) and \( X \to U \to \cdots \to Y \) are in another DAG \( \mathcal{G}_2 \in [\mathcal{G}^*, \mathcal{K}] \), then there exists a multivariate Gaussian density \( f \over \mathbf{E}(\mathcal{G}^*) \) such that \( f_1(y \mid do(x)) \neq f_2(y \mid do(x)) \), where \( f_1(y \mid do(x)) \) and \( f_2(y \mid do(x)) \) are interventional distributions computed from two causal models \((\mathcal{G}_1, f(\mathbf{V})) \) and \((\mathcal{G}_2, f(\mathbf{V})) \), respectively.

**Proof.** Let \( f \) be a multivariate Gaussian density determined by the following linear Gaussian structural equation model,

\[
X_i = \sum_{X_j \in pa(X_i, \mathcal{G}_1)} \beta_{ji}X_j + \epsilon_i,
\]

where \( \beta_{ji} = 0 \) if \( X_j \to X_i \) is neither \( X \to U \) nor the edges on the corresponding path of \( \pi \) in \( \mathcal{G}_2 \) and \( 0 < \beta_{ji} < 1 \) otherwise, \( \epsilon_i \) are Gaussian noises with zero means and variances that makes every variable has variance one. (This is possible if we set \( \beta_{ji} \)'s small enough.) It is clear that \( f \) is Markovian to \( \mathcal{G}_2 \), and thus Markovian to \( \mathcal{G}_1 \) as \( \mathcal{G}_1 \) and \( \mathcal{G}_2 \) are Markov equivalent. Moreover, denote by \( \mathcal{G}_i' \) the DAGs obtained by removing from \( \mathcal{G}_i \) the edges that are neither on the corresponding path of \( \pi \) nor \( X \to U \). (\( i = 1, 2 \)), it can be checked that \( f \) is Markovian to \( \mathcal{G}_i' \) and \( f_i(y \mid do(x)) = f_i'(y \mid do(x)) \), where \( f_i'(y \mid do(x)) \) is the interventional distributions computed from the causal model \((\mathcal{G}_i', f(\mathbf{V})) \), \( i = 1, 2 \).

Using the backdoor criterion, it can be verified that \( E_1(y \mid do(X = 1)) = \sigma_{xy} \) and \( E_2(y \mid do(X = 1)) = (\sigma_{xy} - \sigma_{xw}\sigma_{wy})/(1 - \sigma_{xw}^2) \). By Wright's rule (Wright, 1921), it can be checked that \( \sigma_{xy} - (\sigma_{xy} - \sigma_{xw}\sigma_{wy})/(1 - \sigma_{xw}^2) \) equals to the product of the edge weights along the path \( X \leftarrow W \to
We first prove that (ii) holds. Based on Perković (2020, Theorem 3.6), the sufficiency of the identification condition holds, since \([G^*,\mathcal{K}] \subseteq [\mathcal{H}]\) and the causal effect of \(X\) on \(Y\) is identifiable from \(\mathcal{H}\) when the condition holds.

To prove the necessity, let \(\pi\) be a possibly causal path from \(X \in \mathbf{X}\) to \(Y \in \mathbf{Y}\) in \(\mathcal{H}\) where the first edge from the side of \(X\) is undirected. Denote by \(\pi^* = (X, W, U, ..., Y), k \geq 1\), a shortest subsequence of \(\pi\) such that \(\pi^*\) is also a possibly causal path from \(X\) to \(Y\) where the first edge from the side of \(X\) is undirected. It is clear that \(\pi^*(W, Y)\) is unshielded. By Lemma 12, there is a DAG \(G_2 \in [G^*,\mathcal{K}]\) such that \(ch(W, \pi_2) = sib(W, \mathcal{H}) \cup ch(W, \mathcal{H})\). Hence, the corresponding path of \(\pi^*\) in \(G_2\) is \(X \leftarrow W \rightarrow U \rightarrow \cdots \rightarrow Y\), according to the first Meek’s rule.

If \(X\) is not adjacent to \(U\) in \(\mathcal{H}\), then we consider a DAG \(G_1 \in [G^*,\mathcal{K}]\) where \(ch(X, G_1) = sib(X, \mathcal{H}) \cup ch(X, \mathcal{H})\). By Lemma 12, such a DAG exists. Since \(X\) is not adjacent to \(U\), \(\pi^*\) is unshielded, and thus the corresponding path of \(\pi^*\) in \(G_1\) is \(X \rightarrow W \rightarrow U \rightarrow \cdots \rightarrow Y\). By Corollary 4, the causal effect of \(X\) on \(Y\) is not identifiable.

If \(X\) is adjacent to \(U\), then \(X \rightarrow U\) is in \(\mathcal{H}\), since otherwise, \(X - U\) and \(\pi^*(U, Y)\) form a possibly causal path shorter than \(\pi^*\), which is contradicted to our assumption. If \(W \rightarrow U\) is in \(\mathcal{H}\), then we again consider a DAG \(G_1 \in [G^*,\mathcal{K}]\) where \(ch(X, G_1) = sib(X, \mathcal{H}) \cup ch(X, \mathcal{H})\). In \(G_1\), the corresponding path of \(\pi^*\) is \(X \rightarrow W \rightarrow U \rightarrow \cdots \rightarrow Y\). If \(W - U\) is in \(\mathcal{H}\), then we consider the DAG \(G_1 \in [G^*,\mathcal{K}]\) where \(ch(U, G_1) = sib(U, \mathcal{H}) \cup ch(U, \mathcal{H})\). Since \(X \rightarrow U\) and \(U \rightarrow W\) are in \(G_1\), \(X \rightarrow W\) is in \(G_1\). Thus, according to Lemma 14, the causal effect of \(X\) on \(Y\) is not identifiable.

\section*{C.21 Proof of Corollary 3}

Proof. We first prove that \((ii) \Rightarrow (i)\). Assume that \(X \rightarrow Y\) exists in every DAG in \([G^*,\mathcal{K}]\), but \(X - Y\) is in \(G^*\), then the causal effect of \(Y\) on \(X\) is not identifiable in \([G^*]\) but becomes identifiable in \([G^*,\mathcal{K}]\). In fact, the causal effect of \(Y\) on \(X\) is 0 in every DAG in \([G^*,\mathcal{K}]\).

Conversely, if the common directed causal relations of the DAGs in \([G^*,\mathcal{K}]\) are all encoded by directed edges in \(G^*\), then by the definition of causal MPDAG, \(\mathcal{H} = G^*\). By Theorem 9, an effect is identifiable in \([G^*]\) if and only if it is identifiable in \([G^*,\mathcal{K}]\). This completes the proof of \((i) \Rightarrow (ii)\).

Next, suppose that \(\mathcal{K}\) is derived from a consistent causal background knowledge set \(\mathcal{B}\). If there is a direct causal constraint in \(\mathcal{B}\) which does not hold for all DAGs in \([G^*]\), then it is clear that an unidentifiable effect becomes identifiable in \([G^*,\mathcal{K}]\), as statement \((ii)\) holds. If there is a non-ancestral causal constraint in \(\mathcal{B}\) which does not hold for all DAGs in \([G^*]\), then by Theorem 3, statement \((ii)\) also holds. Finally, since \(X \rightarrow Y\) implies \(Y \rightarrow X\), \(\mathcal{B}\) is equivalent to \((Y \rightarrow X) \cup \mathcal{B}\) with respect to \(G^*\). Thus, if \(Y \rightarrow X\) does not hold for all DAG in \([G^*]\), then statement \((ii)\) holds.

Finally, the proof of Theorem 9 follows a similar argument to that for Perković et al. (2017, Lemma C.1).
C.22 Proof of Theorem 10

Before proving Theorem 10, we first introduce some technical lemmas.

Lemma 15 (Perković et al. (2017), Lemma C.2). Let \( \mathcal{H} \) be a causal MPDAG, and \( X, Y \) are disjoint subsets of vertices of \( \mathcal{H} \). Suppose that the causal effect of \( X \) on \( Y \) is identifiable in \( [\mathcal{H}] \), then

(i) \( Z \cap \text{Forb}(X, Y, \mathcal{H}) = \emptyset \) implies that \( Z \cap \text{Forb}(X, Y, \mathcal{G}) = \emptyset \) for any DAG \( \mathcal{G} \in [\mathcal{H}] \), and

(ii) \( Z \cap \text{Forb}(X, Y, \mathcal{H}) \neq \emptyset \) implies that in \( \mathcal{H} \) there exist \( X \in X, Y \in Y, U \in Z \cap \text{Forb}(X, Y, \mathcal{H}) \) and \( W \) such that there are a directed path from \( X \) to \( W \) and unshielded possibly causal paths from \( W \) to \( Y \) and \( U \), respectively.

Lemma 16 (Perković et al. (2017), Lemma C.3). Let \( \mathcal{H} \) be a causal MPDAG, and \( X, Y \) are disjoint subsets of vertices of \( \mathcal{H} \). Suppose that the causal effect of \( X \) on \( Y \) is identifiable in \( [\mathcal{H}] \) and \( Z \cap \text{Forb}(X, Y, \mathcal{H}) = \emptyset \), then there is a proper definite status non-causal path from \( X \in X \) to \( Y \in Y \) which is not blocked by \( Z \) in \( \mathcal{H} \) implies that \( Z \) is not an adjustment set for \( (X, Y) \) in any DAG \( \mathcal{G} \in [\mathcal{H}] \).

Lemmas 15 and 16 result the following Corollaries 5 and 6, respectively.

Corollary 5. Let \( \mathcal{H} \) be an MPDAG representing \( \mathcal{G}^*, \mathcal{K} \) for a CPDAG \( \mathcal{G}^* \) and a set of consistent DCCs \( \mathcal{K} \), and \( X, Y \) are disjoint subsets of vertices of \( \mathcal{H} \). Suppose that the causal effect of \( X \) on \( Y \) is identifiable in \( [\mathcal{G}^*, \mathcal{K}] \), then

(i) \( Z \cap \text{Forb}(X, Y, \mathcal{H}) = \emptyset \) implies that \( Z \cap \text{Forb}(X, Y, \mathcal{G}) = \emptyset \) for any DAG \( \mathcal{G} \in [\mathcal{G}^*, \mathcal{K}] \), and

(ii) \( Z \cap \text{Forb}(X, Y, \mathcal{H}) \neq \emptyset \) implies that in \( \mathcal{H} \) there exist \( X \in X, Y \in Y, U \in Z \cap \text{Forb}(X, Y, \mathcal{H}) \) and \( W \) such that there are a directed path from \( X \) to \( W \) and unshielded possibly causal paths from \( W \) to \( Y \) and \( U \), respectively.

Corollary 6. Let \( \mathcal{H} \) be an MPDAG representing \( \mathcal{G}^*, \mathcal{K} \) for a CPDAG \( \mathcal{G}^* \) and a set of consistent DCCs \( \mathcal{K} \), and \( X, Y \) are disjoint subsets of vertices of \( \mathcal{H} \). Suppose that the causal effect of \( X \) on \( Y \) is identifiable in \( [\mathcal{G}^*, \mathcal{K}] \) and \( Z \cap \text{Forb}(X, Y, \mathcal{H}) = \emptyset \), then there is a proper definite status non-causal path from \( X \in X \) to \( Y \in Y \) which is not blocked by \( Z \) in \( \mathcal{H} \) implies that \( Z \) is not an adjustment set for \( (X, Y) \) in any DAG \( \mathcal{G} \in [\mathcal{G}^*, \mathcal{K}] \).

The above corollaries hold since \( [\mathcal{G}^*, \mathcal{K}] \subseteq [\mathcal{H}] \) and Theorem 9 proves that the causal effect of \( X \) on \( Y \) is identifiable in \( [\mathcal{G}^*, \mathcal{K}] \) if and only if it is identifiable in \( [\mathcal{H}] \). We omit the proofs here.

The proof of Theorem 10 is analogue to that of Perković et al. (2017, Theorem 4.4).

Proof of Theorem 10. Based on Theorem 4.4 in Perković et al. (2017) and the fact that \( [\mathcal{G}^*, \mathcal{B}] \subseteq [\mathcal{H}] \), it is clear that \( Z \) satisfies the b-adjustment criterion relative to \( (X, Y) \) in \( \mathcal{H} \) implies that \( Z \) is an adjustment set for \( (X, Y) \) with respect to \( \mathcal{G}^* \) and \( \mathcal{B} \). To prove the other direction, we use the proof by contradiction. First, Theorem 9 indicates that the first condition holds. Assuming the first condition holds but the second condition fails to hold, then by Corollary 5, there exist \( X \in X, Y \in Y, U \in Z \cap \text{Forb}(X, Y, \mathcal{H}) \) and \( W \) such that there are a directed path from \( X \) to \( W \) and unshielded possibly causal paths from \( W \) to \( Y \) and \( U \), respectively. According to Lemma 12,
there is a DAG $\mathcal{G} \in [\mathcal{G}^*, \mathcal{B}]$ such that every sibling of $W$ is a child of $W$ in $\mathcal{G}$. Thus, the unshielded possibly causal paths from $W$ to $Y$ and $U$ are directed in $\mathcal{G}$, which means $\mathbf{Z} \cap \text{Forb}(\mathbf{X}, \mathbf{Y}, \mathcal{G}) \neq \emptyset$ for $\mathcal{G}$. Consequently, by Perković (2020, Theorem 4.4), $\mathbf{Z}$ is not an adjustment set for $(\mathbf{X}, \mathbf{Y})$ in $\mathcal{G}$. Finally, the necessity of the third condition is guaranteed by Corollary 6.

\[ \square \]

C.23 Proof of Theorem 11

Maathuis et al. (2009) proved that,

**Lemma 17** (Maathuis et al. (2009), Lemma 3.1). Given a CPDAG $\mathcal{G}^*$, a treatment $X$, and $\mathbf{S} \subseteq sib(X, \mathcal{G}^*)$, there is a DAG $\mathcal{G} \in [\mathcal{G}^*, \mathcal{B}]$ such that $pa(X, \mathcal{G}) = \mathbf{S} \cup pa(X, \mathcal{G}^*)$ and $ch(X, \mathcal{G}) = sib(X, \mathcal{G}^*) \cup ch(X, \mathcal{G}^*) \setminus \mathbf{S}$ if and only if the induced subgraph of $\mathcal{G}^*$ over $\mathbf{S}$ is complete.

Given a CPDAG $\mathcal{G}^*$, a treatment $X$ and $\mathbf{S} \subseteq sib(X, \mathcal{G}^*)$, and suppose that there is a DAG $\mathcal{G} \in [\mathcal{G}^*, \mathcal{B}]$ such that $pa(X, \mathcal{G}) = \mathbf{S} \cup pa(X, \mathcal{G}^*)$ and $ch(X, \mathcal{G}) = sib(X, \mathcal{G}^*) \cup ch(X, \mathcal{G}^*) \setminus \mathbf{S}$. Regarding $\mathbf{S} \to X$ and $X \to sib(X, \mathcal{G}^*) \setminus \mathbf{S}$ as direct causal constraints and denote them by $\mathbf{K}$, the MPDAG $\mathcal{H}$ of $[\mathcal{G}^*, \mathbf{K}]$ is a chain graph (He and Geng, 2008, Theorem 6). Suppose that, apart from $\mathbf{K}$, we have another DCC set $\mathbf{K}'$. The following lemma extends Theorem 4 and gives a sufficient and necessary condition to check whether $\mathbf{K}'$ is consistent with $\mathcal{G}^*$ given $\mathbf{K}$ (that is, $\mathbf{K}' \cup \mathbf{K}$ is consistent with $\mathcal{G}^*$).

**Lemma 18.** Let $\mathcal{G}^*$ be a CPDAG, $X$ be a variable in $\mathcal{G}^*$ and $\mathbf{S} \subseteq sib(X, \mathcal{G}^*)$. Let $\mathbf{K} = \{S \to X \mid S \in \mathbf{S}\} \cup \{X \to C \mid C \in sib(X, \mathcal{G}^*) \setminus \mathbf{S}\}$ and assume that $\mathbf{K}$ is consistent with $\mathcal{G}^*$. Denote by $\mathcal{H}$ the MPDAG of $[\mathcal{G}^*, \mathbf{K}]$. For any DCC set $\mathbf{K}'$, the following two statements are equivalent.

(i) $\mathbf{K}'$ is consistent with $\mathcal{G}^*$ given $\mathbf{K}$.

(ii) Any connected undirected induced subgraph of $\mathcal{H}$ has a potential leaf node with respect to $\mathbf{K}'$ and $\mathcal{H}$.

Note that, in the main text the potential leaf node is defined over a CPDAG instead of an MPDAG. Therefore, for the sake of rigor, we extend the related definitions to chain graph causal MPDAG in the following, where a chain graph causal MPDAG is a causal MPDAG which itself is a chain graph.

**Definition 14’.** Given a chain graph causal MPDAG $\mathcal{H}$ and a set of DCCs $\mathbf{K}$ over $\mathbf{V}(\mathcal{H})$, a reduced form of $\mathbf{K}$ with respect to $\mathcal{H}$, denoted by $\mathbf{K}(\mathcal{H})$, is defined as follows.

$$
\mathbf{K}(\mathcal{H}) := \{\kappa_t \overrightarrow{\rightarrow} (\kappa_h \cap \text{sib}(\kappa_t, \mathcal{H})) \mid \kappa \in \mathbf{K} \text{ and } \kappa_h \cap \text{ch}(\kappa_t, \mathcal{H}) = \emptyset\}.
$$

(10)

Similar to Proposition 5, it is easy to verify that a DAG in $[\mathcal{H}]$ satisfies all constraints in $\mathbf{K}(\mathcal{H})$ if and only if it satisfies all constraints in $\mathbf{K}$.

**Definition 15’.** Given an undirected induced subgraph $\mathcal{U}$ of a chain graph causal MPDAG $\mathcal{H}$ over $\mathbf{V}(\mathcal{U}) \subseteq \mathbf{V}(\mathcal{H})$, and a set of DCCs $\mathbf{K}$ over $\mathbf{V}(\mathcal{H})$, the restriction subset of $\mathbf{K}$ on $\mathcal{U}$ given $\mathcal{H}$ is defined by

$$
\mathbf{K}(\mathcal{U} \mid \mathcal{H}) := \{\kappa \in \mathbf{K}(\mathcal{H}) \mid \{\kappa_t\} \cup \kappa_h \subseteq \mathbf{V}(\mathcal{U})\}.
$$

(11)
Definition 16'. Let $\mathcal{H}$ be a chain graph causal MPDAG and $\mathcal{K}$ be a set of DCCs over $\mathcal{V}(\mathcal{H})$. Given an undirected induced subgraph $U$ of $\mathcal{H}$ and a vertex $X$ in $U$, $X$ is called a potential leaf node in $U$ with respect to $\mathcal{K}$ and $\mathcal{H}$, if $X$ is a simplicial vertex in $U$ and $X$ is not the tail of any clause in $\mathcal{K}(U \mid \mathcal{H})$.

Proof of Lemma 18. The proof is similar to that of Theorem 4. We first prove the necessity. If $\mathcal{K}'$ is consistent with $\mathcal{G}^*$ given $\mathcal{K}$, then there exists a DAG $\mathcal{G} \in [\mathcal{H}]$ satisfying all constraints in $\mathcal{K}'$. Let $\mathcal{U}$ be an arbitrary connected undirected induced subgraph of $\mathcal{H}$, and denote the induced subgraph of $\mathcal{G}$ over $\mathcal{V}(\mathcal{U})$ by $\mathcal{G}_{\text{sub}}$. Since any induced subgraph of a DAG is still a DAG, $\mathcal{G}_{\text{sub}}$ is a DAG, and thus it must have a leaf node $V_{\text{leaf}}$. As we assume that $\mathcal{H}$ is a chain graph, following exactly the same argument for proving Lemma 9, we can show that $V_{\text{leaf}}$ is a potential leaf node in $U$ with respect to $\mathcal{K}'$ and $\mathcal{H}$.

We next prove the sufficiency. Since $\mathcal{H}$ is a chain graph, no orientation of the edges not oriented in $\mathcal{H}$ will create a directed cycle which includes an edge or edges that were oriented in $\mathcal{H}$. Moreover, based on statement (iii) of Theorem 1, no orientation of an edge not directed in $\mathcal{H}$ can create a new $v$-structure with an edge that was oriented in $\mathcal{H}$. Then, following the same argument for proving Lemma 10, we can show that $\mathcal{K}'$ is consistent with $\mathcal{G}^*$ given $\mathcal{K}$ if and only if $\mathcal{K}'(C \mid \mathcal{H})$ is consistent with $C$ for any chain component $C$ of $\mathcal{H}$. The desired result comes from the same construction of PEO given in the proof of Theorem 4.

In order to prove Theorem 11, we prove the following Theorem 11’, which includes the result provided in Theorem 11.

Theorem 11’. Let $\mathcal{K}$ be a set of DCCs consistent with a CPDAG $\mathcal{G}^*$, and $\mathcal{H}$ be the MPDAG of $[\mathcal{G}^*, \mathcal{K}]$. For any vertex $X$ and $S \subseteq \text{sub}(X, \mathcal{H})$, let

$$T = \{X\} \cup ((\text{pa}(X, \mathcal{H}) \cup S) \cap \text{sub}(X, \mathcal{G}^*)),$$

and

$$D_X = \{u \to X \mid u \in \text{pa}(X, \mathcal{H}) \cup S\} \cup \{X \to v \mid v \in \text{sub}(X, \mathcal{H}) \cup \text{ch}(X, \mathcal{H}) \setminus S\}.$$

Then, the following statements are equivalent.

(i) There is a DAG $\mathcal{G}$ in $[\mathcal{G}^*, \mathcal{K}]$ such that $\text{pa}(X, \mathcal{G}) = S \cup \text{pa}(X, \mathcal{H})$ and $\text{ch}(X, \mathcal{G}) = \text{sub}(X, \mathcal{H}) \cup \text{ch}(X, \mathcal{H}) \setminus S$.

(ii) The induced subgraph of $\mathcal{H}$ over $S$ is complete and the restriction subset of $\mathcal{K} \cup D_X$ on $\mathcal{G}^*(\mathcal{M}_T)$ given $\mathcal{G}^*$ is consistent with $\mathcal{G}^*(\mathcal{M}_T)$ for all maximal clique $\mathcal{M}_T$ of $\mathcal{G}^*$ containing $T$.

(iii) The restriction subset of $\mathcal{K} \cup D_X$ on $\mathcal{G}^*(\text{sub}(X, \mathcal{G}^*))$ given $\mathcal{G}^*$ is consistent with $\mathcal{G}^*(\text{sub}(X, \mathcal{G}^*))$.

Proof of Theorem 11’. By Theorem 4, statement (i) implies statement (iii) and statement (iii) $\Rightarrow$ (ii). Thus, we only prove (ii) $\Rightarrow$ (i) in the following.

To prove (ii) $\Rightarrow$ (i), it suffices to show that $\mathcal{K} \cup D_X$ is consistent with $\mathcal{G}^*$. According to Lemma 10, we can consider each chain component of $\mathcal{G}^*$ separately. Therefore, without loss of generality, we can assume that $\mathcal{G}^*$ is a connected chordal graph, and that $\mathcal{K}$ is already in its reduced form with respect to $\mathcal{G}^*$. This means we have that,
(P1) for any \( \kappa \in \mathcal{K} , \kappa_h \subseteq sib(\kappa_t, \mathcal{G}^*) = \text{adj}(\kappa_t, \mathcal{G}^*) \), and the consistency of \( \mathcal{K} \) with \( \mathcal{G}^* \) indicates that \( \kappa_h \neq \emptyset \).

It can be seen from the definition of consistency that checking the consistency of \( \mathcal{K} \cup D_X \) with \( \mathcal{G}^* \) is equivalent to the following two-steps procedure:

**Step 1.** checking whether \( D_X \) is consistent with \( \mathcal{G}^* \), and if the consistency holds, then

**Step 2.** checking whether \( \mathcal{K} \setminus D_X \) is consistent with \( \mathcal{G}^* \) given \( D_X \).

Note that, the intersection of \( \mathcal{K} \) and \( D_X \) may not be empty. Clearly, \( \mathcal{K} \cup D_X \) is consistent if and only if neither of the above two steps returns a negative answer.

We first prove that \( D_X \) is consistent with \( \mathcal{G}^* \), meaning that step 1 returns a positive answer. Based on statement (ii), the induced subgraph of \( \mathcal{H} \) over \( \mathcal{S} \) is complete, indicating that the induced subgraph of \( \mathcal{G}^* \) over \( \mathcal{S} \) is complete as \( \mathcal{H} \) and \( \mathcal{G}^* \) has the same skeleton. If \( pa(X, \mathcal{H}) = \emptyset \), then \( pa(X, \mathcal{H}) \cup \mathcal{S} \) induces a complete subgraph. If \( pa(X, \mathcal{H}) \neq \emptyset \), then for any \( p \in pa(X, \mathcal{H}) \) and \( S \subseteq \mathcal{S} \), \( p \) and \( S \) are adjacent in \( \mathcal{H} \), since otherwise \( X \to S \) should appear in \( \mathcal{H} \) due to the maximality of \( \mathcal{H} \). Moreover, since we have assumed that \( \mathcal{G}^* \) is a connected chordal graph, \( \mathcal{H} \) has no v-structure as discussed in Appendix C.1, and thus, \( pa(X, \mathcal{H}) \) induces a complete subgraph. Therefore, it holds that,

(P2) \( pa(X, \mathcal{H}) \cup \mathcal{S} \) induces a complete subgraph of \( \mathcal{G}^* \).

By Lemma 17 and the definition of \( D_X \), \( D_X \) is consistent with \( \mathcal{G}^* \).

Below we will show that \( \mathcal{K} \setminus D_X \) is consistent with \( \mathcal{G}^* \) given \( D_X \). Note that, since \( D_X \) contains direct causal constraints only, if we denote the MPDAG representing \( [\mathcal{G}^*, D_X] \) by \( \mathcal{C}^* \), then \( \mathcal{C}^* \) is a chain graph MPDAG and \( [\mathcal{C}^*] = [\mathcal{G}^*, D_X] \) (He and Geng, 2008, Theorem 6). Now, consider the following four subsets of \( \mathcal{K} \setminus D_X \):

\[
\begin{align*}
\mathcal{K}_p &= \{ \kappa \in \mathcal{K} \setminus D_X \mid \exists d \in \kappa_h, \kappa_t \to d \text{ is in } \mathcal{C}^* \}, \\
\mathcal{K}_u &= \{ \kappa \in \mathcal{K} \setminus D_X \mid \forall d \in \kappa_h, \kappa_t \to d \text{ is in } \mathcal{C}^* \}, \\
\mathcal{K}_c &= \{ \kappa \in \mathcal{K} \setminus D_X \mid \forall d \in \kappa_h, d \to \kappa_t \text{ is in } \mathcal{C}^* \}, \\
\mathcal{K}_r &= \mathcal{K} \setminus D_X \setminus (\mathcal{K}_p \cup \mathcal{K}_u \cup \mathcal{K}_c).
\end{align*}
\]

It is easy to verify that \( \mathcal{K}_p, \mathcal{K}_u, \mathcal{K}_c \) and \( \mathcal{K}_r \) are disjoint and

\[
\mathcal{K}_r = \{ \kappa \in \mathcal{K} \setminus D_X \mid \exists d \in \kappa_h, d \to \kappa_t \text{ is in } \mathcal{C}^* \text{ and } \exists d \in \kappa_h, d \to \kappa_t \text{ is in } \mathcal{C}^* \}.
\]

Since the DCCs in \( \mathcal{K}_p \) are already satisfied given \( \mathcal{C}^* \), to prove that \( \mathcal{K} \setminus D_X \) is consistent with \( \mathcal{G}^* \) given \( D_X \), it suffices to show that \( \mathcal{K}_u \cup \mathcal{K}_c \cup \mathcal{K}_r \) is consistent with \( \mathcal{G}^* \) given \( D_X \).

We will give a proof by contradiction. Assuming that \( \mathcal{K}_u \cup \mathcal{K}_c \cup \mathcal{K}_r \) is not consistent with \( \mathcal{G}^* \) given \( D_X \), then either \( \mathcal{K}_c \neq \emptyset \) or there exists a connected undirected induced subgraph \( \mathcal{W} \) of \( \mathcal{C}^* \) such that \( \mathcal{W} \) has no potential lead node with respect to \( \mathcal{K}_u \cup \mathcal{K}_r \) and \( \mathcal{C}^* \), as indicated by Lemma 18.

**Case 1.** Suppose that \( \mathcal{K}_c \neq \emptyset \). Let \( \kappa \in \mathcal{K}_c \) be an arbitrary DCC. By the definitions of \( \mathcal{K}_c \) and \( \mathcal{C}^* \), as well as the maximality of \( \mathcal{C}^* \), it holds that,
Case 1-2. If $\mathcal{G}^*_t$ with respect to $G^*$ and $D_X$, denoted by $U_t$, satisfies that $\kappa_t \subseteq \text{pa}(\kappa_t, \mathcal{G}^*) = \text{adj}(\kappa_t, U_t)$.

$\text{pa}(\kappa_t, \mathcal{G}^*) = \text{adj}(\kappa_t, U_t)$ is because we have assumed that $\mathcal{G}^*$ does not contain any directed edge. By (P1), $\kappa_t \neq \emptyset$, and thus $\text{adj}(\kappa_t, U_t) \neq \emptyset$ and $U_t$ is not a singleton graph (that is, $U_t$ has at least two vertices).

We first show that $X \in \mathbf{V}(U_t)$. Assume, for the sake of contradiction, that $X \notin \mathbf{V}(U_t)$, then the restriction subset of $D_X$ on $U_t$ given $\mathcal{G}^*$ is empty, as every DCC in $D_X$ has $X$ as its tail or head. Thus, $U_t$ is not a maximal orientation component for $\kappa_t$ with respect to $D_X$ and $\mathcal{G}^*$, since $U_t$ is chordal and any connected chordal graph has at least two simplicial vertices. This leads to a contradiction.

Recall that $U_t$ is connected, hence $X \in \mathbf{V}(U_t)$ implies that $\text{adj}(X, U_t) \neq \emptyset$. The remaining proof is quite lengthy. We will consider two subcases: $\text{adj}(X, U_t) \subseteq \text{pa}(X, \mathcal{H}) \cup S = \text{pa}(X, \mathcal{C}^*)$ and $\text{adj}(X, U_t) \not\subseteq \text{pa}(X, \mathcal{H}) \cup S = \text{pa}(X, \mathcal{C}^*)$, and show that in both subcases statement (ii) does not hold. That is, the restriction subset of $\mathcal{K} \cup D_X$ on $\mathcal{G}^*(M_T)$ given $\mathcal{G}^*$ is not consistent with $\mathcal{G}^*(M_T)$ for some $M_T$. This completes the proof for case 1.

Case 1-1. If $\text{adj}(X, U_t) \subseteq \text{pa}(X, \mathcal{H}) \cup S = \text{pa}(X, \mathcal{C}^*)$, then $\text{adj}(X, U_t)$ is a clique in $U_t$ based on (P2). Thus, $X$ is a simplicial vertex in $U_t$. On the other hand, $\text{adj}(X, U_t) \subseteq \text{pa}(X, \mathcal{H}) \cup S$ implies that $D_X(U_t) = \{u \rightarrow X \mid u \in \text{adj}(X, U_t)\}$, hence $X$ is a potential leaf node in $U_t$ with respect to $D_X$ and $\mathcal{G}^*$. By the definition of $U_t$, it holds that $X = \kappa_t$. Thus, $\{X\} \cup \kappa_t \subseteq \{X\} \cup \text{pa}(X, \mathcal{H}) \cup S \subseteq \mathcal{M}_T$ for some maximal clique $\mathcal{M}_T$ of $\mathcal{G}^*$ containing $T$. Recall that $\kappa \in \mathcal{K}_c \subseteq \mathcal{K}$, the restriction subset of $\mathcal{K} \cup D_X$ on $\mathcal{G}^*(M_T)$ given $\mathcal{G}^*$ contains $X \rightarrow \kappa_t$ and $\kappa_t \rightarrow X$ both, which is not consistent with $\mathcal{G}^*(M_T)$.

Case 1-2. If $\text{adj}(X, U_t) \not\subseteq \text{pa}(X, \mathcal{H}) \cup S = \text{pa}(X, \mathcal{C}^*)$, then $\text{adj}(X, U_t) \cap \text{ch}(X, \mathcal{C}^*) \neq \emptyset$. We first claim that,

(P4) none of the vertices in $\mathbf{V}(U_t) \setminus (\{\kappa_t, X\} \cup \text{pa}(X, \mathcal{C}^*))$ (possibly empty) is simplicial in $U_t$.

In fact, with respect to $D_X$ and $\mathcal{G}^*$, only $X$ and the vertices in $\text{adj}(X, U_t) \cap \text{pa}(X, \mathcal{C}^*)$ (possibly empty) can be the tails of DCCs in $D_X(U_t)$. By the definition of potential leaf node and $U_t$, the vertices in $\mathbf{V}(U_t) \setminus (\{\kappa_t, X\} \cup \text{pa}(X, \mathcal{C}^*))$ are non-simplicial as they are not potential leaf nodes in $U_t$ with respect to $D_X$ and $\mathcal{G}^*$. Now, denote by $L$ the set of potential leaf nodes of $U_t$ with respect to $\mathcal{K}_c$ and $\mathcal{G}^*$, then $L \subseteq \{\kappa_t, X\} \cup \text{pa}(X, \mathcal{C}^*)$ based on (P4) as the vertices in $L$ are simplicial in $U_t$. However, as $\kappa_t \subseteq \text{pa}(\kappa_t, \mathcal{C}^*) = \text{adj}(\kappa_t, U_t)$, if $X = \kappa_t$, then $\text{adj}(X, U_t) = \text{pa}(X, \mathcal{C}^*)$, contradicted to the assumption of case 1-2. Hence, $X \neq \kappa_t$. Since $\kappa \in \mathcal{K}_c(U_t)$, $\kappa_t$ is not a potential leaf node in $U_t$ with respect to $\mathcal{K}_c$ and $\mathcal{G}^*$. Thus, it holds that,

(P5) the set of potential leaf nodes of $U_t$ with respect to $\mathcal{K}_c$ and $\mathcal{G}^*$, denoted by $L$, satisfies that $L \subseteq \{X\} \cup \text{pa}(X, \mathcal{C}^*)$.

Case 1-2-1. If $X$ is simplicial in $U_t$, then $\text{adj}(X, U_t)$ is a clique in $U_t$. Recall that $\text{adj}(X, U_t) \cap \text{ch}(X, \mathcal{C}^*) \neq \emptyset$, we next consider two possibilities depends on whether a vertex in $\text{adj}(X, U_t) \cap \text{ch}(X, \mathcal{C}^*)$ is simplicial.
First, suppose that there is a \( c \in \text{adj}(X, \mathcal{U}_t) \cap \text{ch}(X, \mathcal{C}^*) \) which is simplicial in \( \mathcal{U}_t \), then by (P4), \( c \notin \mathbf{V}(\mathcal{U}_t) \setminus (\{\kappa_t, X\} \cup \text{pa}(X, \mathcal{C}^*)) \), indicating that \( c = \kappa_t \). Thus, \( \kappa_t \in \text{adj}(X, \mathcal{U}_t) \).

(i) \( \text{adj}(X, \mathcal{U}_t) = \{\kappa_t\} \). We claim that this is an impossible case. In fact, it holds that \( \text{adj}(\kappa_t, \mathcal{U}_t) = \{X\} \), since otherwise, the vertices in \( \text{adj}(\kappa_t, \mathcal{U}_t) \) are adjacent to \( X \) due to the simplicity of \( \kappa_t \), which is contradicted to \( |\text{adj}(X, \mathcal{U}_t)| = 1 \). Thus, \( \kappa_h = \{X\} \) and \( \kappa_t \to X \) is in \( \mathcal{H} \), which is contradicted to the assumption that \( \kappa_t \in \text{ch}(X, \mathcal{C}^*) = \text{ch}(X, \mathcal{H}) \cup \text{sib}(X, \mathcal{H}) \setminus \mathbf{S} \).

(ii) \( \text{adj}(X, \mathcal{U}_t) \setminus \{\kappa_t\} \neq \emptyset \) and \( \text{adj}(X, \mathcal{U}_t) \setminus \{\kappa_t\} = \text{pa}(X, \mathcal{C}^*) \). Since \( \kappa_t, X \) are both simplicial in \( \mathcal{U}_t \), \( \kappa_h \subseteq \text{adj}(\kappa_t, \mathcal{U}_t) = \{X\} \cup \text{adj}(X, \mathcal{U}_t) \setminus \{\kappa_t\} = \{X\} \cup \text{pa}(X, \mathcal{C}^*) = \mathbf{T} \). Hence, \( \{\kappa_t\} \cup \mathbf{T} \) is a clique in \( \mathcal{G}^* \). It is then straightforward to check that the restriction subset of \( \mathcal{K} \cup D_X \) on \( \mathcal{G}^*(\mathbf{M}_\mathbf{T}) \) given \( \mathcal{G}^* \) is not consistent with \( \mathcal{G}^*(\mathbf{M}_\mathbf{T}) \) for any \( \mathbf{M}_\mathbf{T} \) containing \( \{\kappa_t\} \cup \mathbf{T} \).

(iii) \( \text{adj}(X, \mathcal{U}_t) \setminus \{\kappa_t\} \neq \emptyset \) and \( \text{adj}(X, \mathcal{U}_t) \setminus \{\kappa_t\} \subseteq \text{pa}(X, \mathcal{C}^*) \). Below we show that this is also an impossible case. For any \( p \in \text{pa}(X, \mathcal{C}^*) \) which is not in \( \mathcal{U}_t \), \( p \) is not adjacent to \( \kappa_t \), since otherwise, \( p \to \kappa_t \) is in \( \mathcal{C}^* \) by Rule 1 of Meek's rules and \( p \) should be included in \( \mathcal{U}_t \). Denote by \( \mathcal{T} \) the induced subgraph of \( \mathcal{G}^* \) over \( \{p, \kappa_t\} \cup \text{adj}(\kappa_t, \mathcal{U}_t) \). As \( \text{adj}(\kappa_t, \mathcal{U}_t) \subseteq \{X\} \cup \text{pa}(X, \mathcal{C}^*) \) and \( \{X\} \cup \text{pa}(X, \mathcal{C}^*) \) induces a complete subgraph of \( \mathcal{G}^* \), \( p \in \text{pa}(X, \mathcal{C}^*) \) is adjacent to every vertex in \( \text{adj}(\kappa_t, \mathcal{U}_t) \). Therefore, \( p \) and \( \kappa_t \) are all and only simplicial vertices in \( \mathcal{T} \). Moreover, due to the consistency of \( \mathcal{K}_c \) and the fact that \( \kappa \in \mathcal{K}_c \), \( \mathcal{T} \) is an orientation component for \( p \) with respect to \( \mathcal{K}_c \) and \( \mathcal{G}^* \). Therefore, \( \text{adj}(\kappa_t, \mathcal{U}_t) \to p \) are in \( \mathcal{H} \). In particular, \( X \to p \) is in \( \mathcal{H} \), which is contrary to the assumption that \( p \in \text{pa}(X, \mathcal{C}^*) \subseteq \text{pa}(X, \mathcal{H}) \cup \text{sib}(X, \mathcal{H}) \).

(iv) \( \text{adj}(X, \mathcal{U}_t) \setminus \{\kappa_t\} \neq \emptyset \) and \( \text{adj}(X, \mathcal{U}_t) \cap \text{ch}(X, \mathcal{C}^*) \setminus \{\kappa_t\} \neq \emptyset \). This case is not possible either. Notice that none of the vertices in \( \text{adj}(X, \mathcal{U}_t) \cap \text{ch}(X, \mathcal{C}^*) \setminus \{\kappa_t\} \) is simplicial in \( \mathcal{U}_t \), we have that \( \mathcal{U}_t \) is not complete, and thus \( \mathcal{U}_t \) must have two non-adjacent simplicial vertices. Since \( X \) and \( \kappa_t \) are two adjacent simplicial vertices in \( \mathcal{U}_t \), there must exist another simplicial vertex \( w \) in \( \mathcal{U}_t \) which is not adjacent to \( X \) and not adjacent to \( \kappa_t \). However, as \( w \neq X \) and \( w \) is not adjacent to \( X \), \( w \) is not the tail of any DCC in \( D_X \). It implies that \( w \neq \kappa_t \) is a potential leaf node of \( \mathcal{U}_t \) with respect to \( D_X \) and \( \mathcal{G}^* \). This leads to a contradiction since we assume that \( \mathcal{U}_t \) is the maximal orientation component for \( \kappa_t \) with respect to \( D_X \) and \( \mathcal{G}^* \).

Next, suppose that none of the vertices in \( \text{adj}(X, \mathcal{U}_t) \cap \text{ch}(X, \mathcal{C}^*) \) is simplicial in \( \mathcal{U}_t \). Denote by \( \mathbf{R} \) (possibly empty) the set of simplicial vertices in \( \mathcal{U}_t \) which are adjacent to \( X \). Let \( \mathcal{T} \) be the induced subgraph of \( \mathcal{U}_t \) over \( \mathbf{V}(\mathcal{U}_t) \setminus \mathbf{R} \). We will show that,

(P6) \( \mathcal{T} \) is an orientation component for \( X \) with respect to \( \mathcal{K}_c \) and \( \mathcal{G}^* \).

Since \( X \) is a simplicial node in \( \mathcal{U}_t \), \( X \) must be simplicial in \( \mathcal{T} \). Hence, by Theorem 4 and the consistency of \( \mathcal{K}_c \), it suffices to show that for any \( Y \in \mathbf{V}(\mathcal{T}) \setminus \{X\} \), \( Y \) is not a potential leaf node in \( \mathcal{T} \) with respect to \( \mathcal{K}_c \) and \( \mathcal{G}^* \). The proof consists of two claims:

(i) For any \( Y \in \mathbf{V}(\mathcal{T}) \setminus \{X\} \), \( Y \) is not simplicial in \( \mathcal{U}_t \) implies that \( Y \) is not simplicial in \( \mathcal{T} \). Suppose that there exists a \( Y \in \mathbf{V}(\mathcal{T}) \setminus \{X\} \) which is not simplicial in \( \mathcal{U}_t \) but simplicial in \( \mathcal{T} \), then \( \text{adj}(Y, \mathcal{U}_t) \cap \text{adj}(Y, \mathcal{T}) \neq \emptyset \). This implies that \( \mathbf{R} \neq \emptyset \) as \( \text{adj}(Y, \mathcal{U}_t) \cap \text{adj}(Y, \mathcal{T}) \subseteq \mathbf{V}(\mathcal{U}_t) \setminus \mathbf{V}(\mathcal{T}) = \mathbf{R} \). On the other hand, since every vertex in \( \mathbf{R} \) is simplicial in \( \mathcal{U}_t \), \( \mathbf{R} \subseteq \text{adj}(Y, \mathcal{U}_t) \), meaning that \( \text{adj}(Y, \mathcal{U}_t) \cap \text{adj}(Y, \mathcal{T}) = \mathbf{R} \). Moreover, \( \mathbf{R} \subseteq \text{adj}(X, \mathcal{U}_t) \) implies that \( Y \) is also
adjacent to $X$. Notice that $\text{adj}(Y, T)$ is a clique and $X \in \text{adj}(Y, T)$, $\text{adj}(Y, U_t)$ is also a clique, which is contradicted to our assumption.

(ii) For any $Y \in V(T) \setminus \{X\}$, $Y$ is simplicial in $U_t$ implies that $Y$ is the tail of some DCC in $\mathcal{K}_c(T)$. In fact, if $Y \notin R \cup \{X\}$ is simplicial in $U_t$, then it is simplicial in $T$, and there is a DCC in $\mathcal{K}_c(U_t)$ whose tail is $Y$, since otherwise, $Y$ is a potential leaf node in $U_t$ with respect to $\mathcal{K}_c$ and $G^*$, which means $Y \in \text{adj}(X, U_t) \cap \text{pa}(X, C^*)$ and thus $Y \in R$, according to (P5). If $Y$ is not the tail of any DCC in $\mathcal{K}_c(T)$, then $\text{adj}(Y, T) \subseteq \text{adj}(Y, U_t)$, meaning that $\text{adj}(Y, U_t) \cap R \neq \emptyset$. Since the vertices in $R$ are simplicial in $U_t$, and $R \subseteq \text{adj}(X, U_t)$, $Y$ is adjacent to $X$ in $U_t$. Finally, as $Y$ is simplicial in $U_t$, by the construction, we have $Y \in R$ and hence $Y \notin V(T)$, which is contradicted to our assumption.

In conclusion, $T$ is an orientation component for $X$ with respect to $\mathcal{K}_c$ and $G^*$. Note that $\text{adj}(X, U_t) \cap \text{ch}(X, C^*) \neq \emptyset$ and $\text{adj}(X, U_t) \cap \text{ch}(X, C^*) \cap R = \emptyset$, $\text{adj}(X, U_t) \cap \text{ch}(X, C^*) \subseteq \text{adj}(X, T)$. Hence, $\text{adj}(X, U_t) \cap \text{ch}(X, C^*) \rightarrow X$ are in $\mathcal{H}$, which is contradicted to the assumption that $\text{ch}(X, C^*) \subseteq \text{ch}(X, \mathcal{H}) \cup \text{sib}(X, \mathcal{H}) \setminus S$.

Case 1-2-2. Suppose that $X$ is not simplicial in $U_t$. We first show that there is a $\phi \in \text{adj}(X, U_t) \cap \text{pa}(X, C^*)$ which is a potential leaf node in $U_t$ with respect to $\mathcal{K}_c$ and $G^*$. In fact, with respect to $\mathcal{K}_c$ and $G^*$, $U_t$, which is a connected undirected induced subgraph of $G^*$, must have a potential leaf node, since $\mathcal{K}_c \subseteq \mathcal{K}$ and $\mathcal{K}$ is consistent with $G^*$. By (P5), these potential leaf nodes are in $\{X\} \cup \text{pa}(X, C^*)$. However, as $X$ is not simplicial in $U_t$ by our assumption, the potential leaf nodes are all in $\text{pa}(X, C^*)$.

Now let $\phi \in \text{adj}(X, U_t) \cap \text{pa}(X, C^*)$ be a potential leaf node in $U_t$ with respect to $\mathcal{K}_c$ and $G^*$. Denote by $R$ (possibly empty) the set of simplicial vertices in $U_t$ which are adjacent to $\phi$. Clearly, $\{\phi\} \cup R$ is a clique of $U_t$. Let $T$ be the induced subgraph of $U_t$ over $V(U_t) \setminus R$. By the similar argument given to prove (P6), we can prove that $T$ is an orientation component for $\phi$ with respect to $\mathcal{K}_c$ and $G^*$. Note that $X \in \text{adj}(\phi, U_t)$ and $X \notin R$, $X \in \text{adj}(\phi, T)$. Hence, $X \rightarrow \phi$ is in $\mathcal{H}$, which is contradicted to the assumption that $\phi \in \text{pa}(X, \mathcal{H}) \cup S$.

Case 2. Suppose that $\mathcal{K}_c = \emptyset$, then there exists a connected undirected subgraph $W$ of $C^*$ such that $W$ has no potential lead node with respect to $\mathcal{K}_u \cup \mathcal{K}_r$ and $C^*$ (Lemma 18). Note that, since $C^*$ is a chain graph, for any DCC in $\mathcal{K}_u$, its heads and tail are in the same chain component of $C^*$. As $\mathcal{K}$ is consistent with $G^*$, $\mathcal{K}_u \subseteq \mathcal{K}$ is also consistent with $G^*$. Then, by Lemma 18, we can conclude that,

(P7) $\mathcal{K}_u$ is consistent with $G^*$ given $D_X$ because $\mathcal{K}_u(C^*) = \mathcal{K}_u = \mathcal{K}_u(G^*)$ and any connected undirected induced subgraph of $C^*$ is also a connected undirected induced subgraph of $G^*$.

Since $W$ is undirected and connected, $W$ must be an induced subgraph of some chain component of $C^*$. Denote by $A$ the set of all potential leaf nodes of $W$ with respect to $\mathcal{K}_u$ and $C^*$. As $\mathcal{K}_u$ is consistent with $G^*$ given $D_X$, $A \neq \emptyset$. Notice that, $(\mathcal{K}_u \cup \mathcal{K}_r)(W | C^*) = \mathcal{K}_u(W | C^*) \cup \mathcal{K}_r(W | C^*)$, $W$ has no potential leaf node with respect to $\mathcal{K}_u \cup \mathcal{K}_r$ and $C^*$ implies that every vertex in $A$ is the tail of some DCC in $\mathcal{K}_r(W | C^*)$. That is,

(P8) for any $a \in A$ there is a DCC $\kappa := (a \xrightarrow{or} \kappa_h) \in \mathcal{K}_r$ such that (i) $\kappa_h \cap \text{sib}(a, C^*) \neq \emptyset$ and $\kappa_h \cap \text{sib}(a, C^*) \subseteq V(W)$, (ii) $\kappa_h \setminus V(W) \neq \emptyset$ and $\kappa_h \setminus V(W) \subseteq \text{pa}(a, C^*)$, and (iii) $\kappa_h \subseteq V(W) \cup \text{pa}(a, C^*)$.
Now consider $G^*$ and $D_X$. For any $a \in A$, let $U_a$ be the maximal orientation component for $a$ with respect to $D_X$ in $G^*$. It is clear that $pa(a, C^*) = adj(a, U_a)$. Since $C^*$ is a chain graph causal MPDAG and $A \subseteq V(W)$ and $W$ is an induced subgraph of some chain component of $C^*$, by Theorem 1, $pa(a, C^*) = pa(a', C^*)$ for any $a, a' \in A$. Thus, $adj(a, U_a) = adj(a', U_{a'})$ for any $a, a' \in A$.

On the other hand, following the same argument for case 1, it can be shown that $X \in V(U_a)$ for any $a \in A$. Moreover, if $adj(X, U_a) \cap ch(X, C^*) = \emptyset$ for some $a \in A$, then we can prove that $X$ is a potential leaf node in $U_a$ with respect to $D_X$ and $G^*$, which means $X = a$, and consequently, $X \in V(W)$. As $W$ is an induced subgraph of some chain component of $C^*$ but $X$ has no siblings in $C^*$, $V(W) = \{X\}$. This is impossible since $V(W) = \{X\}$ implies that $\kappa_h \cap sib(a, C^*) = \emptyset$, contrary to (P8). Therefore, we have that,

\[(P9) \text{ for all } a \in A, \text{ adj}(X, U_a) \cap ch(X, C^*) \neq \emptyset.\]

Moreover, following the same argument for proving (P4), it can be shown that,

\[(P10) \text{ none of the vertices in } V(U_a) \setminus (\{a\} \cup pa(X, C^*)) \text{ (possibly empty) is simplicial in } U_a.\]

The rest of the proof is similar to that for case 1-2. Let

$$F = V(W) \bigcup_{a \in A} V(U_a),$$

and

$$N = \bigcup_{a \in A} V(U_a) \setminus (\{X\} \cup A \cup pa(X, C^*)).$$

Denote by $F$ the induced subgraph of $G^*$ over $F$. Firstly, since $V(U_a) \subseteq F$ and $N \subseteq F$, by (P10), it holds that

\[(P11) \text{ none of the vertices in } N \text{ is simplicial in } F.\]

Moreover, by the definition of $A$, every vertex in $V(W) \setminus A$ is either non-simplicial in $W$, or the tail of a DCC in $K_u(W \mid C^*)$. Thus,

\[(P12) w \in V(W) \setminus A \text{ is non-simplicial in } W \text{ implies that } w \text{ is non-simplicial in } F, \text{ and } w \in V(W) \setminus A \text{ is the tail of a DCC in } K_u(W \mid C^*) \text{ implies that } w \text{ is also the tail of a DCC in } K_u(W \mid G^*) \text{ based on (P7)}.\]

Finally, for set $A$, we have that,

\[(P13) \text{ for any } a \in A, \text{ a is simplicial in } F, \text{ and is also the tail of some DCC in } K_r(F \mid G^*).\]

The first claim comes from the simplicity of $a$ in $W$ as well as the fact that

$$adj(a, F) = adj(a, W) \bigcup_{a' \in A} adj(a', U_{a'}) = adj(a, W) \cup adj(a, C^*) = adj(a, W) \cup pa(a, C^*),$$

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where the second equality holds because \( \text{adj}(a, \mathcal{U}_a) = \text{adj}(a', \mathcal{U}_a) \) for any \( a, a' \in A \), and the third equality holds because of the definition of \( \mathcal{U}_a \). The second claim holds because of the above equation and (P8)-(iii).

Below we will consider two subcases depending on whether \( X \) is simplicial in \( F \).

**Case 2-1 (analogue to case 1-2-1).** If \( X \) is simplicial in \( F \), then \( \text{adj}(X, F) \) is a clique in \( F \). Recall that (P9) says that \( \text{adj}(X, \mathcal{U}_a) \cap ch(X, \mathcal{C}^*) \neq \emptyset \) for all \( a \in A \), we have \( \text{adj}(X, F) \cap ch(X, \mathcal{C}^*) \neq \emptyset \) based on the definition of \( F \).

If there is a \( c \in \text{adj}(X, F) \cap ch(X, \mathcal{C}^*) \) which is simplicial in \( F \), then \( c \in V(W) \) based on (P11), (P12) and (P13). Since \( \mathcal{C}^* \) is a chain graph and \( W \) is an induced subgraph of some chain component in \( \mathcal{C}^* \), \( X \to V(W) \) in \( \mathcal{C}^* \). That is, \( V(W) \subseteq ch(X, \mathcal{C}^*) \cap \text{adj}(X, F) \). As \( X \) is simplicial, \( V(W) \) is a clique in \( F \).

(i) \( \text{adj}(X, F) = V(W) \). If there is an \( a \in A \subseteq V(W) \) such that \( pa(a, \mathcal{C}^*) \setminus \{X\} \neq \emptyset \), then the vertices in \( pa(a, \mathcal{C}^*) \setminus \{X\} \) are adjacent to \( X \), since \( a \) is simplicial in \( F \) and \( pa(a, \mathcal{C}^*) \subseteq V(\mathcal{U}_a) \subseteq V(F) \). This is contradicted to \( \text{adj}(X, F) = V(W) \), and thus, \( pa(a, \mathcal{C}^*) = \{X\} \). Since \( pa(w, \mathcal{C}^*) = pa(w', \mathcal{C}^*) \) for any \( w, w' \in V(W) \), we have \( pa(V(W), \mathcal{C}^*) = \{X\} \). It can be shown by (P12) and (P13) that the induced subgraph of \( G^* \) over \( \{X\} \cup V(W) \) is an orientation component for \( X \) with respect to \( K_u \cup K_r \) and \( G^* \), thus \( V(W) \to X \) are in \( H \), which is contradicted to the assumption that \( V(W) \subseteq ch(X, \mathcal{C}^*) \subseteq ch(X, H) \cup \text{sib}(X, H) \setminus S \).

(ii) \( \text{adj}(X, F) \setminus V(W) = pa(X, \mathcal{C}^*) \). We claim that the restriction subset of \( K \cup D_X \) on \( G^*(M_T) \) given \( G^* \) is not consistent with \( G^*(M_T) \) for any \( M_T \) containing \( T \cup V(W) \). In fact, every vertex in \( T \cup V(W) = \{X\} \cup pa(X, \mathcal{C}^*) \subseteq V(W) \) is the tail of some DCC in the restriction subset of \( K \cup D_X \) on \( G^*(T \cup V(W)) \) given \( G^* \), because (1) \( pa(X, \mathcal{C}^*) \to X \) and \( X \to V(W) \) are in the restriction subset of \( D_X \) on \( G^*(T \cup V(W)) \) given \( G^* \), (2) every vertex in \( V(W) \setminus A \) is the tail of some DCC in the restriction subset of \( K_u \) on \( G^*(T \cup V(W)) \) given \( G^* \) according to (P12), and (3) every vertex in \( A \) is the tail of some DCC in the restriction subset of \( K_r \) on \( G^*(T \cup V(W)) \) given \( G^* \) according to (P13) and (P8).

(iii) \( \text{adj}(X, F) \setminus V(W) \subseteq pa(X, \mathcal{C}^*) \). Let \( p \in pa(X, \mathcal{C}^*) \) such that \( p \notin \text{adj}(X, F) \). It is clear that none of the vertices in \( V(W) \) is adjacent to \( p \), since otherwise, \( p \to V(W) \) are in \( \mathcal{C}^* \), and in particular, \( p \to A \) are in \( \mathcal{C}^* \) and \( p \) should be included in \( F \). By the similar argument for proving case 1-2-1 we can show that the induced subgraph of \( G^* \) over \( \{p, X\} \cup \text{adj}(X, F) \) is an orientation component for \( p \) with respect to \( K_u \cup K_r \). In fact, (1) \( p \) is simplicial in the induced subgraph of \( G^* \) over \( \{p, X\} \cup \text{adj}(X, F) \) since \( p \) is adjacent to the vertices in \( \{X\} \cup \text{adj}(X, F) \setminus V(W) \) and \( \{X\} \cup \text{adj}(X, F) \) is a clique, (2) every vertex in \( \{X\} \cup \text{adj}(X, F) \setminus V(W) \) is non-simplicial in the induced subgraph of \( G^* \) over \( \{p, X\} \cup \text{adj}(X, F) \) since \( p \) is not adjacent to any \( w \in V(W) \) but both \( p \) and \( w \) are neighbors of the vertices in \( \{X\} \cup \text{adj}(X, F) \setminus V(W) \), (3) every vertex in \( V(W) \setminus A \) is the tail of some DCC in \( K_u(W \cup G^*) \), and (4) \( V(W) \cup pa(a, \mathcal{C}^*) \subseteq \{p, X\} \cup \text{adj}(X, F) \) for every \( a \in A \) (since the simplicity of \( a \) in \( F \) implies that \( pa(a, F) \subseteq \text{adj}(X, F) \)) and (P8) implies that every \( a \in A \) is the tail of some DCC in the restriction subset of \( K_r \) on \( G^*(\{p, X\} \cup \text{adj}(X, F)) \) given \( G^* \). Therefore, \( X \to p \) is in \( H \), which leads to a contradiction.

(iv) \( \text{adj}(X, F) \cap ch(X, \mathcal{C}^*) \setminus V(W) \neq \emptyset \). Let \( c \in \text{adj}(X, F) \setminus V(W) \) such that \( c \in ch(X, \mathcal{C}^*) \). It is clear that \( c \in N \), and consequently, \( c \) is not simplicial in \( F \) by (P11). This indicates
that $\mathcal{F}$ is not complete, and thus, there is a simplicial vertex $w$ in $\mathcal{F}$ which is not adjacent to $X$. However, this is impossible since every simplicial vertex in $\mathcal{F}$ should be in $\mathcal{F} \setminus \mathcal{N} \subseteq V(W) \cup pa(X, \mathcal{C}^*) \cup \{X\}$, which is either $X$ or adjacent to $X$.

Now assume that none of the vertices in $adj(X, \mathcal{F}) \cap ch(X, \mathcal{C}^*)$ is simplicial in $\mathcal{F}$. Denote by $R$ (possibly empty) the set of simplicial vertices in $\mathcal{F}$ which are adjacent to $X$. Following the same argument for proving (P6), we can show that the induced subgraph of $\mathcal{F}$ over $\mathcal{F} \setminus R$ is an orientation component for $X$ with respect to $\mathcal{K}_u \cup \mathcal{K}_r$ and $\mathcal{G}^*$. Hence, $adj(X, \mathcal{F}) \cap ch(X, \mathcal{C}^*) \rightarrow X$ are in $\mathcal{H}$, which leads to a contradiction.

Case 2-2 (analogue to case 1-2-2). Suppose that $X$ is not simplicial in $\mathcal{F}$. Denote by $L$ the set of potential leaf nodes in $\mathcal{F}$ with respect to $\mathcal{K}_u \cup \mathcal{K}_r$ and $\mathcal{G}^*$. Since $\mathcal{K}_u \cup \mathcal{K}_r$ is consistent with $\mathcal{G}^*$, $L \neq \emptyset$. Based on (P11), (P12), (P13) and the definition of potential leaf node, $L \subseteq \{X\} \cup pa(X, \mathcal{C}^*)$. Moreover, since $X$ is not simplicial in $\mathcal{F}$, $L \subseteq pa(X, \mathcal{C}^*)$. Therefore, there is a $\phi \in adj(X, \mathcal{F}) \cap pa(X, \mathcal{C}^*)$ which is a potential leaf node in $\mathcal{F}$ with respect to $\mathcal{K}_u \cup \mathcal{K}_r$. Denote by $R$ (possibly empty) the set of simplicial vertices in $\mathcal{F}$ which are adjacent to $\phi$. Following the same proof for case 1-2-2, it can be checked that the induced subgraph of $\mathcal{F}$ over $\mathcal{F} \setminus R$ is an orientation component for $\phi$ with respect to $\mathcal{K}_u \cup \mathcal{K}_r$ and $\mathcal{G}^*$. Hence, $X \rightarrow \phi$ is in $\mathcal{H}$, which leads to a contradiction.

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