Effect Identification in Cluster Causal Diagrams

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Abstract

One pervasive task found throughout the empirical sciences is to determine the effect of interventions from non-experimental data. It is well-understood that assumptions are necessary to perform causal inferences, which are commonly articulated through causal diagrams (Pearl, 2000). Despite the power of this approach, there are settings where the knowledge necessary to specify a causal diagram over all observed variables may not be available, particularly in complex, high-dimensional domains. In this paper, we introduce a new type of graphical model called cluster causal diagrams (for short, C-DAGs) that allows for the partial specification of relationships among variables based on limited prior knowledge, alleviating the stringent requirement of specifying a full causal diagram. A C-DAG specifies relationships between clusters of variables, while the relationships between the variables within a cluster are left unspecified. We develop the foundations and machinery for valid causal inferences over C-DAGs. In particular, we first define a new version of the d-separation criterion and prove its soundness and completeness. Secondly, we extend these new separation rules and prove the validity of the corresponding do-calculus. Lastly, we show that a standard identification algorithm is sound and complete to systematically compute causal effects from observational data given a C-DAG.

1. Introduction

One of the central tasks found in data-driven disciplines is to infer cause and effect relationships using observational (non-experimental) data collected from the phenomenon under investigation. These relations are considered essential in the construction of explanations and for making decisions about interventions that have never been implemented (Pearl, 2000; Spirtes et al., 2000; Bareinboim & Pearl, 2016; Peters et al., 2017; Pearl & Mackenzie, 2018). However, there are still practical challenges that limit the applicability of causal theory and tools. Many of them stem from the fact that causal inferences require prior knowledge about the underlying data generating mechanisms (Pearl, 2000), which in many real world settings are not fully understood.

Standard tools for causal analysis and effect identification such as d-separation, do-calculus, and the ID-algorithm require qualitative knowledge about the causal and confounding relationships among observed variables. Such knowledge is typically articulated through the language of graphical models in what is known as a causal diagram (e.g., see Fig. 1(a)). Intuitively, a causal diagram $G$ has a directed edge from $X$ to $Y$ if $Y$ “listens” to the value of $X$; in terms of the underlying causal system, $X$ appears as an argument of the mechanism of $Y$. The importance of this notion has been emphasized in the literature by Pearl: “This listening metaphor encapsulates the entire knowledge that a causal network conveys; the rest can be derived, sometimes by leveraging data” (Pearl & Mackenzie, 2018, p. 129).

Once the causal diagram is fully articulated based on domain knowledge, the empirical researcher can use standard causal inference tools to infer the effect of a treatment $X$ on an outcome $Y$, which is formally written as the interventional distribution $P(Y|do(X = x))$. Determining whether the do-distribution is inferable from the combination of the causal diagram $G$ and the observational distribution $P(V)$, where $V$ represents the set of observed variables, is known as the identification problem. This problem has been extensively studied in the literature and a number of conditions have been proposed. These include symbolic methods such as Pearl’s celebrated do-calculus (Pearl, 1995) as well as algorithmic strategies (Galles & Pearl, 1995; Tian & Pearl, 2002; Spirtes & Pearl, 2006; Huang & Valtorta, 2006; Lee et al., 2019), to cite a few.

Despite the power of such approaches, limited scientific knowledge may hinder the full specification of causal diagrams, especially in complex, high-dimensional settings.
Electronic health records, for example, include data on lab tests, drugs, demographic information, and other clinical attributes, but medical knowledge is not yet advanced enough to lead to the construction of causal diagrams amongst all of these variables, limiting use of the graphical approach to inferring causality (Kleinberg & Hripcsak, 2011).

In many cases, however, contextual or temporal information about variables is available, which may partially inform how these variables are situated in a causal diagram relative to other key variables. Consider, for example, the causal diagram in Fig. 1(a) illustrating the mechanisms behind the effect of lisinopril (X), a treatment for hypertension, on the outcome of having a stroke (Y). Researchers may know that variables like age (A), blood pressure (B), comorbidities (C), medication history (D), and sleep quality (S) temporally before lisinopril is prescribed or a stroke occurs. They may even suspect that some of these pretreatment (or cluster) variables in some way, as X variables are causes of C comorbidities (may know that variables like age (A), blood pressure (B), comorbidities (C) mediate the effect of lisinopril (D) shown in Fig. 1(a)).

In this paper, our goal is to develop a framework for identification of causal effects in partially understood domains such as the above example. By and large, we will focus on formalizing the problem of causal effect identification considering that the researcher does not have prior knowledge to specify the full causal diagram or causal relationships over all variables, but does have prior knowledge to partially specify causal relationships between variables in different clusters or groups. First, we formally define and characterize a novel class of graphs called cluster causal diagram (or C-DAG, for short), which will allow for encoding of partially understood causal relationships between abstracted clusters, representing a group of variables among which causal relationships are not understood or specified. Within a cluster, any relationships between variables are possible, so a C-DAG represents an equivalence class of causal diagrams compatible with the knowledge available. Then, we develop the foundations and machinery for valid causal inference, akin to Pearl’s d-separation and do-calculus for when such a coarser graphical representation of the system is provided based on the limited prior knowledge available. These are fundamental first steps in terms of causal semantics and graphical conditions to perform causal inferences over clusters of variables. The new proposed semantics provide the basis for the development of more practical and relaxed causal inferences and learning tools.

Specifically, we outline our technical contributions below.

1. We introduce a new class of graphs called cluster causal diagrams (or C-DAGs) over a set of clusters of variables where the relationships amongst the variables inside the clusters are left unspecified (Definition 3.1). We show that despite C-DAGs’ abstracted representation of possibly numerous underlying paths, separation rules can be developed to account for the clusters. We prove the soundness and completeness of the d-separation rules extended to C-DAGs (Theorem 4.6).

2. We prove that the inference rules known as Pearl’s do-calculus are sound and complete for the coarse representation of C-DAGs (Theorems 5.1 and 5.3).

3. We prove that interventional distributions admit a convenient factorization following the C-DAG’s structure (Theorem 5.4). This factorization can be used to show that the ID-algorithm is sound and complete to systematically infer causal effects from the combination of an observational distribution and partial domain knowledge encoded as a C-DAG (Theorem 5.5).

1.1. Related work

Since a group of variables may constitute a semantically meaningful entity, causal models over abstracted clusters of variables have attracted increasing attention for the development of more interpretable tools (Schölkopf et al., 2021). Recent developments on causal abstraction have focused on the distinct problem of investigating functions that map a cluster of (micro-) variables to a single (macro-) variable, while preserving some causal properties (Chalupka et al., 2015; 2016; Rubenstein et al., 2017; Beckers & Halpern, 2019). The result is a new structural causal model defined
on a higher level of abstraction, but with causal properties similar to those in the low-level model. By contrast, our work proposes a new graphical representation of a class of compatible causal diagrams, representing limited causal knowledge when the full structural causal model is unknown.

Algorithms for causal discovery from observational data can be an alternative for when background knowledge is not sufficient to fully delineate a causal diagram (Pearl, 2000; Spirtes et al., 2000; Peters et al., 2017). In general, it is not possible to fully recover the causal diagram based solely on observational data, without making strong assumptions about the underlying causal model, including causal sufficiency (all relevant variables have been measured), the form of the functions (e.g., linearity, additive noise), and the distributions of the error terms (e.g. Gaussian, non-Gaussian, etc) (Glymour et al., 2019). Then, there are cases where a meaningful causal diagram cannot be learned and background knowledge is necessary for its construction. Our work focuses on establishing a language and corresponding machinery to encode partial causal knowledge and infer causal effects over clusters, alleviating some challenges in causal modeling in high-dimensional settings.

2. Preliminaries

We introduce in this section the necessary concepts and notation used throughout the paper.

Notation. A single variable is denoted by a (non-boldface) uppercase letter $X$ and its realized value by a small letter $x$. A boldfaced uppercase letter $X$ denotes a set (or a cluster) of variables. We use kinship terminology (e.g., parents, children, descendants, ancestors) to denote various relationships in a graph $G$. These kinship relations are defined along the full edges in the graph, ignoring bidirected edges. We use $Pa(X)_{G}$, $An(X)_{G}$, and $De(X)_{G}$ to represent the sets of parents, ancestors, and descendants in $G$, respectively. A vertex $V$ is said to be active on a path relative to a set $Z$ if 1) $V$ is collider and $V$ or any of its descendants are in $Z$ or 2) $V$ is a non-collider and is not in $Z$. A path $p$ is said to be active given (or conditioned on) $Z$ if every vertex on $p$ is active relative to $Z$. Otherwise, $p$ is said to be inactive. Given a graph $G$, $X$ and $Y$ are d-separated by $Z$ if every path between $X$ and $Y$ is inactive given $Z$. We denote this d-separation by $(X \perp Y \mid Z)_{G}$. The mutilated graph $G_{\overline{X}}$ is the result of removing from $G$ edges coming into variables in $X$ and going out of variables in $Z$.

Structural Causal Models. We use the language of Structural Causal Models (SCMs) (Pearl, 2000, pp. 204-207) as our semantical framework. Formally, an SCM $M$ is a 4-tuple $(U, V, F, P(U))$, where $U$ is a set of exogenous (latent) variables and $V$ is a set of endogenous (measured) variables. $F$ is a collection of functions $\{f_{i}\}_{i=1}^{V}$ such that each endogenous variable $V_{i} \in V$ is determined by a function $f_{i} \in F$, where $f_{i}$ is a mapping from the respective domain of $U_{i} \cup Pa(V_{i})$ to $V_{i}$, where $U_{i} \subseteq U$ and $Pa(V_{i}) \subseteq V \setminus V_{i}$. The uncertainty is encoded through a probability distribution over the exogenous variables, $P(U)$. Each SCM $M$ induces a directed acyclic graph (DAG) $G(V, E)$ with bidirected edges, known as a causal diagram, that encodes the structural relations among $V \cup U$, where every $V_{i} \in V$ is a vertex, there is a directed edge $(V_{j} \rightarrow V_{i})$ for every $V_{i} \in V$ and $V_{j} \in Pa(V_{i})$, and there is a dashed bidirected edge $(V_{j} \leftrightarrow V_{i})$ for every pair $V_{i}, V_{j} \in V$ such that $U_{i} \cap U_{j} \neq \emptyset$ ($V_{i}$ and $V_{j}$ have a common exogenous parent). Performing an action $X=x$ is represented through the do-operator, $do(X=x)$, which represents the operation of fixing a set $X$ to a constant $x$ regardless of their original mechanisms. Such an intervention induces a submodel $M_{x}$, which is $M$ with $f_{X}$ replaced to $x$ for every $X \in X$. The post-interventional distribution induced by $M_{x}$ is denoted by $P(V \setminus x|do(x))$.

3. C-DAGs: Definitions and Properties

We now formally introduce cluster causal diagrams, which define a coarser graphical representation of an SCM where variables are grouped as entities called clusters. In this definition, every variable is a part of exactly one cluster, where a variable may be "grouped" in a cluster by itself and all vertices in a C-DAG are clusters.

Definition 3.1 (Cluster Causal Diagram or C-DAG). Consider an SCM $M = (V, U, F, P(U))$ and the corresponding causal diagram $G(V, E)$. Given a partition $C = \{C_{1}, \ldots, C_{k}\}$ of $V$, construct a graph $G_{C}(C, E_{C})$ over $C$ with a set of edges $E_{C}$ defined as follows:

1. An edge $C_{i} \rightarrow C_{j}$ is in $E_{C}$ if there exists some $V_{i} \in C_{i}$ and $V_{j} \in C_{j}$ such that $V_{i} \in Pa(V_{j})$;
2. A dashed bidirected edge $C_{i} \leftrightarrow C_{j}$ is in $E_{C}$ if there exists some $V_{i} \in C_{i}$ and $V_{j} \in C_{j}$ such that there is a bidirected edge $V_{i} \leftrightarrow V_{j}$.

If $G_{C}(C, E_{C})$ contains no cycles, then we say that $C$ is an admissible partition of $V$. We then call $G_{C}$ a cluster causal diagram, or C-DAG, compatible with $G$.

Throughout the paper, we will use the same symbol (e.g. $C_{i}$) to represent both a cluster node in a C-DAG, $G_{C}$, and the set of variables contained in the cluster in a compatible causal diagram, $G$.

Interestingly, a causal diagram is a C-DAG where each variable forms its own cluster, which means that all clusters are of size one. As discussed, in practice, all such relationships may be unknown or burdensome to explicitly define, as is common in fields like medicine and the social sciences.
Revisiting the medical example discussed earlier, Fig. 1(a) illustrates a possible causal diagram modeling the effect of lisinopril \((X)\) on the outcome of having a stroke \((Y)\). As proposed, if not all the relationships specified in Fig. 1(a) are known, researchers cannot construct a full causal diagram, but may still have enough knowledge to create a C-DAG given the partial knowledge that the covariates occur temporally before lisinopril is prescribed or a stroke occurs and the suspicion that some of the pre-treatment variables are causes of \(X\) and \(Y\). Specifically, we can create the cluster \(Z = \{A, B, C, D\}\) with all the covariates and then construct a C-DAG with edges \(Z \rightarrow X\) and \(Z \rightarrow Y\). Further, the researchers may also suspect that some of the variables in \(Z\) are confounded with \(X\) and others with \(Y\), an uncertainty that is encoded in the C-DAG through the bidirected edges \(Z \leftrightarrow X\) and \(Z \leftrightarrow Y\). With the additional knowledge that sleep quality \((S)\) is measured after the treatment is applied (i.e., post-treatment), and acts as a mediator between the treatment and outcome, the C-DAG in Fig. 1(b) can be constructed.

Following Pearl’s construction of an edge being drawn from one variable \(X\) to another \(Y\) in a causal diagram if \(Y\) “listens” to the value of \(X\), intuitively, the edges are drawn from one cluster \(X\) to another \(Y\) in a C-DAG if at least one variable in \(Y\) “listens” to the value of at least one variable in \(X\). Consider again the causal diagram \(G\) in Fig. 1(a) over the set of observables \(V = \{X, Y, A, B, C, D, S\}\). As previously discussed, a C-DAG over the partition \(C = \{\{X\}, \{Y\}, \{Z\}, \{S\}\}\), where \(Z = \{A, B, C, D\}\), is shown in Fig. 1(b). A different partition \(C' = \{\{X\}, \{Y\}, \{Z\}, \{D, W\}\}\) with \(W = \{S, B\}\) and \(Z = \{A, C\}\) leads to the C-DAG shown in Fig. 1(c). Note that both \(G_{C_2}\) and \(G_{C_3}\) are considered valid C-DAGs because no cycles are created. Alternatively, if we consider partition \(C'' = \{\{X\}, \{Y\}, \{Z\}, \{W\}\}\), where \(W = \{S, B\}\) and \(Z = \{A, C\}\), this would lead to the graph shown in Fig. 1(d). The edge \(X \rightarrow W\) is present since \(S \in W\) is a function of \(i.e., \) listen to \(X\); the edge \(X \rightarrow Z\) is present because \(C \in Z\) listens to \(B \in W\); the edge \(Z \rightarrow X\) is present since \(X\) listens to \(D \in Z\). These edges together create a cycle, therefore \(G_{C''}\) is not a valid C-DAG.

A C-DAG can be seen as an equivalence class of causal diagrams, and represents a collection of causal diagrams that share the relationships among the clusters while allowing for any possible relationships among the variables within each cluster. For instance, the two causal diagrams \(G_1\) in Fig. 2(a) and \(G_2\) in (b) can be represented by the C-DAG \(G_{C_1}\) in (c), and can therefore be thought of as being members of the equivalence class represented by \(G_{C_1}\). Note that a seemingly active path in a C-DAG (e.g., \(X \leftrightarrow Z \rightarrow Y\) in \(G_{C_1}\)) does not necessarily correspond to an active path in a compatible causal diagram. We consider the case of backdoor paths, i.e., paths between \(X\) and \(Y\) with an arrowhead into \(X\). All such paths are active in \(G_{C_2}\), but the only backdoor path, \(X \leftarrow Z_1 \rightarrow Z_2 \leftarrow Z_3 \rightarrow Y\), in \(G_{C_1}\) is inactive. This property of C-DAGs prevents us from saying that a d-connection in a C-DAG corresponds to a d-connection in all compatible causal diagrams in the equivalence class. On the other hand, we show in the next section a pleasant and surprising result (Theorem 4.6) that d-separations in a C-DAG do hold in all compatible causal diagrams. This powerful result is indeed critical to deriving causal inference rules and algorithms that are applicable to all the causal diagrams compatible with a given C-DAG (Theorems 5.1-5.5) regardless of the unknown relationships within each cluster.

The criteria set forth in Def. 3.1 ensure that a C-DAG, \(G_{C}\), has two properties that will prove critical later on. Namely, they preserve adjacencies, and preserve directed paths in any compatible causal diagram, \(G\), as stated below. Given space constraints, all proofs are provided in Appendix. 3.

**Proposition 3.2. (Preservation of adjacencies)** Let \(G_{C}(C, E_{C})\) be a C-DAG compatible with a causal diagram \(G(V, E)\). Consider distinct clusters \(C_i, C_j \in C\). If \(V_i, V_j \in V\) are adjacent in \(G\) and belong to \(C_i, C_j\) respectively, then \(C_i\) and \(C_j\) are adjacent in \(G_{C}\). Further, if \(C_i\) and \(C_j\) are adjacent in \(G_{C}\), then there exists \(V_i \in C_i\) and \(V_j \in C_j\) such that \(V_i\) and \(V_j\) are adjacent in \(G\).

**Proposition 3.3. (Preservation of directed paths)** Let \(G_{C}(C, E_{C})\) be a C-DAG compatible with a causal diagram \(G(V, E)\) and \(C_i, C_j \in C\) be two distinct clusters. If two variables \(V_i \in C_i\) and \(V_j \in C_j\) are connected in \(G\) by a directed path from \(V_i\) to \(V_j\), then the clusters \(C_i\) and \(C_j\) are connected by a directed path from \(C_i\) to \(C_j\) in \(G_{C}\).

Proposition 3.2 states that any adjacency between variables is preserved in a compatible C-DAG. Proposition 3.3 states that connections via directed paths are preserved, implying that order and ancestral relationships are preserved. These results will prove helpful in extending causal inference tools to C-DAGs, including d-separation and do-calculus.
4. D-Separation in C-DAGs

D-separation is a central result that allows inferences with causal diagrams, which has been used in the context of probabilistic (Pearl, 1988) and causal reasoning (Pearl, 1995). In this section, we investigate extending d-separation rules to C-DAGs. In a causal diagram $G$, whenever sets $X$ and $Y$ are d-separated by a set $Z$, $X$ is independent of $Y$ given $Z$ in the distribution $P(V)$. This establishes a link between the causal assumptions encoded in the graph (in the form of missing edges) and the observed data. Since a C-DAG represents a class of compatible causal diagrams, we must make sure that a d-separation statement in a C-DAG must hold in all the compatible causal diagrams.

Let $X$, $Y$, $Z$ be clusters in the C-DAG $G_C$. Let the symbol $*$ represent either an arrow head or tail. Let $p$ be a path in $G_C$ between $X$ and $Y$ that goes only through $Z$. We say that $p$ is inactive in $G_C$ if in all causal diagrams $G$ compatible with $G_C$, all corresponding paths are inactive according to the d-separation rules. Note that if $p$ is in the form $X \leftarrow Z \rightarrow Y$ (i.e., $Z$ is a non-collider), then the corresponding paths in $G$ are those between $X$ and $Y$ going only through variables in $Z$ and containing the edge $Z \rightarrow Y$ for some $Z \in Z$ and some $Y \in Y$. Alternatively, if $p$ is in the form $X \leftarrow Z \rightarrow Y$ (i.e., $Z$ is a collider), then the corresponding paths in $G$ are those between $X$ and $Y$ going only through variables in $Z$ and containing the edge $X \rightarrow Z$ for some $X \in X$ and some $Z \in Z$ and the edge $Z \rightarrow Y$ for some $Z' \in Z$ and some $Y \in Y$.

We say $p$ is either active or inactive if in some compatible causal diagram $G$ all the paths between $X$ and $Y$ going through only variables in $Z$ are inactive, while in some compatible causal diagram $G$ there exists at least one active path between $X$ and $Y$ going through only variables in $Z$.

Next, we study the separation rules under two possible scenarios for $Z$, as a non-collider, or as a collider or a descendant of a collider.

Cluster as a Non-Collider (Chains & Forks)

Consider a C-DAG where $Z$ is a non-collider between $X$ and $Y$ as shown in Fig. 3(a) and (d).

The causal diagrams (b) and (c) in Fig. 3, over $V = \{X, Z_1, Z_2, Z_3, Y\}$, are compatible with the C-DAG in Fig. 3(a), where $X = \{X\}$, $Z = \{Z_1, Z_2, Z_3\}$, and $Y = \{Y\}$. Note that in diagram (b) the path between $X$ and $Y$ is active when $Z$ is not conditioned on. However, in diagram (c), the path between $X$ and $Y$ is inactive, even though the abstracted cluster $Z$ is a non-collider.

Similarly, in Fig. 3, the causal diagrams (e) and (f) over $V = \{X, Z_1, Z_2, Z_3, Y\}$ are compatible with the C-DAG $G_C$ in (d), where $X = \{X\}$, $Z = \{Z_1, Z_2, Z_3\}$, and $Y = \{Y\}$. In diagram (e), the path is active while in diagram (f) the path is inactive when $Z$ is not conditioned on.

From these examples, it is clear that when a cluster $Z$ acts as a non-collider between two other clusters $X$ and $Y$, the path between $X$ and $Y$ through $Z$ may be either active or inactive.

**Remark 4.1.** In a C-DAG, the path $X \leftrightarrow Z \rightarrow Y$ may be either active or inactive when $Z$ is not conditioned on.

Conditioning on a cluster will be considered as equivalent to conditioning on all the variables in it. In all diagrams (b), (c), (e) and (f), the path between $X$ and $Y$ is inactive when conditioning on $\{Z_1, Z_2, Z_3\}$ and we show that this property will hold regardless of the connections within a cluster as stated in the following lemma.

**Lemma 4.2.** In a C-DAG, the path $X \leftrightarrow Z \rightarrow Y$ is inactive when non-collider $Z$ is conditioned on.

Cluster as a Collider or a Descendant of a Collider

Consider a C-DAG where $Z$ is a collider between $X$ and $Y$ as shown in Fig. 3(g), or a descendant of a collider $W$ between $X$ and $Y$ as shown in Fig. 3(j).

The causal diagrams (h) and (i) in Fig. 3 over $V = \{X, Z_1, Z_2, Z_3, Y\}$ are compatible with the C-DAG in Fig. 3(g), where $X = \{X\}$, $Z = \{Z_1, Z_2, Z_3\}$, and $Y = \{Y\}$. The path between $X$ and $Y$ is active when conditioning on $\{Z_1, Z_2, Z_3\}$ in diagram (h), but it is inactive in diagram (i).

Similarly, the causal diagrams (k) and (l) in Fig. 3 over $V = \{X, W_1, W_2, Z_1, Z_2, Y\}$ are compatible with the C-DAG in Fig. 3(j), where $X = \{X\}$, $Z = \{Z_1, Z_2\}$, $W = \{W_1, W_2\}$, and $Y = \{Y\}$. In diagram (k), the path from $X$ and $Y$ is active when conditioning on $\{Z_1, Z_2\}$, while in diagram (l) the path is inactive when conditioning on $\{Z_1, Z_2\}$.

These examples illustrate that when a cluster $Z$ acts as a collider or a descendant of a collider between two other clusters $X$ and $Y$, the path between $X$ and $Y$ through $Z$ may be either active or inactive when conditioning on $Z$.

**Remark 4.3.** In a C-DAG, the path $X \leftrightarrow Z \leftrightarrow Y$ may be either active or inactive when $Z$ or some descendant of $Z$ is conditioned on.

Note that the path between $X$ and $Y$ is inactive in all diagrams (h), (i), (k), and (l). We show this property holds in general regardless of the connections within a cluster as stated in the following lemma.

**Lemma 4.4.** In a C-DAG, the path $X \leftrightarrow Z \leftrightarrow Y$ is inactive when none of the descendants of $Z$ (nor $Z$) are conditioned on.
The following result states the soundness and completeness when a path between two clusters is not d-separated in C-DAGs.

The above discussion and lemmas illustrate how the original d-separation rules relate to C-DAGs. In other words, when a path between two clusters is not d-separated in C-DAGs, the path between corresponding variables may or may not be active in a compatible causal diagram. These observations together lead to the following definition:

**Definition 4.5 (d-Separation in C-DAGs).** A path \( p \) in a C-DAG \( G_C \) is said to be d-separated (or blocked) by a set of clusters \( Z \subset C \) if and only if \( p \) contains

1. a triplet \( C_i \leftarrow \cdots \leftarrow C_m \rightarrow C_j \) such that the non-collider cluster \( C_m \) is in \( Z \), or
2. a triplet \( C_i \leftarrow \cdots \leftarrow C_m \leftarrow \cdots \leftarrow C_j \) such that neither the collider cluster \( C_m \) nor any of its descendants is in \( Z \).

A set of clusters \( Z \) is said to d-separate two sets of clusters \( X, Y \subset C \), denoted by \( (X \perp\!
\!
\!\!\!\perp Y \mid Z)_{G_C} \), if and only if \( Z \) blocks every path from a cluster in \( X \) to a cluster in \( Y \).

The following result states the soundness and completeness of the d-separation rules in C-DAGs. In other words, whenever a d-separation holds in a C-DAG according to these rules, it holds for all causal diagrams compatible with it. Moreover, whenever a d-separation does not hold in a C-DAG, it means that there exists at least one causal diagram compatible with it for which the same d-separation statement does not hold.

**Theorem 4.6. (Soundness and completeness of d-separation).** Consider a C-DAG \( G_C \), and let \( X, Z, Y \subset C \). If \( X \) and \( Y \) are d-separated by \( Z \) in \( G_C \), then, in any causal diagram \( G \) compatible with \( G_C \), \( X \) and \( Y \) are d-separated by \( Z \) in \( G \), that is,

\[
(X \perp\!
\!
\!\!\!\perp Y \mid Z)_{G_C} \implies (X \perp\!
\!
\!\!\!\perp Y \mid Z)_G.
\] (1)

If \( X \) and \( Y \) are not d-separated by \( Z \) in \( G_C \), then, there exists a causal diagram \( G \) compatible with \( G_C \) where \( X \) and \( Y \) are not d-separated by \( Z \) in \( G \).

Naturally, operating over a C-DAG may be less informative than a fully specified causal diagram (due to the paths that may be either active or inactive in a compatible causal diagram), yet some strong statements about conditional independence relations can still be obtained from a C-DAG. From the understanding of d-separation in causal diagrams, we can see that the d-separation rules for clusters allow us to read off conditional independencies from an even broader set of distributions. While a d-separation between sets of variables \( X \) and \( Y \) given \( Z \) in a causal diagram, \( G \), implies that \( X \) is independent of \( Y \) conditional on \( Z \) in every distribution induced by \( G \), a d-separation between clusters \( X \) and \( Y \) given \( Z \) in a C-DAG \( G_C \) implies that \( X \) is independent of \( Y \) conditional on \( Z \) in every distribution compatible with any \( G \) compatible with \( G_C \). All in all, there is a natural tradeoff between how variables are clustered and the strength of the statements that can be made about a larger class of models.

### 5. Causal Identification in C-DAGs

The aforementioned d-separation criterion allows us to decide from a C-DAG \( G_C \) whether two sets of clusters \( X \)
and \( Y \) are d-separated given a third set \( Z \) in any compatible causal diagram \( G \). This will be essential to establishing conditions for causal identifiability in C-DAGs.

### 5.1. Do-Calculation in C-DAGs

A fundamental tool used in causal inference is Pearl's celebrated do-calculus (Pearl, 1995). The do-calculus has been used extensively for solving a variety of causal effect identification tasks. Armed with the understanding coming from the d-separation rules in C-DAGs, next we extend the do-calculus rules to C-DAGs.

**Theorem 5.1.** (Do-calculus in C-DAGs). Let \( G_C \) be a C-DAG compatible with a causal diagram \( G \) associated with an SCM \( M \). For any disjoint subsets of clusters \( X, Y, Z, W \subseteq C \), the following three rules hold:

**Rule 1:** \( P(y|do(x), z, w) = P(y|do(x), w) \)

if \( (Y \perp \!\!\!\perp Z|X, W)_{G_C} \)

**Rule 2:** \( P(y|do(x), do(z), w) = P(y|do(x), z, w) \)

if \( (Y \perp \!\!\!\perp Z|X, W)_{G_C} \)

**Rule 3:** \( P(y|do(x), do(z), w) = P(y|do(x), w) \)

if \( (Y \perp \!\!\!\perp Z|X, W)_{G_C} \)

where \( G_C \) is obtained from \( G_C \) by removing the edges into \( X \) and out of \( Z \), and \( Z(W) \) is the set of \( Z \)-clusters that are non-ancestors of any \( W \)-cluster in \( G_C \).

Note that in the above do-calculus rules, \( X, Y, Z, W \) represent sets of cluster nodes in \( G_C \) in the d-separation tests \( (Y \perp \!\!\!\perp Z|X, W)_{G_C} \), while in the distribution \( P(\cdot) \) statements, \( X, Y, Z, W \) represent the sets of variables contained in the corresponding sets of clusters.

Given the soundness and completeness of the d-separation rules in C-DAGs, the main question to be solved in order to show the soundness of do-calculus in C-DAGs is whether the mutilation operations in a C-DAG to create \( G_C \) and \( G_C \) carry over to the compatible causal diagrams. We obtain the following result toward this goal.

**Lemma 5.2.** If a C-DAG \( G_C \) is compatible with a causal diagram \( G \), then, for \( X, Z \subseteq C \), the mutilated C-DAG \( G_C \) is compatible with the mutilated causal diagram \( G_C \).

Theorem 5.1 then follows from Propositions 3.2 and 3.3, Theorem 4.6, and Lemma 5.2. In addition, we show that the do-calculus rules in C-DAGs are complete as follows:

**Theorem 5.3.** (Completeness of do-calculus). If a do-calculus rule does not apply in a C-DAG \( G_C \), then there exists a causal diagram \( G \) compatible with \( G_C \) for which it also does not apply.

Equipped with d-separation and do-calculus in C-DAGs, causal inference algorithms developed for a variety of tasks that rely on a known causal diagram can potentially be extended to C-DAGs (Bareinboim & Pearl, 2016). In this paper, we study the problem of identifying causal effects from observational data in C-DAGs.

### 5.2. ID-Algorithm

There exists a complete algorithm to determine whether \( P(y|do(x)) \) is identifiable from the combination of the causal diagram \( G \) and the observational distribution \( P(V) \) (Tian, 2002; Shpitser & Pearl, 2006; Huang & Valtorta, 2006). This identification algorithm, or ID-algorithm for short, is based on the factorization of the interventional distributions according to the graphical structure, known as the truncated factorization product, i.e.:

\[
P(v \setminus x|do(x)) = \sum_u P(u) \prod_{k: v_k \in \text{pa}_{v_k}, u_k} P(v_k|\text{pa}_{v_k}, u_k).
\]

We show that the truncated factorization holds in C-DAGs as well, in the following sense.

**Theorem 5.4.** (Truncated factorization in C-DAGs.) Let \( G_C \) be a C-DAG compatible with a causal diagram \( G \) associated with an SCM \( M = (U, V, F, P(U)) \). For any \( X \subseteq C \), the following holds:

\[
P(c \setminus x|do(x)) = \sum_u P(u) \prod_{k: C_k \in C \setminus X} P(c_k|\text{pa}_{C_k}, u_k'),
\]

where \( \text{pa}_{C_k} \) are the parents of \( C_k \) in \( G_C \) and \( U_k' \subseteq U \) such that, for any \( i, j \), \( U_i' \cap U_j' \neq \emptyset \) if and only if there is a bidirected edge \( (C_i, C_j) \) between \( C_i \) and \( C_j \) in \( G_C \).

In Eq. (3), \( X, C, C_k, \text{pa}_{C_k} \) are the sets of variables contained in the corresponding sets of clusters.

Theorem 5.4 shows that C-DAGs are Causal Bayesian Networks, where a cluster with \( N \) variables is treated as an \( N \)-dimensional random variable. This result allows us to prove that the ID-algorithm is sound and complete to systematically infer causal effects from the observational distribution \( P(V) \) and partial domain knowledge encoded as a C-DAG \( G_C \) (since ID relies on the truncated factorization).

**Theorem 5.5.** (Soundness and Completeness of ID-algorithm). The ID-algorithm is sound and complete when applied to a C-DAG \( G_C \) for identifying causal effects of the form \( P(y|do(x)) \) from the observational distribution \( P(V) \), where \( X \) and \( Y \) are sets of clusters in \( G_C \).

The ID algorithm returns a formula for identifiable \( P(y|do(x)) \) that is valid in all causal diagrams compatible
with the C-DAG $G_C$. The completeness result ensures that if the ID-algorithm fails to identify $P(y|do(x))$ from $G_C$, then there exists a causal diagram $G$ compatible with $G_C$ where the effect $P(y|do(x))$ is not identifiable.

### 5.3. Effect Identification in C-DAGs

We now use the aforementioned results and show examples of identification in C-DAGs in practice. Due to the coarsening of the diagram by clusters, it is possible an effect will be identifiable in some causal graph $G$, but will not be identifiable by the clustering yielding $G_C$.

#### Identification in Fig. 1.

In diagram (a) the effect of $X$ on $Y$ is identifiable through backdoor adjustment (Pearl, 2000, pp. 79-80) over the set of variables $\{B, D\}$. In the C-DAG in Fig. 1(b), with cluster $Z = \{A, B, C, D\}$, the effect of $X$ on $Y$ is identifiable through front-door adjustment (Pearl, 2000, p. 83) over $S$, given by $P(y|do(x)) = \sum_s \sum_{x'} P(y(x', s)|x') P(x')$. Because this front-door adjustment holds for the C-DAG in Fig. 1(b) with which diagram (a) is compatible, this front-door adjustment identification formula is equivalent to the adjustment in the case of diagram (a) and gives the correct causal effect in any other compatible causal diagram. In the C-DAG in (c), the loss of separations from the creation of clusters $Z = \{A, B, C, D\}$ and $W = \{B, S\}$ render the effect no longer identifiable, indicating that there exists another graph compatible with (c) for which the effect cannot be identified.

#### Identification in Fig. 4.

In diagram (a), the effect of $\{X_1, X_2\}$ on $\{Y_1, Y_2\}$ is identifiable by backdoor adjustment over $\{Z_1, Z_2\}$ as follows: $P(y_1, y_2|do(x_1, x_2)) = \sum_{z_1, z_2} P(y_1, y_2|x_1, x_2, z_1, z_2)P(z_1, z_2)$. Note, however, that the backdoor path cannot be blocked in the C-DAG $G_1$ (b) with clusters $X = \{X_1, X_2\}$, $Y = \{Y_1, Y_2\}$, and $Z = \{Z_1, Z_2\}$. In this case, the effect $P(y|do(x))$ is not identifiable. If the covariates $Z_1$ and $Z_2$ are not clustered together as shown in the C-DAG $G_{C_2}$ (c), the backdoor paths relative to $X$ and $Y$ can still be blocked despite the unobserved confounders between $Z_1$ and $X$ and between $Z_2$ and $Y$. So the effect $P(y|do(x))$ is identifiable by backdoor adjustment over $\{Z_1, Z_2\}$ as follows: $P(y|do(x)) = \sum_{x_1, x_2} P(y|x_1, z_1, z_2)P(z_1, z_2)$. If the treatments $X_1$ and $X_2$ are not clustered together as shown in the C-DAG $G_{C_2}$ (d), then the joint effect of $X_1$ and $X_2$ on the cluster $Y$ is identifiable and given by the following expression: $P(y|do(x_1, x_2)) = \sum_{x_1, x_2} P(y|x_1, x_2, z)P(x_1, z)$.

An additional example of identification of causal effects in C-DAGs with clustered treatments and outcomes is shown in Appendix ??.
We hope the new machinery for C-DAGs will allow researchers to represent complex systems in a simplified way, allowing for more relaxed causal inferences when substantive knowledge is largely unavailable and coarse.

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