Causal DAG Summarization

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ABSTRACT

Causal inference aids researchers in discovering cause-and-effect relationships, leading to scientific insights. Accurate causal estimation requires identifying confounding variables to avoid false discoveries. Pearl's causal model uses causal DAGs to identify confounding variables, but incorrect DAGs can lead to unreliable causal conclusions. However, for high dimensional data, the causal DAGs are often complex beyond human verifiability. Graph summarization is a logical next step, but current methods for general-purpose graph summarization are inadequate for causal DAG summarization. This paper addresses these challenges by proposing a causal graph summarization objective that balances graph simplification for better understanding while retaining essential causal information for reliable inference. We develop an efficient greedy algorithm and show that summary causal DAGs can be directly used for inference and are more robust to misspecification of assumptions, enhancing robustness for causal inference. Experimenting with six real-life datasets, we compared our algorithm to three existing solutions, showing its effectiveness in handling high-dimensional data and its ability to generate summary DAGs that ensure both reliable causal inference and robustness against misspecifications.

1 INTRODUCTION

Causal inference is central to informed decision-making in fields such as economics, sociology, and medicine, helping analysts unravel complex cause-effect relationships [30, 42, 99]. It has become increasingly critical in machine learning (ML), where it supports efforts to ensure algorithmic fairness [84], data debiasing and cleaning [111, 111, 112], improving explainable AI [11, 28, 60, 61], and enhancing robustness [52, 85, 96]. Moreover, causal inference is a major theme in recent data management research [13, 56, 57, 79, 83], and has been incorporated into various tasks including data discovery [27, 107], query result explanation [82, 106], data exploration [50], hypothetical reasoning [26], and large system diagnostics [7, 29, 35].

Drawing causal conclusions from data fundamentally hinges on access to background knowledge and assumptions, as data alone cannot establish causality [70, 81]. A principled way to encode such background knowledge is through Causal Directed Acyclic Graphs (DAGs)[70]. These graphs explicitly represent assumed causal relationships, enabling systematic reasoning about interventions. Causal DAGs can be used together with graphical criteria such as the backdoor criterion, frontdoor criterion, or in general, Pearl's *do*-calculus[70] to determine whether the effect of interventions can be answered using data and the available background knowledge. If so, they help identify the right set of confounding variables and causal pathways to control for, ensuring sound causal inference given the background knowledge.

However, the soundness and robustness of causal inferences hinges on the availability of high-quality causal DAGs, which are often not readily available. These DAGs are typically constructed using domain knowledge [16, 54, 100] or through causal discovery methods [20, 34, 89, 103, 113]. The elicitation process is costly, error-prone [65], and time-consuming. Causal discovery methods, while useful, are fundamentally restrictive as they identify a class of DAGs compatible with observed data rather than a singular, definitive model [34]. Moreover, existing discovery methods often do not perform well on real-world data and require significant human intervention for verification [21, 39, 92]. Handling high-dimensional data complicates the process, increasing the need for efficient methods to simplify and verify causal models while retaining essential information [67]. We illustrate this with an example:

Example 1. Consider the application of diagnosing system performance for a cloud-based data warehouse service. Specifically, consider a dataset collected from the monitoring views in Amazon Redshift Serverless [8]. This dataset includes performance metrics and query-extracted features such as the number of unique tables and columns. This data offers opportunities to answer crucial causal queries for optimizing performance. For example, understanding the impact of caching on latency (i.e., `Result Cache Hit` on `Elapsed Time`) can help tune caching mechanisms to reduce query times. Similarly, analyzing the effect of join complexity on the query planner's performance (i.e., `Num Joins` on `Plan Time`) can optimize query execution strategies. However, constructing the necessary causal DAGs to answer such questions requires a principled approach, as they are not readily available.

Figure 1 shows an example causal DAG among a set of variables from just one monitoring view [6] and a few query features, chosen for illustration. This is just a small part of the overall dataset, which is highly dimensional. To answer the above causal queries, `Query Template` is a critical confounder that must be adjusted for because it influences both the query performance metrics (e.g., `Elapsed Time`) and the caching mechanisms (e.g., `Result Cache Hit`). Failing to adjust for this can lead to biased estimations and incorrect conclusions. Hence, any misspecification in the causal DAG that does not identify this variable as a confounder can yield incorrect confounders and result in flawed inferences, making domain expert verification essential for each existing or missing edge. This task can be overwhelming, even in this small example with only 12 nodes, as it involves inspecting 66 potential edges, one per pair of nodes. In real-life applications, the number of variables can often be much higher. □

Graph summarization is a logical next step, as it reduces the number of nodes and edges, making it easier for users to verify and inspect causal DAGs in high-dimensional datasets. In this paper, we propose a graph summarization technique tailored for causal inference. It simplifies high-dimensional causal DAGs into manageable forms without compromising essential causal information, thereby improving interpretability. Using our technique, one can summarize an initial causal DAG (constructed using partial domain knowledge or causal discovery) for simpler verification and elicitation. Additionally, the summary causal DAG can be directly used for causal inference and is more robust to misspecification of assumptions. Our approach thereby improves *interpretability*, *verifiability*, and *robustness* in causal inference, facilitating the adoption of these techniques in practice.

Graph summarization has been extensively studied, with state-of-the-art methods designed to efficiently generate concise representations aimed at minimizing reconstruction errors [46, 105], or facilitating accurate query answering [51, 90]. However, we argue that while general-purpose methods are adept at managing massive graphs, they are inadequate for summarizing causal graphs, a task that demands the preservation of causal information crucial for reliable inference. Our approach introduces a causal DAG summarization objective, which balances simplifying the graph for enhanced comprehensibility and retaining essential causal information. We illustrate this with an example:

Example 2. Consider Fig. 2a, which shows the summary graph generated by SSumM [46] for the causal DAG of Fig. 1. SSumM is a top-performing general-purpose graph summarization method known for effectively balancing conciseness and accuracy. However, it exhibits cycles and self-loops, characteristics that are incompatible with causal inference, making it unsuitable for this purpose. For example, computing the causal effect of `Num Joins` on `Plan time` is impossible due to the bidirectional edge between their cluster nodes [1]. An in-depth comparison with another graph summarization method [97] is provided in Section 8. We show that although this method can be adapted to generate summary DAGs compatible with causal inference principles, it does not optimally preserve critical causal information, reducing the accuracy of the inference over the summary DAG.

In contrast, Fig.2b shows the 5-node summary DAG generated by our approach. Unlike the summary graph from SSumM, our summary DAG preserves critical causal information, offering a more interpretable summary that can be directly used for inference. This summary DAG makes it easier to verify the soundness of assumptions it encodes. Furthermore, using this summary DAG for inference is inherently more robust to misspecification. This is because our summarization process involves merging nodes, resulting in a summary DAG that is compatible with a set of possible DAGs. This summary DAG preserves robust information (that holds in all compatible DAGs) for answering causal queries. Using the summary DAG for confounder detection intuitively leads to a more conservative set of confounders to control for, as it may lead to adjusting for redundant attributes that do not hurt the analysis. Hence, if the original DAG missed an edge, our summarization

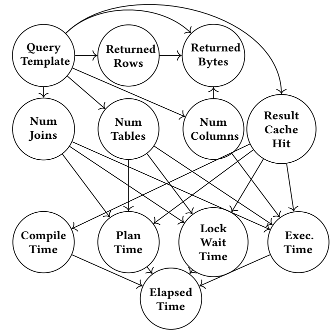
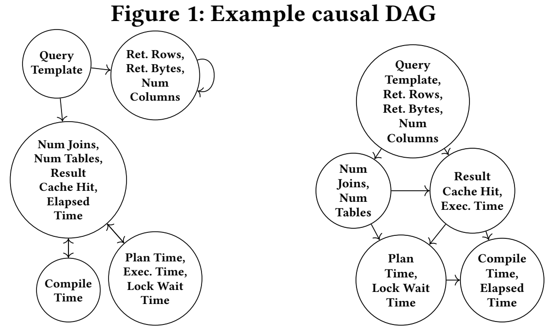


Figure 1: Example causal DAG



(a) A not useful Summary Graph (b) Our generated Summary DAG

Figure 2: 5-node summary graphs for the DAG in Fig. 1.

algorithm still creates the necessary connections to maintain causal integrity. □

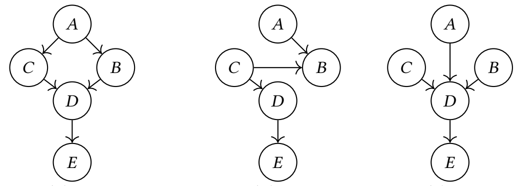
Our main contributions are summarized as follows.

Causal DAG Summarization. We introduce the problem of summarizing causal DAGs that maintain the utility of the model for reliable causal inference (Section 3). This process necessitates preserving the causal information encoded in the input DAG. Causal DAGs encode information through missing edges, which implies Conditional Independence (CI) constraints. The problem of causal DAG summarization is therefore formalized as finding a summary DAG that maintains, to the greatest extent possible, CI statements while meeting a size constraint on the number of nodes. We prove that this problem is NP-hard.

Summary Causal DAGs. We introduce the concept of *summary causal DAGs* derived by grouping nodes within the original DAG via *node contractions*. Node contraction, while inherently leading to information loss, enables summary DAGs to compactly encapsulate potential causal DAGs from which the summary DAG could have originated. We show that contracting nodes results in a reduction of causal information in a causal DAG, akin to adding edges to the input causal DAG. Based on this connection, we develop a sound and complete algorithm for identifying all CIs encoded by a summary DAG. This is crucial for utilizing summary causal DAG for causal inference. (Section 4).

The CaGreS Algorithm. We devise an efficient greedy algorithm called CaGreS. A key feature of CaGreS is its methodical approach to choosing which node pair to contract. This process is informed by the connection between node contraction and the addition of edges to the input causal DAG, prioritizing node pairs that add the fewest edges upon contraction. Additionally, CaGreS incorporates

[1]Other available graph summarization methods (e.g., [105]) exhibit similar weaknesses, making them unsuitable for summarizing causal DAGs.



(a) $\mathcal{G}_1$ (b) $\mathcal{G}_2$ (c) $\mathcal{G}_3$

Figure 3: Three causal DAGs over the same set of nodes.

several optimizations, including caching mechanisms, making it a practical tool for generating summary causal DAGs (Section 5).

Causal Inference over Summary Causal DAGs. We show that summary causal DAGs can be directly utilized for causal inference. We establish that Pearl's *do-calculus* framework [70], which provides a set of sound and complete rules for reasoning about the effects of interventions using causal DAGs, remains sound and complete for summary DAGs. By examining the connection between node contractions and the addition of edges, we offer clear insights into how these modifications affect the soundness and completeness of do-calculus within the framework of summary DAGs (Section 6).

Experimental Evaluation. We demonstrate via a case study how summary DAGs offer robustness against errors in the input causal DAG (Section 7). We further conduct an extensive experimental study over synthetic and six real-life datasets, demonstrating the effectiveness of CaGreS compared to three existing solutions and two variations of CaGreS as additional comparison points. Our results demonstrate the robust quality of CaGreS. The results further show the efficiency of CaGreS in handling high-dimensional datasets and its ability to generate summary DAGs that ensure reliable inference (Section 8).

Related work is discussed in Section 9 and we conclude in Section 10.

2 BACKGROUND

We consider a single-relation database over a schema $\mathbb{A}$. We use upper case letters to denote a variable from $\mathbb{A}$ and bold symbols to represent a set of variables. The broad goal of causal inference is to estimate the effect of an *exposure variable* $T \in \mathbb{A}$ (e.g., `Num Joins`) on an *outcome variable* $O \in \mathbb{A}$ (e.g., `Elapsed Time`). We use Pearl's model for conducting such inference using observational data [70].

To get an unbiased estimate for the causal effect of the exposure T on the outcome O, one must mitigate the effect of *confounding variables*, i.e., variables that can affect the exposure assignment and outcome [70]. For instance, when estimating how the query execution time affects the elapsed time, one would avoid a source of *confounding bias* by considering the number of columns and tables. Pearl's causal model provides ways to account for these confounding variables to get an unbiased causal estimate from observational data using *causal DAGs* [70]. Causal DAGs provide a simple way of graphically representing causal relationships within a set of variables. A causal DAG $\mathcal{G}$ for the variables in $\mathbb{A}$ is a specific type of a Bayesian network and is formally defined as follows:

Causal DAG. A Bayesian network is a DAG $\mathcal{G}$ in which nodes represent random variables and edges express direct dependence between the variables. Each node X_i is associated with the conditional distribution $\mathbb{P}(X_i|\pi(X_i))$, where $\pi(X_i)$ is the set of parents of X_i in $\mathcal{G}$. The joint distribution over all variables $\mathbb{P}(X_1, \ldots, X_n)$, is given by the product of all conditional distributions. That is,

$$\mathbb{P}(X_1, \ldots, X_n) = \prod_{i=1}^{n} \mathbb{P}(X_i|\pi(X_i)) \tag{1}$$

A causal DAG is a Bayesian network where edges signify direct causal influence rather than statistical dependence. We say that X is a potential cause of Y if there is a directed path from X to Y. Fig. 3 shows three example causal DAGs over the same set of variables.

***d*-Separation & Conditional Independence.** A *trail* t=$(X_1, \ldots, X_n)$ is a sequence of nodes s.t. there is a a distinct edge between X_i and X_{i+1} for every i. That is, $(X_i{\rightarrow}X_{i+1}){\in}\mathsf{E}(\mathcal{G})$ or $(X_i{\leftarrow}V_{X+1}){\in}\mathsf{E}(\mathcal{G})$ for every i. A node X_i is said to be *head-to-head* with respect to t if $(X_{i-1}{\rightarrow}X_i){\in}\mathsf{E}(\mathcal{G})$ and $(X_i{\leftarrow}X_{i+1}){\in}\mathsf{E}(\mathcal{G})$. A trail $t = (X_1, \ldots, X_n)$ is *active* given $\mathbf{Z}{\subseteq}\mathcal{X}$ if (1) every X_i that is a head-to-head node with respect to t either belongs to $\mathbf{Z}$ or has a descendant in $\mathbf{Z}$, and (2) every X_i that is not a head-to-head node w.r.t. t does not belong to $\mathbf{Z}$. If a trail t is not active given $\mathbf{Z}$, then it is *blocked* given $\mathbf{Z}$ [70].

Causal DAGs encode a set of Conditional Independence statements (CIs) that can be read off the graph using d-separation [70]. These statements describe the absence of an active trail between two sets of variables when conditioning on other variables. In Fig. 3(a), some examples of CIs are: $(\mathtt{B} \perp\!\!\!\perp_d \mathtt{C} \mid \mathtt{A})$, and $(\mathtt{D} \perp\!\!\!\perp_d \mathtt{A} \mid \mathtt{BC})$.

In causal DAGs, the information encoded by missing edges implies the set of CIs the DAG represents. Namely, removing edges can undermine the causal model as it implies CIs that do not necessarily hold in the distribution. On the other hand, existing edges indicate *potential* causal dependence. This implies that adding edges to a causal DAG, provided acyclicity is maintained, does not necessarily compromise validity [70].

The Recursive Basis. The *Recursive Basis* (RB) [33] for a causal DAG comprises a set of at most n CIs, signifying that each node is conditionally independent of its non-descendants nodes given its parents. This succinct set of CIs holds significance, as it can be used for constructing the causal DAG, and all other CIs encoded in the causal DAG can be deduced from it (see full details in the Appendix).

Formally, given a causal DAG $\mathcal{G}$, let $\langle X_1, \ldots, X_n \rangle$ denote a complete topological order over $\mathsf{V}(\mathcal{G})$. Equation 1 implicitly encodes a set of n CIs, called the RB for $\mathcal{G}$, defined as follows:

$$\Sigma_{\mathrm{RB}}(\mathcal{G}) \stackrel{\mathrm{def}}{=} \{(X_i \perp\!\!\!\perp X_1 \ldots X_{i-1} \backslash \pi(X_i) \mid \pi(X_i)) : i \in [n]\} \tag{2}$$

It has been shown [32, 33, 101] that both the semi-graphoid axioms (given in the Appendix) and the d-separation criterion are sound and complete for inferring CIs from the RB (and this is exactly the same set of CIs the causal DAG encodes).

Example 3. Consider the causal DAG $\mathcal{G}_1$ in Fig. 3(a). In the nodes' topological order, A precedes B and C, which in turn, precedes D. The last node is E. The RB of $\mathcal{G}_1$ is given in Table 1. Given the topological order over the nodes and the RB, $\mathcal{G}_1$ can be fully constructed. Further, any CI statement encoded in $\mathcal{G}_1$ can be implied from this RB by using the semi-graphoid axioms. □

ATE& do-Calculus. The do-operator, a fundamental concept in causal inference, is used to denote interventions on variables in a causal model. It represents the intervention on a variable to observe the resulting change in an outcome variable while holding the external factors constant. In computing the *Average Treatment Effect* (ATE) [70], a popular measure of causal estimate, the *do*-operator is applied to represent the treatment assignment for treatment and control groups. The ATE quantifies the average causal effect of a treatment T on an outcome variable O in a population:

$$ATE(T,O) = \mathbb{E}[O \mid do(T=1)] - \mathbb{E}[O \mid do(T=0)] \qquad (3)$$

To compute the causal effect of a treatment T on an outcome O, identifying and adjusting for confounders is crucial to revealing the true causal relationship. The backdoor criterion [70] serves as a sufficient condition for this purpose by specifying a set $\mathbf{Z}$ that, when conditioned upon, blocks all backdoor paths between T and O. This criterion offers a practical way to adjust for confounders within the causal DAG framework. However, it is part of the larger *do*-calculus system, a more generic axiomatic framework designed for reasoning about interventions and their effects within causal models. The *do*-calculus comprises three rules that facilitate the substitution of probability expressions containing the *do*-operator with standard conditional probabilities [70]. This system underpins a systematic methodology for deriving causal relationships from observational data. Given its soundness and completeness, this framework offers a broad toolkit for causal inference. Since these concepts are not directly employed in this paper, we do not delve into a detailed review of them here.

3 PROBLEM FORMULATION

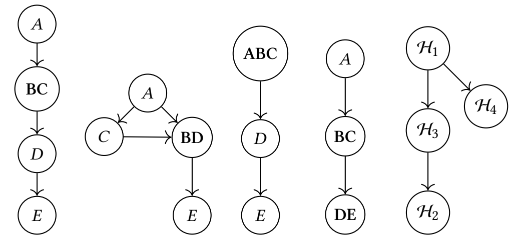
Our goal is to distill an input causal DAG into a more interpretable summary DAG by grouping nodes while preserving its utility for reliable causal inference. To achieve this, the summary causal DAG should meet the following criteria:

Size Constraint: The summary DAG should be concise to reduce the cognitive load on the analyst while providing a clear view of the causal relationships [14]. We therefore introduce a size constraint to enhance the summary DAG's intelligibility, ensuring the core complexity of the original DAG is maintained in a simplified form.

Preserving Causal Information: The summary DAG must maintain the causal dependencies present in the original causal DAG, including the directionality of those dependencies. If variable A has a directed causal path to variable B in the original DAG, this directional relationship should be faithfully preserved in the summary DAG. The summary DAG should also preserve the conditional independencies represented in the original DAG. If variables A and B are conditionally independent, this lack of dependence should be reflected in the summary DAG. Lastly, the summary DAG should not introduce any spurious conditional independencies that the original causal DAG does not imply.

Our objective must be to preserve the utility of the summary causal DAG for causal inference. As mentioned, in causal DAGs, the information encoded by missing edges implies the set of CIs the DAG represents. Therefore, removing edges can undermine the causal model as it implies CIs that do not necessarily hold in the original DAG. On the other hand, existing edges indicate *potential* causal dependence. This implies that adding edges to a causal DAG, provided acyclicity is maintained, does not necessarily compromise validity. We, therefore, rigorously enforce conditions on the summary DAG to ensure that the directionality is faithfully preserved in the summary DAG and assert that the summary DAG should preserve, to the greatest extent possible, a subset of the independence assumptions encoded in the original DAG. We show that, with these considerations, the summary causal DAG remains a viable tool for causal inference (Section 6).

We first formalize the concept of a summary causal DAG, then rigorously formalize the problem of causal DAG summarization.



(a) $\mathcal{H}_1$ **(b)** $\mathcal{H}_2$ **(c)** $\mathcal{H}_3$ **(d)** $\mathcal{H}_4$ **(e) Order**

Figure 4: 4 summary causal DAGs for $\mathcal{G}_1$ and the partial order among them.

Table 1: The recursive bases of the summary DAGs in Figure 4

Graph	Recursive Basis
$\mathcal{G}_1$	$(C \perp\!\!\!\perp B \mid A), (D \perp\!\!\!\perp A \mid BC), (E \perp\!\!\!\perp ABC \mid D)$
$\mathcal{H}_1$	$(D \perp\!\!\!\perp A \mid BC), (E \perp\!\!\!\perp ABC \mid D)$
$\mathcal{H}_2$	$(E \perp\!\!\!\perp AC \mid BD)$
$\mathcal{H}_3$	$(E \perp\!\!\!\perp ABC \mid D)$
$\mathcal{H}_4$	$(DE \perp\!\!\!\perp A \mid BC)$

3.1 Summary Causal DAGs

A *summary graph* is obtained by grouping nodes of the input graph based on a given partition of the nodes. The resulting graph retains the essential connectivity and structural information of the original graph but with a reduced number of nodes. We obtain a summary graph by applying *node contraction* operations [72].

Given a graph $\mathcal{G}$, the contraction of a pair of nodes $U, V \in \mathsf{V}(\mathcal{G})$ is the operation that produces a graph $\mathcal{H}$ in which the two nodes U and V are replaced with a single node $\mathbf{C}=\{U,V\} \in \mathsf{V}(\mathcal{H})$, where $\mathbf{C}$ is now neighbors with nodes that U and V were originally adjacent to (edge directionality is preserved). If U and V were connected by an edge, the edge is removed upon contraction.

Definition 1 (Summary-DAG)**.** A summary DAG of a DAG $\mathcal{G}$ is a pair $(\mathcal{H}, f)$, where $\mathcal{H}$ is a DAG with nodes $\mathsf{V}(\mathcal{H})$, edges $\mathsf{E}(\mathcal{H})$, and $f : \mathsf{V}(\mathcal{G}) \to \mathsf{V}(\mathcal{H})$ is a function that partitions the nodes $\mathsf{V}(\mathcal{G})$ among the nodes $\mathsf{V}(\mathcal{H})$, such that: If $(U,V) \in \mathsf{E}(\mathcal{G})$, then $f(U)=f(V)$ or $(f(U), f(V)) \in \mathsf{E}(\mathcal{H})$. We define the inverse $f^{-1}:\mathsf{V}(\mathcal{H}) \to 2^{\mathsf{V}(\mathcal{G})}$ as follows: $f^{-1}(X) \stackrel{\text{def}}{=} \{V \in \mathsf{V}(\mathcal{G}) : f(V)=X\}$

To simplify the notations, we omit f whenever possible.

Example 4. Consider Fig. 3(a) which depicts a DAG $\mathcal{G}_1$. After contracting B and C, the resulting summary DAG $\mathcal{H}_1$ is displayed in Fig. 4(a). In $\mathcal{H}_1$, the nodes B and C have been contracted into the node $\mathbf{BC}$. Namely, $f(B) = f(C) = \mathbf{BC}$, and $f^{-1}(\mathbf{BC}) = \{B, C\}$. ◻

A causal DAG $\mathcal{G}$ is said to be *compatible* with a summary DAG $\mathcal{H}$, if, there exists a function f that partitions the nodes $\mathsf{V}(\mathcal{G})$ among the nodes $\mathsf{V}(\mathcal{H})$, such that: If $(U,V) \in \mathsf{E}(\mathcal{G})$, then $f(U)=f(V)$ or $(f(U), f(V)) \in \mathsf{E}(\mathcal{H})$. Namely, $\mathcal{H}$ is a summary DAG of $\mathcal{G}$.

Definition 2 (Compatibility)**.** Let $(\mathcal{H}, f)$ be a summary DAG. A DAG $\mathcal{G}$ is *compatible* with $\mathcal{H}$ if $\mathcal{H}$ is a summary DAG for $\mathcal{G}$. We use $\{\mathcal{G}_i\}_{\mathcal{H}}$ to denote the set of all causal DAGs compatible with $\mathcal{H}$.

We also use the term compatibility to describe the relationship between two causal DAGs sharing the same set of nodes, where the edges of one are fully contained in the set of edges of another graph. Let $\mathcal{G}$ be a causal DAG and let $\mathcal{G}'$ be a causal DAG where $\mathsf{V}(\mathcal{G})=\mathsf{V}(\mathcal{G}')$. We say that $\mathcal{G}'$ is a *supergraph* of $\mathcal{G}$ if $\mathsf{E}(\mathcal{G})\subseteq\mathsf{E}(\mathcal{G}')$. In this case, we also say that $\mathcal{G}$ is *compatible* with $\mathcal{G}'$.

Example 5. Consider again Fig. 3. Both $\mathcal{G}_1$ and $\mathcal{G}_2$ are compatible with the summary DAG $\mathcal{H}_1$ shown in Fig. 4(a) (achieved by contracting B and C). However, $\mathcal{G}_3$ is not compatible with $\mathcal{H}_1$, since the edge between D and A is not preserved. ◻

We are interested in finding acyclic summary graphs. Thus, we prove a simple lemma that characterizes node contractions that maintain acyclicity.

Lemma 3.1. *Let $\mathcal{G}$ be a DAG, and let $V, U\in\mathsf{V}(\mathcal{G})$. Let $\mathcal{H}_{VU}$ denote the summary graph that results from $\mathcal{G}$ by contracting V and U. Then $\mathcal{H}_{VU}$ contains a directed cycle if and only if $\mathcal{G}$ contains a directed path P from V to U (or U to V), where $|P|\geq 2$.*

A *summary causal DAG* is a specific type of summary graph obtained through node contraction operations over a given causal DAG $\mathcal{G}$ and ensures acyclicity. Namely, only contractions involving nodes without a directed path of length ≥ 2 are permitted.

As mentioned, the RB of a causal DAG comprises a set of at most n CIs (where $n=|\mathsf{V}(\mathcal{G})|$), signifying that each node is conditionally independent of its preceding nodes[2] given its parents. This succinct set of CIs holds significance, because it enables the derivation of all other CIs represented in the causal DAG.

The RB of a summary causal DAG is defined in a manner akin to the RB of a causal DAG, as denoted by Eq. (2). The only difference is that in a summary causal DAG, a node may represent a subset of nodes of the original DAG. To illustrate, Table 1 shows the RBs of summary causal DAGs depicted in Figure 4.

3.2 The Causal DAG Summarization Problem

As mentioned, we aim to reduce the size of an input causal DAG by partitioning its nodes into sets of nodes, while retaining maximal causal information. We covered the two criteria of our problem before proceeding with formalizing it.

Size Constraint A size constraint on a summary graph is a key motivating constraint for graph summarization work and may be imposed on the number of edges, nodes, storage space, minimum description length, etc. [49]. In this work, we focus on a node-based size constraint, as limited-size graphs are generally more accessible for inspection [14, 38]. Moreover, it is relatively straightforward for analysts to set and adjust a limit on the number of nodes [97].

Causal Information Preservation As mentioned, if two variables have a directed path between them in the original DAG, then this relationship should be faithfully preserved in the summary DAG. Indeed, this follows from the definition of a summary DAG (Def. 1).

Given two summary DAGs derived from the same causal DAG $\mathcal{G}$ (i.e., $\mathcal{G}$ is compatible with both summary DAGs), both adhering to the size constraint, we prefer the one that preserves, to a larger degree, the set of CIs represented in $\mathcal{G}$. To this end, we devise a measure to compare summary DAGs based on their RBs. When comparing two summary DAGs $\mathcal{H}_1$ and $\mathcal{H}_2$, we assert that $\mathcal{H}_1$ is *superior* to $\mathcal{H}_2$ if the RB of $\mathcal{H}_2$ is implied by the RB of $\mathcal{H}_1$. Namely, all the CIs encoded by $\mathcal{H}_2$ can also be deduced from $\mathcal{H}_1$. We are searching for a maximal summary causal DAG, namely, that its RB is not implied by any other valid summary DAG.

Let $\Omega\stackrel{\text{def}}{=}\{X_1, \ldots, X_n\}$ be a set of jointly distributed random variables with distribution $\mathbb{P}$ (i.e., nodes of the original DAG). Formally,

Definition 3 (I-Map)**.** A DAG $\mathcal{G}$ is an *I-Map* for $\mathbb{P}$ if for every disjoint sets $\mathbf{X}, \mathbf{Y}$, and $\mathbf{Z}$ it holds that $(\mathbf{X} \perp\!\!\!\perp_d \mathbf{Y} \mid \mathbf{Z})_{\mathcal{G}}$ only if $(\mathbf{X} \perp\!\!\!\perp_{\mathbb{P}} \mathbf{Y} \mid \mathbf{Z})$.

We denote by $\mathcal{G}(\mathbb{P})$ the set of DAGs that are an I-Map for $\mathbb{P}$. Let $\mathcal{G}_1$ and $\mathcal{G}_2$ be two DAGs that are I-Maps for $\mathbb{P}$. We say that $\mathcal{G}_2$ is superior to $\mathcal{G}_1$, in notation $\mathcal{G}_2\succ\mathcal{G}_1$, if for every $\sigma\in\Sigma_{\text{RB}}(\mathcal{G}_1)$, it holds that $\Sigma_{\text{RB}}(\mathcal{G}_2) \implies \sigma$. Note that the relation $\succ$ does not necessarily form a complete order. We say that $\mathcal{G}$ is *maximal for* $\mathbb{P}$ if $\mathcal{G}$ is an I-Map for $\mathbb{P}$, and there does not exist any $\mathcal{G}'\in\mathcal{G}(\mathbb{P})$ such that $\mathcal{G}'\succ\mathcal{G}$. Our goal is to find a summary DAG that is maximal for $\mathbb{P}$, give a constraint on the number of nodes.

Example 6. Consider the causal DAG $\mathcal{G}_1$ in Fig. 3(a). Fig. 4(a) presents a 4-size summary DAG $\mathcal{H}_1$ for $\mathcal{G}_1$. The RBs of both DAGs are shown in Table 1. Clearly, $\Sigma_{\text{RB}}(\mathcal{H}_1)\subset\Sigma_{\text{RB}}(\mathcal{G}_1)$, and hence $\mathcal{H}_1$ is an I-Map for $\mathbb{P}$. Fig. 4(b) presents $\mathcal{H}_2$, another 4-size summary DAG for $\mathcal{G}_1$, where $\Sigma_{\text{RB}}(\mathcal{H}_2)=\{(E \perp\!\!\!\perp AC|BD)\}$. From the semi-graphoid axioms, it holds that $(E \perp\!\!\!\perp ABC|D) \implies (E \perp\!\!\!\perp AC|BD)$. Thus, $\mathcal{H}_1\succ\mathcal{H}_2$. Hence, $\mathcal{H}_1$ is a superior summary DAG. Similarly, Figures 4(c) and 4(d) illustrate $\mathcal{H}_3$ and $\mathcal{H}_4$, 3-size summary DAGs for $\mathcal{G}_1$. Their RBs are given in Table 1. The partial order among all summary DAGs is presented in Fig. 4(e). Despite $\mathcal{H}_3$ having only three nodes, it surpasses $\mathcal{H}_2$. However, $\mathcal{H}_3$ and $\mathcal{H}_4$ are incomparable, i.e., neither $\Sigma_{\text{RB}}(\mathcal{H}_3) \implies \Sigma_{\text{RB}}(\mathcal{H}_4)$ nor $\Sigma_{\text{RB}}(\mathcal{H}_4) \implies \Sigma_{\text{RB}}(\mathcal{H}_3)$. ◻

We define the causal DAG summarization problem as follows:

Problem 1 (Causal DAG Summarization)**.** Given a causal DAG $\mathcal{G}$ defined over a joint distribution $\mathbb{P}$, and a bound k, find a summary causal DAG $\mathcal{H}$ s.t. (i) the number of nodes in $\mathcal{H}$ is $\leq k$; (ii) $\mathcal{G}$ is compatible with $\mathcal{H}$, $\mathcal{H}\in\mathcal{G}(\mathbb{P})$ and is maximal for $\mathbb{P}$.

Example 7. Consider again the causal DAG in Fig. 1. We set k=5. Fig. 2b depicts an optimal summary causal DAG. Namely, the RB of any other summary causal DAG with 5 or fewer nodes is not superior to RB of this 5-node summary causal DAG. ◻

We show that the causal DAG summarization problem is *NP*-hard via a reduction from the k-Min-Cut problem [37].

Theorem 3.2. *The causal DAG summarization problem is NP-hard.*

4 NODE-CONTRACTION AS EDGE ADDITION

Next, we establish the connection between node contractions and the addition of edges to the input causal DAG. This connection will be used to read off, from a given summary causal DAG, all the CIs it encodes. It also serves as a pivotal factor in guiding our algorithm for selecting promising node pairs to merge. Additionally,

[2] according to a given full topplogical order of the nodes

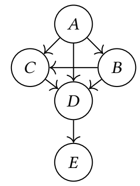


Figure 5: The canonical causal DAG of $\mathcal{H}_3$ (Fig. 4(c))

in Section 6, we will leverage this connection to demonstrate how causal inference can be directly conducted over summary DAGs.

4.1 The Canonical Causal DAG

Given a summary causal DAG $\mathcal{H}$, we define its corresponding canonical causal DAG, denoted as $\mathcal{G}_{\mathcal{H}}$. In this causal DAG, cluster nodes are decomposed into distinct nodes connected by edges. We show that the RB of the canonical causal DAG is *equivalent* to that of $\mathcal{H}$. We first define the notion of equivalence for sets of CIs.

Definition 4 (CI Sets Equivalence)**.** Let $\mathbf{S}$ and $\mathbf{T}$ denote two sets of CIs over the variable-set $\{X_1, \ldots, X_n\}$. We say that $\mathbf{S} \Longrightarrow \mathbf{T}$ if $\mathbf{S} \Longrightarrow \sigma$ for every CI $\sigma \in \mathbf{T}$. We say that $\mathbf{S}$ and $\mathbf{T}$ are *equivalent*, in notation $\mathbf{S} \equiv \mathbf{T}$, if $\mathbf{S} \Longrightarrow \mathbf{T}$ and $\mathbf{T} \Longrightarrow \mathbf{S}$.

Next, we formally define the notion of the *canonical causal DAG* for a given summary DAG.

Definition 5 (Canonical Causal DAG)**.** Let $(\mathcal{H}, f)$ be a summary DAG for a causal DAG $\mathcal{G}$. Let $\langle X_1, \ldots, X_n \rangle$ denote a complete topological order over $\mathsf{V}(\mathcal{G})$. We define the canonical causal DAG associated with $(\mathcal{H}, f)$, denoted $\mathcal{G}_{\mathcal{H}}$ as follows: $\mathsf{V}(\mathcal{G}_{\mathcal{H}}) = \mathsf{V}(\mathcal{G})$, and

$$
\begin{aligned}
(X_i, X_j) \in \mathsf{E}(\mathcal{G}_{\mathcal{H}}) \text{ if and only if } \quad & (X_i, X_j) \in \mathsf{E}(\mathcal{G}) \\
\text{or} \quad & (f(X_i), f(X_j)) \in \mathsf{E}(\mathcal{H}) \\
\text{or} \quad & f(X_i) = f(X_j) \text{ and } i < j
\end{aligned}
$$

We observe that, by definition, $\mathcal{G}_{\mathcal{H}}$ is compatible with the summary DAG $(\mathcal{H}, f)$.

Example 8. Consider the summary DAG $\mathcal{H}_3$ in Figure 4(c). Its canonical causal DAG $\mathcal{G}_{\mathcal{H}_3}$ is depicted in Figure 5. Assume that in the topological order A precedes B which in turn precedes C. All nodes within the cluster node $\mathbf{ABC}$ are connected by edges in $\mathcal{G}_{\mathcal{H}_3}$, according to the topological order. Since the cluster node $\mathbf{ABC}$ is the parent of D in $\mathcal{H}_3$, in $\mathcal{G}_{\mathcal{H}_3}$ all A, B and C are parents of D. □

We show that the RB of the canonical causal DAG $\mathcal{G}_{\mathcal{H}}$ is equivalent to that of the summary DAG $\mathcal{H}$ obtained by node contractions to a causal DAG $\mathcal{G}$. In other words, node contractions can be conceptualized as the addition of edges to the input causal DAG, since $\mathsf{V}(\mathcal{G}_{\mathcal{H}})=\mathsf{V}(\mathcal{G})$ and $\mathsf{E}(\mathcal{G})\subseteq\mathsf{E}(\mathcal{G}_{\mathcal{H}})$ (i.e., $\mathcal{G}_{\mathcal{H}}$ is a supergraph of $\mathcal{G}$).

Theorem 4.1. *Let $\mathcal{H}$ be a summary causal DAG, and $\mathcal{G}_{\mathcal{H}}$ is its corresponding canonical causal DAG. We have: $\Sigma_{RB}(\mathcal{H}) \equiv \Sigma_{RB}(\mathcal{G}_{\mathcal{H}})$.*

Continuing with Example 8, the RB of $\mathcal{G}_{\mathcal{H}_3}$ is $(E \perp\!\!\!\perp ABC|D)$, which is identical to that of $\mathcal{H}_3$ (see Table 1).

4.2 s-Separation

We introduce the notion of *s-separation*, an extension of d-separation, tailored to identify CIs encoded by a summary DAG. Intuitively, a summary DAG represents a collection of causal DAGs that are compatible with it, meaning that it could have been obtained from any of those DAGs (similar to *possible worlds* in probabilistic database [23]). Each of these DAGs encodes a different set of CIs. The set of CIs encoded by a summary DAG is defined as the intersection of CIs that holds in all compatible DAGs. In this way, we can ensure we restrict ourselves only to CIs that are certainly present in a particular context and can be reliably used for inference.

The validity of a CI statement, as derived from summary DAG $\mathcal{H}$, is given by the following definition:

Definition 6 (Validity of a CI in a summary DAG)**.** A CI statement is deemed *valid* in a summary causal DAG $\mathcal{H}$ if and only if it is implied by all causal DAGs within $\{\mathcal{G}_i\}_{\mathcal{H}}$.

s-separation captures all certain CIs that hold across all DAGs in $\{\mathcal{G}_i\}_{\mathcal{H}}$. We propose the following criterion for s-separation to encapsulate this notion of validity.

Definition 7 (s-separation)**.** Given a summary DAG $(\mathcal{H}, f)$ and disjoint subsets $\mathbf{X}, \mathbf{Y}, \mathbf{Z} \subseteq \mathsf{V}(\mathcal{H})$, we say that $\mathbf{X}$ and $\mathbf{Y}$ are s-separated in $\mathcal{H}$ by $\mathbf{Z}$, denoted by $(\mathbf{X} \perp\!\!\!\perp_S \mathbf{Y} \mid \mathbf{Z})_{\mathcal{H}}$, iff $f^{-1}(\mathbf{X})$ and $f^{-1}(\mathbf{Y})$ are d-separated by $f^{-1}(\mathbf{Z})$ in every causal DAG within $\{\mathcal{G}_i\}_{\mathcal{H}}$.

We say that $\mathbf{X}$ and $\mathbf{Y}$ are s-connected in $(\mathcal{H}, f)$ by $\mathbf{Z}$, if there exists a causal DAG $\mathcal{G} \in \{\mathcal{G}_i\}_{\mathcal{H}}$, such that $f^{-1}(\mathbf{X})$ and $f^{-1}(\mathbf{Y})$ are d-connected in $\mathcal{G}$ by $f^{-1}(\mathbf{Z})$.

4.2.1 **s-separation Algorithm.** Given a summary causal DAG $\mathcal{H}$, we aim to derive the set of CIs it encodes. A naive approach would be to employ d-separation algorithms [70]. However, $\mathcal{H}$ can potentially encompass more CIs than those discerned through d-separation alone, as demonstrated in the following example.

Example 9. Referring back to Fig. 3, $(B \perp\!\!\!\perp_d E \mid D)$ and $(C \perp\!\!\!\perp_d E \mid B, D)$, and thus also $(B, C \perp\!\!\!\perp_d E \mid D)$, all hold in $\mathcal{G}_1$ and $\mathcal{G}_2$. Likewise, $(\mathbf{BC} \perp\!\!\!\perp_d E \mid D)$ holds in $\mathcal{H}_1$ (Fig. 4(a)) where $f^{-1}(\mathbf{BC})=\{B, C\}$. However, since $\mathcal{H}_1$ does not contain B or C as separate nodes, we cannot establish $(B \perp\!\!\!\perp_d E \mid D)$ or $(C \perp\!\!\!\perp_d E \mid B, D)$ from $\mathcal{H}_1$. □

To address this, a simple solution is to find the set of CIs shared across all causal DAGs compatible with $\mathcal{H}$. However, this approach is costly, as it necessitates examining all compatible causal DAGs. We, therefore, present a simple algorithm for s-separation that leverages the connection between a summary DAG and its canonical causal DAG. This algorithm operates as follows: Given a summary DAG $\mathcal{H}$, establish a topological order for its nodes.[3] Using this order, construct the canonical causal DAG $\mathcal{G}_{\mathcal{H}}$. Next, apply d-separation over $\mathcal{G}_{\mathcal{H}}$ and return the resulting CI set. We demonstrate that this algorithm is sound and complete.

Theorem 4.2 (Soundness and Completeness of s-separation). *In a summary DAG $(\mathcal{H}, f)$, let $\mathbf{X}, \mathbf{Y}, \mathbf{Z} \subseteq \mathsf{V}(\mathcal{H})$ be disjoint sets of nodes. If $\mathbf{X}$ and $\mathbf{Y}$ are d-separated by $\mathbf{Z}$ in $\mathcal{H}$, then in any causal DAG $\mathcal{G} \in \{\mathcal{G}_i\}_{\mathcal{H}}$, $f^{-1}(\mathbf{X})$ and $f^{-1}(\mathbf{Y})$ are d-separated by $f^{-1}(\mathbf{Z})$. That is:*

$$(\mathbf{X} \perp\!\!\!\perp_d \mathbf{Y}|\mathbf{Z})_{\mathcal{H}} \Longrightarrow (f^{-1}(\mathbf{X}) \perp\!\!\!\perp_d f^{-1}(\mathbf{Y})|f^{-1}(\mathbf{Z}))_{\mathcal{G}} \Longrightarrow (\mathbf{X} \perp\!\!\!\perp_s \mathbf{Y}|\mathbf{Z})_{\mathcal{H}}$$

If $\mathbf{X}$ and $\mathbf{Y}$ are d-connected by $\mathbf{Z}$ in $\mathcal{H}$, then there exists a DAG $\mathcal{G} \in \{\mathcal{G}_i\}_{\mathcal{H}}$, s.t $f^{-1}(\mathbf{X})$ and $f^{-1}(\mathbf{Y})$ are d-connected by $f^{-1}(\mathbf{Z})$ in $\mathcal{G}$.

[3] The order of nodes within a cluster is considered arbitrary, or it may be determined based on the topological order of the input causal DAG if such information is preserved.

Algorithm 1: The CaGreS Algorithm

```
input  : A causal DAG 𝒢 and a number k.
output : A summary causal DAG ℋ with k nodes.
1  ℋ ← 𝒢
2  /* Merge node-pairs in which their cost is ≤ 1         */
3  ℋ ← LowCostMerges(ℋ)
4  while size(ℋ.nodes) > k do
5      min_cost ← ∞
6      (X, Y) ← Null
7      for (U, V) ∈ ℋ.nodes do
8          if IsValidPair (U, V, ℋ) then
9              cost_UV ← GetCost(U, V, ℋ)
10             if cost_UV < min_cost then
11                 min_cost ← cost_UV
12                 (X, Y) ← (U, V)
13             if cost_UV == min_cost then
14                 Randomly decide if to replace X and Y with U and V
15         ℋ.Merge(X, Y)
16 return ℋ
```

Algorithm 2: The GetCost Procedure

```
input  : A summary causal DAG ℋ and a pair of nodes U and V.
output : The cost of contracting U and V.
1  cost ← 0
2  /* New edges among the nodes in the cluster             */
3  if ℋ.HasEdge(U, V) == False then
4      cost ← cost +size(U) · size(V)
5  /* New parents                                          */
6  parents_U ← ℋ.predecessors(U)
7  parents_U.RemoveSharedParents(V)
8  cost ← cost + size(parents_U) · size(V)
9  parents_V ← ℋ.predecessors(V)
10 parents_V.RemoveSharedParents(U)
11 cost ← cost + size(parents_V) · size(U)
12 /* New children                                         */
13 children_U ← ℋ.successors(U)
14 children_U.RemoveSharedChildren(V)
15 cost ← cost + size(children_U) · size(V)
16 children_V ← ℋ.successors(V)
17 children_V.RemoveSharedChildren(U)
18 cost ← cost + size(children_V) · size(U)
19 return cost
```

5 THE CAGRES ALGORITHM

We introduce an algorithm, named CaGreS for the causal DAG summarization problem. Although lacking theoretical guarantees, CaGreS effectively meets the size constraint and efficiently produces high-quality summary causal DAGs in practice. A brute force approach explores all summary DAGs with up to k nodes; for each candidate, it materializes its RB and selects one with a maximal RB. It finds the optimal summary causal DAG, but runs in exponential time due to the exponential number of graphs to explore. CaGreS overcomes this by avoiding iterating over every possible summary DAG and merging nodes based on an estimation of the merging effect on the canonical causal DAG.

Overview The CaGreS algorithm follows a previous line of work [97], using a bottom-up greedy approach to identify promising node pairs for contraction. Its main contribution lies in how it estimates merge costs: It counts the number of edges to be added in the canonical causal DAG for each node pair (a proxy for the RB's effect, as discussed in Section 4). In each iteration, the algorithm contracts the node pair resulting in the minimal number of additional edges. We also introduce optimizations for runtime efficiency, such as semantic constraint, fast low-cost merges, and caching mechanisms.

The CaGreS algorithm is given in Algorithm 1. Given a bound k and an input causal DAG, this algorithm iteratively seeks the next-best pair of nodes to be merged, until the size constraint is met (lines 4-15). The next-best pair of nodes to merge is the node pair whose contraction has the lowest cost (lines 10-12). The algorithm randomly breaks ties (lines 13-14). The GetCost procedure is shown in Algorithm 2. The cost of merging two (clusters of) nodes $\mathbf{U}$ and $\mathbf{V}$ is equal to the number of edges to be added in the corresponding canonical causal DAG: (1) edges to be added between the nodes within the combined cluster $\mathbf{U} \bigcup \mathbf{V}$ (lines 3-4), (2) new parents for the nodes in $\mathbf{U}$ or $\mathbf{V}$ post-merge (lines 6-11), and (3) new children for the nodes in $\mathbf{U}$ or $\mathbf{V}$ after the merge (lines 13-18).

We next propose three optimizations to improve runtime.

Semantic Constraint We can reduce the search space and ensure that only semantically related variables are merged, thereby supporting semantic coherence in the summary DAG. To achieve this, the user may specify which node pairs are allowed to be merged by providing a semantic similarity matrix and a threshold that indicates the maximum distance between two nodes within a cluster. For example, merging `Num Joins` and `Num Tables` is sensible, but merging `Num Columns` and `Elapsed Time` would be challenging to interpret in a summary DAG. The user can assess the semantic similarity using previous work on semantic similarity [36], measured using embedding techniques [59] or large language models [5].

Given a semantic similarity measure $sim(\cdot,\cdot)$ that assigns a value between 0 and 1 to a pair of variables, a score of 0 indicates no semantic relationship, while a score of 1 indicates that the variables are semantically equivalent. For a summary DAG $\mathcal{H}$ and a threshold τ, we say that $\mathcal{H}$ satisfies the semantic constraint if, for every cluster $\mathbf{C} \in \mathsf{V}(\mathcal{H})$, $sim(V_i, V_j) \geq \tau$ for every $V_i, V_j \in \mathbf{C}$. This condition is checked in line 8 of the CaGreS algorithm when validating whether a pair of nodes is suitable for contraction.

Low Cost Merges As a pre-processing step, we contract node pairs with low costs (line 4). This involves merging nodes that share identical children and parents, with a cost of at most 1 (requiring, in the worst case, only the addition of an edge between them in the canonical causal DAG). Additionally, we merge nodes linked along a non-branching path of nodes, each having at most one parent and one child, incurring a cost of 1.

Caching Mechanisms We employ two caching mechanisms. The first is dedicated to storing node pairs deemed invalid for contraction, while the second is utilized for storing cost scores.

We initialize the invalid node pairs cache during the low-cost merge phase. An invalid pair is a pair of nodes with semantic similarity exceeding the threshold or connected by a directed path of length greater than 2 (according to Lemma 3.1). Throughout the execution of CaGreS, whenever we encounter an invalid pair, we add it to the cache. Before computing the cost in each iteration, we verify that the node pair is valid for contraction.

The cost of a node pair **U**, **V** remains unchanged after merging another node pair **X**, **Y** if neither **U** nor **V** are neighbors of **X** or **Y**. Following the merge of **X** and **Y**, we update the cost cache by removing the cost scores of all node pairs involving one of their neighbors. When calculating the cost for a node pair, we check if the score is in the cache. If not, we compute and add it, ensuring the cache reflects node pair mergers' impact on neighboring pairs.

Time Complexity A single cost computation with n=$|\mathsf{V}(\mathcal{G})|$ takes $O(n)$ due to the maximum number of neighbors a node can have. The low-cost merge phase operates in $O(n^3)$ by iterating over every node pair in $\mathcal{G}$ and considering their neighbors. The algorithm undergoes $n{-}k$ iterations, evaluating all node pairs in the current summary DAG with no more than n neighbors. Thus, the overall time complexity is $O((n{-}k){\cdot}n^3)$.

6 DO-CALCULUS IN SUMMARY CAUSAL DAGS

Next, we show that the rules of *do*-calculus are sound and complete in summary causal DAGs. This is vital to ensure that the summary causal DAGs are effective formats that support causal inference by enabling direct causal inference on the summary DAGs. Our proof relies on the connection between node contraction and the addition of edges, namely, on the equivalence between the RB of a summary DAG and its canonical causal DAG (Theorem 4.1). This result is not surprising because the canonical causal DAG is a supergraph of the input causal DAG. Pearl already observed in [70] that: *"The addition of arcs to a causal diagram can impede, but never assist, the identification of causal effects in nonparametric models. This is because such addition reduces the set of d-separation conditions carried by the diagram; hence, if causal effect derivation fails in the original diagram, it is bound to fail in the augmented diagram".*

Given a causal DAG $\mathcal{G}$, for a set of nodes $\mathbf{X} \subseteq \mathsf{V}(\mathcal{G})$, let $\mathcal{G}_{\overline{\mathbf{X}}}$ denote the graph that results from $\mathcal{G}$ by removing all incoming edges to nodes in $\mathbf{X}$, by $\mathcal{G}_{\underline{\mathbf{X}}}$ the graph that results from $\mathcal{G}$ by removing all outgoing edges from the nodes in $\mathbf{X}$. For a set of nodes $\mathbf{X} \subseteq \mathsf{V}(G)\backslash\mathbf{Z}$, we denote by $\mathcal{G}_{\overline{\mathbf{X}}\underline{\mathbf{Z}}}$ the graph that results from $\mathcal{G}$ by removing all incoming edges into $\mathbf{X}$ and all outgoing edges from $\mathbf{Z}$.

Theorem 6.1 (Soundness of Do-Calculus in summary causal DAGs). *Let $\mathcal{G}$ be a causal DAG encoding an interventional distribution $P(\cdot \mid do(\cdot))$, compatible with the summary causal DAG $(\mathcal{H}, f)$. For any disjoint subsets $\mathbf{X},\mathbf{Y},\mathbf{Z},\mathbf{W}{\subseteq}\mathsf{V}(\mathcal{H})$, the following rules hold:*

$$\mathrm{R}_1 : (\mathbf{Y} \perp\!\!\!\perp \mathbf{Z} | \mathbf{X}, \mathbf{W})_{\mathcal{H}_{\overline{\mathbf{X}}}} \implies P(Y \mid do(X), Z, W) = P(Y \mid do(X), W)$$

$$\mathrm{R}_2 : (Y \perp\!\!\!\perp Z | X, W)_{\mathcal{H}_{\overline{\mathbf{X}}\underline{\mathbf{Z}}}} \implies P(Y|do(X), do(Z), W) {=} P(Y|do(X), Z, W)$$

$$\mathrm{R}_3 : (Y \perp\!\!\!\perp Z | X, W)_{\mathcal{H}_{\overline{\mathbf{X}Z(W)}}} \implies P(Y|do(X), do(Z), W) {=} P(Y|do(X), W)$$

where, $\boldsymbol{U} \stackrel{def}{=} (U)$ for every $U \in \mathsf{V}(\mathcal{H})$, and $Z(W)$ is the set of nodes in Z that are not ancestors of any node in W.

Theorem 6.2 (Completeness of Do-Calculus in summary causal DAGs). *Let $(\mathcal{H}, f)$ be a summary causal DAG for $\mathcal{G}$, and let $\boldsymbol{X},\boldsymbol{Y},\boldsymbol{W},\boldsymbol{Z}{\subseteq}\mathsf{V}(\mathcal{H})$ be disjoint sets of variables. If $\boldsymbol{Y}$ is d-connected to $\boldsymbol{Z}$ in $\mathcal{H}_{\overline{\boldsymbol{X}}}$ w.r.t. $\boldsymbol{X}{\cup}\boldsymbol{W}$, then there exists a causal DAG $\mathcal{G}'$ compatible with $\mathcal{H}$, such that $f(Y)$ is d-connected to $f(Z)$ in $\mathcal{G}'_{\overline{f(X)}}$ w.r.t. $f(\boldsymbol{X} \cup \boldsymbol{W})$.*

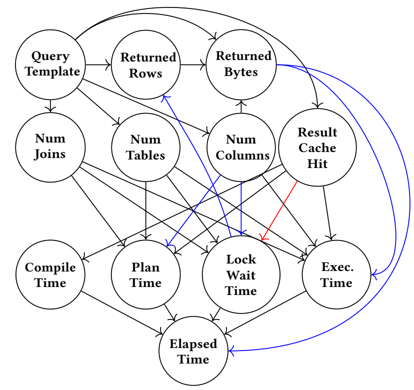
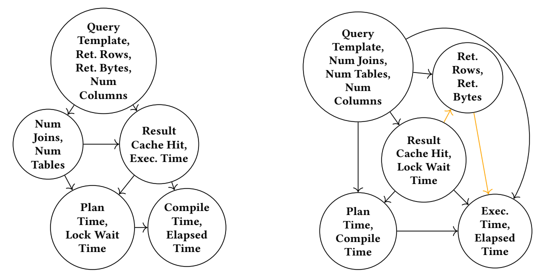


Figure 6: Modifications to the Redshift DAG (Fig. 1).



(a) Summary After Deletion **(b) Summary After Additions**

Figure 7: 5-node summary DAGs after DAG modifications.

ATE Computation over Summary DAGs: To conclude this section, we explain how causal effects (ATE, see in Section 2) can be calculated directly over the summary DAG. If the treatment or outcome is part of a cluster node in the summary DAG $\mathcal{H}$, we proceed as follows: For a node pair U, V, we estimate the causal effect $ATE(U, V)$ over the corresponding canonical causal DAG $\mathcal{G}_{\mathcal{H}}$ (this is valid as demonstrated in Section 6). To reduce the adjustment set's size, we arrange for U to precede all nodes within its cluster node in the $\mathcal{G}_{\mathcal{H}}$. An alternative approach that yields an upper and lower bound involves constraining the causal effect across the summary DAG by considering all subsets in U's cluster in $\mathcal{H}$.

7 ROBUSTNESS AGAINST DAG QUALITY

We evaluate the effectiveness of summary DAGs in providing robustness against a flawed input causal DAG, such as one derived by automated methods [34]. In a case study, we demonstrate that the summary DAG facilitates the handling of errors (i.e., missing and redundant edges) in the input DAG more effectively than directly examining the causal DAG (which may be overwhelming to the user). This study underscores that causal DAG summarization is valuable for addressing quality issues in the input causal DAG, and enhances the robustness against misspecifications.

In particular, we take a closer look at the causal DAG for the Redshift dataset (Fig. 1). We consulted GPT-4 [66] for each pair of variables in the dataset, inquiring about the presence and direction of an edge. This led to a collection of 55 detected edges. Of the original 23 edges, GPT-4 detected 21 correctly and 1 with inverted orientation, failing to detect 1 edge. It also generated additional 33

Table 2: Datasets

Dataset	# Nodes (Variables)	# Edges	# Tuples
REDSHIFT	12	23	9900
FLIGHTS	11	15	1M
ADULT	13	48	32.5K
GERMAN	21	43	1000
ACCIDENTS	41	368	2.8M
URLS	60	310	1.7M

edges (not present in the original DAG). We will show how causal DAG summarization can mitigate the impact of these errors.

Missing Edges: Starting from the DAG for REDSHIFT (Fig. 1), we remove the one edge that GPT-4 failed to detect (`Result Cache Hit` → `Lock Wait Time`), marked in red in Fig. 6. As evident in Fig. 7a, CaGreS produces the same summary DAG for $k = 5$ as in Fig. 2b, providing robustness against this error. The information of which node in the cluster {`Results Cache Hit`, `Exec. Time`} has a directed causal edge to one of the nodes in the cluster {`Plan Time`, `Lock Wait Time`} is lost upon the summarization process. Thus, any causal estimation performed over the summary DAG (as explained in Section 6), considers all possible causal DAGs compatible with this summary DAG, including once where the edge is included. Thus, the impact of this error is reduced.

Extraneous Edges: Starting from the DAG for REDSHIFT (Fig. 1), we add five randomly selected edges from the set of redundant edges produced by GPT-4, marked in blue in Fig. 6. These additional edges reduce the number of CIs entailed by the DAG, which can hurt causal inference accuracy. However, manually pruning possibly extraneous edges would require having the user check each of the (now 28) edges in the DAG for correctness. If we instead summarize the DAG using CaGreS with $k = 5$, the user is faced with the simpler, 9-edge summary DAG shown in Fig. 7b. It is sufficient for the user to detect the 2 suspicious orange edges among these 9 to discover 3 of the 5 extraneous edges. The remaining 2 extraneous edges (from `Num Columns` to `Plan Time` and `Lock Wait Time`) are subsumed grouping `Num Columns` together with other, highly semantically similar, query-related features. As such, graph summarization effectively helps address extraneous edges by facilitating their detection and reducing their impact.

8 EXPERIMENTAL EVALUATION

In this section, we empirically demonstrate the following claims: (**C1**) Our summary DAGs support reliable causal inference. (**C2**) Our objective evaluation method effectively determines superior summary causal DAGs. (**C3**) CaGreS outperforms other methods in causal DAG summarization and achieves efficient performance.

8.1 Experimental Setting

All algorithms are implemented in Python 3.7. Causal effect computation was performed using the DoWhy library [87]. The experiments were executed on a PC with a 4.8GHz CPU, and 16GB memory. Our code and datasets are available at [3].

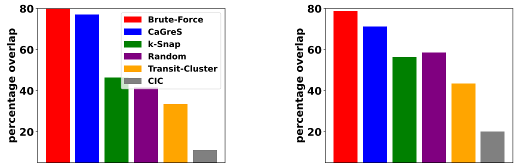
Examined datasets We examine six datasets, as shown in Table 2. Five of the datasets are publicly available themselves, while the remaining one (REDSHIFT) was collected by running a publicly available benchmark on publicly available cloud resources. We use the graph from Figure 1 for REDSHIFTand build the input causal DAG using the approaches outlined in [107] for the remaining datasets. **REDSHIFT**: A dataset collected by running queries from the TPC-DS benchmark [75] on Amazon Redshift Serverless [8]. We execute 100 queries from the query templates benchmark and retrieve the associated entries in the monitoring view [6]. We augment each entry with query-related features (e.g., num joins and tables). **FLIGHTS** [2]: a dataset describing domestic flight statistics in the US. We enriched it with attributes describing the weather, population, and properties of the airline carriers. **ADULT** [1]: a dataset comprises demographic information of individuals including their education, age, and income. **GERMAN** [10]: a dataset contains details of bank account holders, including demographic and financial information. **ACCIDENTS** [62]: This dataset provides information on various factors that are pertinent to the severity of car accidents, including weather conditions and the presence of traffic signs. **URLs** [4]: a dataset containing descriptions of malicious and non-malicious URLs. It encompasses properties such as URL length, the number of digits, and the occurrence of sensitive words.

We also created **synthetic data** using the DoWhy package [87], enabling manipulation of node count, edge count, and data size while retaining knowledge of the causal DAG structure.

Baseline Methods We examine the following baseline methods: **BRUTE-FORCE**: The optimal solution according to Def. 1. This algorithm implements an exhaustive search over all possible summary DAGs that satisfy the constraints. **K-SNAP** [97]: A general-purpose graph summarization algorithm that employs bottom-up node contractions (akin to CaGreS). The primary distinction lies in the objective function: K-SNAP focuses on ensuring homogeneity among nodes within a cluster. We have enhanced K-SNAP to address acyclicity. **TRANSIT-CLUSTER** In [98], the authors proposed Transit Clusters as a specific type of summary causal DAG that maintains identifiability properties under certain conditions. They introduced an algorithm to identify all transit clusters for a graph. For a fair comparison, we consider the transit cluster that meets the constraints and has the maximal RB. **CIC** [64] The authors of [64] proposed a Clustering Information Criterion (CIC), based on information-theoretic measures that represent various complex interactions among variables in a causal DAG. Based on this criterion, they developed a greedy-based approach to learn clustered causal DAGs directly from the data. **RANDOM**: As a sanity check, this algorithm generates a random summary DAG that adheres to the size constraint.

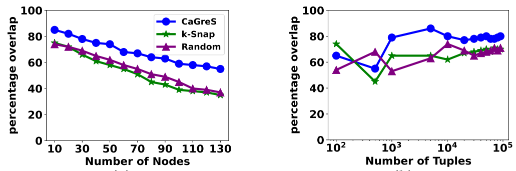
Metrics of evaluation As mentioned, in some cases, summary DAGs are incomparable, meaning that their RBs are not strictly implied by one another. To nevertheless compare their quality, we quantify the number of additional edges in their corresponding canonical causal DAG — edges that are absent in the original DAG. A smaller number of such edges implies a more sparse summary DAG that encodes more CIs. Additionally, with a smaller number of edges, the adjustment sets used to compute causal effects are likely to be smaller and closer to the ones computed over the original causal DAG. As we show, these metrics are highly correlated.

As a default configuration, we set the size constraint k to $\frac{n}{2}$, where n is the number of nodes in the input causal DAG. The runtime cutoff was set at 1 hour.



(a) Flights (b) German

Figure 8: Average percentage overlap with ground truth.



(a) (b)

Figure 9: Average percentage overlap vs. data properties.

8.2 Usability Evaluation (C1)

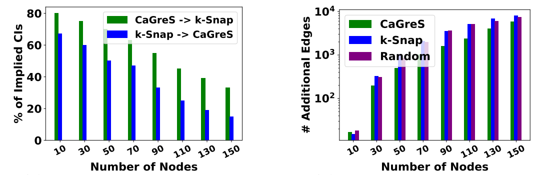
8.2.1 The utility of the summary causal DAGs for causal inference. We assess the utility of the summary causal DAGs for causal inference. To this end, we compare the causal effects estimated within the original DAG with those computed within the summary causal DAGs. Each causal effect estimation yields an interval (of 95% confidence). We compare the intervals derived from the input DAG (the ground truth) with those obtained by the baselines. Given that the adjustment sets in the summary DAGs may differ from those in the original DAG, we anticipate getting different intervals.

Average Percentage Overlap: We report the average percentage of overlap of the causal interval across all node pairs connected by a causal path in the input DAG. A higher percentage overlap indicates greater robustness in causal inference. The results for Flights and German are shown in Fig. 8 (similar trends were observed for the other datasets). CaGreS's average percentage overlap is close to that of Brute-Force, suggesting a high degree of similarity between the two summary DAGs. CaGreS surpasses all other competitors. This underscores the superior suitability of CaGreS for causal inference compared to the baselines.

In what comes next, we use synthetic data, allowing us to manage the number of nodes in the input DAG and database tuples. We omit from presentation the Brute-Force, Transit-Cluster, and CIC baselines as they exceeded our time limit cutoff.

# of attributes: We examine how the number of nodes in the input causal DAG affects the performance. With a larger number of nodes, the task of finding the optimal summary DAG becomes harder. Here, the number of data tuples is fixed at 10K. The results are depicted in Fig. 9(a). For all baselines, with more data attributes, their alignment with the input causal DAG diminishes. Nevertheless, CaGreS consistently outperforms the competing methods.

# of tuples: We examine the effect of data size (# of tuples) on performance. Given that causal effects are statistical measures that are sensitive to the sample size, we anticipate that as the number of tuples grows, the effects evaluated on the summary DAGs will converge towards their counterparts evaluated on the input DAG. Here, the number of nodes in the input causal DAG is fixed at 30. Our findings are shown in Fig. 9 (b). For all baselines, when the data size is small, the results are noisy, and when it increases, the results tend to stabilize. *Again, CaGreS outperforms its competitors.*



(a) Higher bars are better (b) Lower bars are better

Figure 10: Quality metrics vs. the number of nodes.

8.3 Quality Evaluation (C2)

As mentioned, in many cases, there are many summary DAGs with maximal RBs. We, therefore, investigate several evaluation metrics to determine which summary causal DAG is superior: (1) The percentage of CIs in the RB of one summary causal DAG that is implied by the RB of another summary DAG.(2) The number of additional edges in the canonical causal DAG. (3) The size of the adjustment sets in the evaluation of causal estimations. With smaller adjustment sets, the estimation will likely be more accurate. As we will show, these metrics are highly correlated.

We generated a series of random causal with a different number of nodes (five random DAGs for each node count), while keeping all other parameters fixed. We omit from presentation the Brute-Force, Transit-Cluster, and CIC baselines as they exceeded our time limit cutoff. The results are depicted in Fig. 10. Fig. 10(a) depicts the percentage of the CIs in the RB of k-Snap that are implied by that of CaGreS and vice versa. Similar trends were observed for Random, and thus are omitted. A higher percentage of k-Snap's CIs are implied by CaGreS compared to the percentage of CaGreS's CIs that are implied by k-Snap. Hence, while no RB entirely implies the other RB, we can still conclude that the summary DAG of CaGreS is superior to that of k-Snap. Fig. 10(b) depicts the number of additional edges in the . CaGreS consistently yields summary DAGs with fewer additional edges. This is not surprising, as the objective of CaGreS is to minimize the number of such edges. We also considered the average size of the adjustment sets in the computation of causal estimations (omitted from the presentation). We report that CaGreS outperforms the competitors, consistently yielding smaller adjustment sets. As shown above, this results in more accurate causal estimations, as fewer redundant variables are considered. *Since these three metrics are closely interrelated, we deduce that it is appropriate to use the count of additional edges for comparing the quality of summary DAGs.*

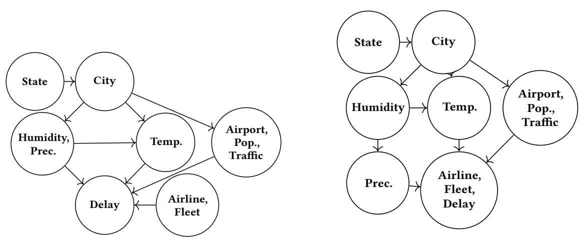
8.4 Effectiveness Evaluation (C3)

We assess CaGreS based on quality and runtime performance.

Case Study: Flights We present the pairwise percentage of the CIs in the RB implied by all baseline pairs. The results are shown in Table 3. The summary DAGs obtained by CaGreS and k-Snap are given in Fig. 11 (The optimal summary DAG by Brute-Force is omitted from presentation). Brute-Force yields the most effective summary DAG, as it implies the highest percentage of CIs of any other baseline. While 60% of the CIs of k-Snap are implied by the RB of CaGreS, only 16% of the CIs of CaGreS are implied by the RB of k-Snap. This superiority of CaGreS over k-Snap is further

Table 3: Pair-wise percentage of the RB's CIs implied.

	Brute-Force	CaGreS	k-Snap	Random	TC	CIC
Brute-Force	-	83.3%	50%	50%	16.6%	16.6%
CaGreS	50%	-	60%	16.6%	0%	16%
k-Snap	0%	16.6%	-	50%	16.6%	0%
Random	16.6%	0%	50%	-	0%	16.6%
TC	0%	0%	16.6%	16.6%	-	50%
CIC	0%	0%	0%	16.6%	0%	-



(a) CaGreS **(b) k-Snap**

Figure 11: Summary causal DAGs for the Flights dataset.

supported by a lower number of additional edges (7 for CaGreS, 13 for Brute-Force, and 14 for k-Snap). Intuitively, this stems from k-Snap's decision to form two 3-size clusters, connected by an edge. In the resulting canonical causal DAG, every pair of nodes within and between the clusters is connected by an edge.

Next, for each dataset, we report the runtime and the number of additional edges in the canonical causal DAG as a quality metric. The results are depicted in Fig. 12. Only CaGreS, k-Snap, and Random can effectively handle input causal DAGs with more than 20 nodes within a responsive runtime. While Random and k-Snap exhibit runtimes comparable to that of CaGreS, the latter consistently produces summary DAGs with fewer additional edges. As shown, this implies more accurate causal estimations. As expected, Brute-Force outperforms CaGreS in terms of quality but is impractical for interactive interaction. CIC exhibits relatively low performance, primarily due to the inclusion of a causal discovery component. Similarly, Transit-Cluster faces limitations in handling input causal DAGs with more than 20 nodes, as the algorithm materializes all transit clusters, and then selects the maximal one.

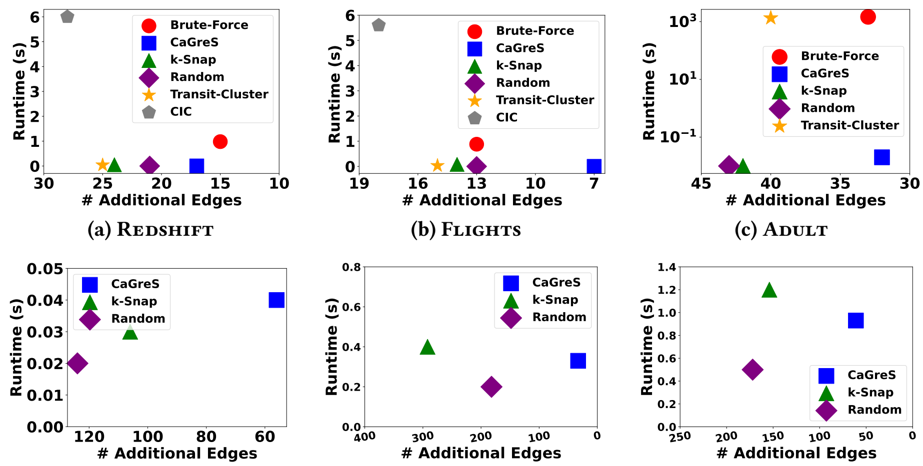
8.4.1 Sensitivity Analysis. We analyze the influence of different parameters on performance. In these experiments, our focus shifts to synthetic data, which enables us to manipulate data-related factors.
Input DAG size We vary the number of nodes in the input DAG. To this end, we generated a series of random DAGs, progressively increasing the number of nodes (5 DAGs per node count) while keeping all other parameters constant. The results are shown in Fig. 13. As expected, k-Snap and CaGreS exhibit a polynomial increase in runtime (Fig. 13(a)). The improvement relative to k-Snap is attributed to our caching mechanisms, particularly beneficial for large causal DAGs. Even when the causal DAG comprises over 100 nodes (i.e., over 100 variables in the data), CaGreS summarizes the DAG in less than 2 minutes. Observe that CaGreS consistently generates summary DAGs with fewer additional edges (Fig. 13(b)), indicating better quality.
Summary size We vary the size constraint k. Here, the node count is set to 50, and the graph density is held constant at 0.3. The results are depicted in Fig.14. The runtime of both CaGreS and k-Snap demonstrate a linear increase with k (Fig. 14(a)). This is because larger k values necessitate more merges. As expected, CaGreS manages to generate summary DAGs corresponding to canonical causal DAGs with fewer edges (Fig. 14(b)).
Graph density We investigate the influence of graph density on performance. We observe a nearly linear increase in runtime for both CaGreS and k-Snap as graph density rises (Figure 15(a)). This is because both algorithms examine the neighboring nodes of each node pair, and with increased density, there are more neighboring nodes. In terms of quality, as density increases, the number of additional edges also rises for both algorithms. However, at high densities (above 0.7), where the graph already includes many edges, there are fewer edges left to be added. Consequently, the number of additional edges decreases (Figure 15(b)).
Data size We report that the data size, i.e., number of tuples, has no effect on the performance of CaGreS and k-Snap. This is because both algorithms only examine the input causal DAGs.

9 RELATED WORK

Summary Causal DAGs. The abstraction of causal models has been studied in literature [85]. Previous work [12, 68] investigated the problem of determining under what assumptions a DAG over sets of variables can represent the same CIs between those individual variables. The authors of [17, 18, 80] explored the problem of determining the causes of a target behavior (a macro-variable) from micro-variables (e.g., image pixels). Other works include chain graphs and ancestral causal graphs [45, 108], which were developed to represent sets of causal diagrams equivalent under specific properties. The authors of [76] presented a method to compress causal graphs by removing nodes to remove redundant information. In contrast, our work studies the problem of causal DAG summarization, wherein certain causal information is inevitably lost, yet the resultant summary DAG maintains reliable causal inference.

The authors of [9] expanded the *do-calculus* framework [70] to clustered causal graphs, a related but distinct concept. Our contribution lies in presenting a more streamlined proof of this principle, relying on the connection between node contraction and edge addition. We also propose an algorithm to generate a summary DAG from a given causal DAG. As discussed in our experiments, two approaches have addressed this problem. Transit-Cluster [98], focuses on clustering mediator variables but lacks control over the summary DAG size. Another approach, the CIC algorithm [64], directly learns a summary DAG from data but does not prioritize preserving independence information.

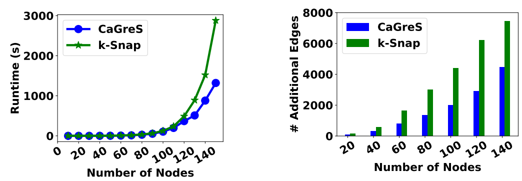
General-Purpose Summary Graphs Graph summarization aims to condense an input graph into a more concise representation. This condensed form not only reduces the graph's size but also facilitates efficient query answering [25, 51, 77, 90], enables enhanced data visualization and pattern discovery [22, 24, 40, 43, 47, 88], and supports extraction of influence dynamics [55]. Various graph summarization techniques have been explored, including grouping nodes based on similarity measures [46, 48, 58, 63, 77, 90, 91, 93, 97, 105, 110], reducing the number bits required to represent graphs [15, 53, 63, 78, 86], and removing unimportant nodes and edges [51, 94]. We argue that existing techniques are ill-suited for the causal DAG summarization problem. Graph summarization objectives differ across applications, often prioritizing minimizing the



(a) Redshift (b) Flights (c) Adult

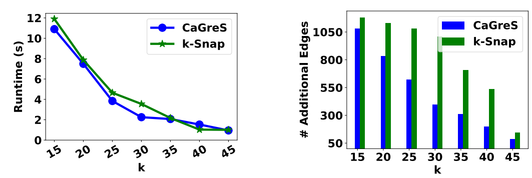
(d) German (e) Accidents (f) URLs

Figure 12: Number of additional edges vs. runtime. The optimal solution should be located in the lower right region.



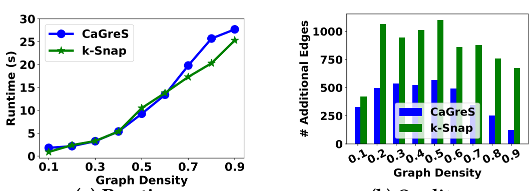
(a) Runtime (b) Quality

Figure 13: Number of nodes vs. running times and quality.



(a) Runtime (b) Quality

Figure 14: Summary size k vs. running times and quality.



(a) Runtime (b) Quality

Figure 15: Graph density vs. running times and quality.

reconstruction error [46, 105], facilitating accurate query answering [51, 90], or enhancing visualizations [40, 43]. Consequently, existing methods inadequately cater to the objective of preserving causal information, often yielding graphs unsuitable for causal inference, as shown in Section 1.

Data Summarization. Data summarization involves distilling meaningful insights from large datasets into a compact, understandable format, which is crucial for uncovering trends and patterns. Related efforts have concentrated on summarizing tabular datasets [41, 44, 102], aiding analysts in extracting insights that might otherwise remain obscured. While our focus is different, its impact is akin, potentially assisting analysts in grasping causal relationships within high-dimensional datasets.

Causal Discovery. Causal discovery is a well-studied problem [34, 107, 109], whose goal is to infer causal relationships among variables. While background knowledge is crucial [71], causal DAGs can be inferred from data under certain assumptions [20, 34]. Existing methods include constraint-based [95] and score-based algorithms [20, 89, 103, 113]. Pashami et al. [69] proposed a clustering-based method, using a cluster-based conflict resolution mechanism to determine the causal relationship among variables. Recent works [16, 100] have explored the use of LLMs for causal discovery. Our aim is to summarize causal DAGs representing relationships in high-dimensional data. Consequently, our work serves as a complementary endeavor to existing research in causal discovery.

10 LIMITATIONS & CONCLUSIONS

A mixed graph, incorporating both directed and undirected edges, is a typical output of causal discovery algorithms [19, 73, 95]. For simplicity in exposition, we concentrated on regular causal DAGs throughout this paper. Nevertheless, our results and algorithms apply to mixed graphs as well.

We note that the user-defined size constraint may significantly influence the generated summary DAG. This parameter might need tuning by the user to achieve a desirable summary DAG. Future research will focus on methods to suggest the optimal value for this parameter. This paper opens up promising future research directions. This includes the development of compact representations of node sets tailored specifically for causal inference, addressing additional size constraints, and refining algorithms with theoretical guarantees.

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A SEMIGRAPHOID-AXIOMS

The semi-graphoid axioms are the following:

(1) Triviality: $I(A;\emptyset|C)$=0.
(2) Symmetry: $I(A;B|C)=0 \Longrightarrow I(A;C|B)=0$.
(3) Decomposition: $I(A;BD|C)=0 \Longrightarrow I(A;B|D)=0$.
(4) Contraction: $I(A;B|C)=0, I(A;D|BC)=0 \Longrightarrow I(A;BD|C)=0$.
(5) Weak Union: $I(A;BD|C)=0 \Longrightarrow I(A;B|CD)=0, I(A;D|BC)=0$.

The semi-graphoid axioms can be summarized using the following identity, which follows from the *chain-rule* for mutual information [104].

$$I(A;BD|C)=0 \text{ if and only if } I(A;B|C)=0 \text{ and } I(A;D|BC)=0 \quad (4)$$

B THE RECURSIVE BASIS

Given a recursive basis and a topological order over the nodes, we can construct the corresponding causal DAG as follows. First, insert the first node X_1. For the second node X_2, if it is independent of X_1, do not add an edge between X_1 and X_2. Otherwise, insert the edge $X_1 \rightarrow X_2$. The same goes for the i-th node X_i. If it is independent of any of its preceding nodes $X_1, \dots X_{i-1}$, do not insert the edge.

Otherwise, insert the edge pointing to X_i. We illustrate this algorithm with the following example.

Consider the recursive basis: $(C \perp\!\!\!\perp B|A), (D \perp\!\!\!\perp A|BC), (E \perp\!\!\!\perp ABC|D)$, with the alphabetical order over the nodes. This is the recursive basis of the causal DAG in Figure 3(a). We first add a node for the variablele A. Since B is not independent of A, we add the edge from A to B. Next, since C is not independent of A, we add an edge from A to C. Since C is independent of B (given A), we do not add an edge from B to C. Next, since D is only independent of A, we add edges from B and C to D (but not from A). Lastly, since E is independent of A, B and C, we only add the edge form D to E. Note that we got the exact same causal DAG in Figure 3(a)

C PROOFS

Next, we provide the missing proofs.

We begin with some basic definitions used in the proofs.

Let $\mathcal{G}$ be a causal DAG. and let $U, V \in \mathsf{V}(\mathcal{G})$ be two nodes. We say that U is a *parent* of V, and V a *child* of U if $(U \rightarrow V) \in \mathsf{E}(\mathcal{G})$. A *directed path* t=$(V_1, \dots, V_n)$ is a sequence of nodes such that there is an edge $(V_i \rightarrow V_{i+1}) \in \mathsf{E}(\mathcal{G})$ for every $i \in \{1, \dots, n-1\}$. We say that V is a *descendant* of U, and U an *ancestor* of V if there is a directed path from U to V. We denote the child-nodes of V in $\mathcal{G}$ as $\mathtt{ch}_{\mathcal{G}}(V)$; the descendants of V (we assume that $V \in \mathtt{Dsc}_{\mathcal{G}}(V)$) as $\mathtt{Dsc}_{\mathcal{G}}(V)$, and the nodes of $\mathcal{G}$ that are not descendants of V as $\mathtt{NDsc}_{\mathcal{G}}(V)$. For a set of nodes $\mathsf{S} \subseteq \mathsf{V}(\mathcal{G})$, we let $\mathtt{Dsc}_{\mathcal{G}}(\mathsf{S}) \stackrel{\text{def}}{=} \bigcup_{U \in \mathsf{S}} \mathtt{Dsc}_{\mathcal{G}}(U)$, and by $\mathtt{NDsc}_{\mathcal{G}}(\mathsf{S}) \stackrel{\text{def}}{=} \bigcap_{U \in \mathsf{S}} \mathtt{NDsc}_{\mathcal{G}}(U)$.

A *trail* t=$(V_1, \dots, V_n)$ is a sequence of nodes such that there is an edge between V_i and V_{i+1} for every $i \in \{1, \dots, n-1\}$. That is, $(V_i \rightarrow V_{i+1}) \in \mathsf{E}(\mathcal{G})$ or $(V_i \leftarrow V_{i+1}) \in \mathsf{E}(\mathcal{G})$ for every $i \in \{1, \dots, n-1\}$. A node V_i is said to be *head-to-head* with respect to t if $(V_{i-1} \rightarrow V_i) \in \mathsf{E}(\mathcal{G})$ and $(V_i \leftarrow V_{i+1}) \in \mathsf{E}(\mathcal{G})$. A trail $t = (V_1, \dots, V_n)$ is *active* given $\mathbf{Z} \subseteq \mathcal{V}$ if (1) every V_i that is a head-to-head node with respect to t either belongs to $\mathbf{Z}$ or has a descendant in $\mathbf{Z}$, and (2) every V_i that is not a head-to-head node w.r.t. t does not belong to $\mathbf{Z}$. If a trail t is not active given $\mathbf{Z}$, then it is *blocked* given $\mathbf{Z}$.

C.1 Proofs for Section 3

Proof of Lemma 3.1. Let P be a directed path from A to B, such that $|P| \geq 2$. Let X be A's successor in P, and Y be B's predecessor in P. By our assumption that $|P| \geq 2$, $X \notin \{A, B\}$, but Y may be the same as X. Now, consider the graph H. By definition, H contains a node AB, with an incoming edge from Y, and an outgoing edge to X. If $X = Y$, we immediately get the cycle $AB \rightarrow X \rightarrow AB$. Otherwise, we consider the subpath P' (of P) from X to Y ($X \underset{P'}{\rightsquigarrow} Y$) in G. This results in the following cycle in H: $Y \rightarrow AB \rightarrow X \underset{P'}{\rightsquigarrow} Y$.

Now, suppose that H contains the cycle C. C must contain the node AB. Otherwise, the cycle is included in G, which leads to a contradiction that G is a DAG. Let Y and X be the incoming and outgoing vertices, respectively, to AB in C. Then, there is a directed path P from X to Y in H that avoids AB. That is, every vertex and edge on the path P belongs to G as well. Hence, P is a directed path from X to Y in G. Since Y is incoming to AB, then Y is incoming to either A or B in G. Assume, wlog, that $Y \rightarrow A \in E$. Since X is an outgoing vertex from AB, then it is outgoing from from either A or B (or both). If X is outgoing from A, then we get the following cycle in G: $Y \rightarrow A \rightarrow X \underset{P}{\rightsquigarrow} Y$. Since G is a DAG, this brings us to a contradiction. Therefore, X must be outgoing from B and not A. But this gives us the following directed path from B to A:

$$A \leftarrow Y \underset{P}{\leftsquigarrow} X \leftarrow B.$$

This completes the proof. □

Next, we show that the causal DAG summarization problem is NP-hard via a reduction from the k-Min-Cut problem [37]. Let G be an undirected graph with weighted edges (i.e., $w : \mathsf{V}(G) \rightarrow \mathbb{R}_{\geq 0}$). The k-Min-Cut problem consists of partitioning $\mathsf{V}(G)$ into k disjoint clusters so as to minimize the sum of weights of the edges joining vertices in different clusters. It is well-known that k-Min-Cut is NP-hard even if $k = 2$ [31]. In other words, deciding whether there exists a k-clustering of $\mathsf{V}(G)$ to clusters $\{V_1, \dots, V_k\}$, where the sum of weights of edges between vertices in distinct clusters is at most a given threshold γ is NP-hard.

Proof of Theorem 3.2. In this proof we make the assumption that $InterSim(\mathsf{S}) = \sum_{u,v \in \mathsf{S}} InterSim(\{u, v\})$ where $\mathsf{S} \subseteq \mathsf{V}(G)$. Given a DAG G, a similarity threshold τ, and its summary graph $\mathcal{H}$, it is easy to verify that $\sum_{\mathsf{S} \in \mathsf{V}(\mathcal{H})} InterSim(\mathsf{S}) \geq \tau$. Therefore, the causal DAG summarization problem is in NP.

We prove hardness by reduction from k-Min-Cut. Let G be an undirected weighted graph, and let $\gamma > 0$ be the threshold for the k-Min-Cut problem. For every pair of vertices $u, v \in \mathsf{V}(G)$, define $InterSim(\{u,v\}) \stackrel{\text{def}}{=} w(u,v)$; define $\tau \stackrel{\text{def}}{=} \sum_{u,v\in\mathsf{V}(G)} w(u,v) - \gamma$. Let G' be the DAG that results from G by orienting its edges such that no directed cycles are generated (this is simple to do by fixing a complete order over the vertices, and orienting the edges accordingly). It is easy to see that there is a k-clustering $\{V_1, \ldots, V_k\}$ of G where the sum of weights of edges between vertices in distinct clusters is at least γ if and only if $\sum_{i=1}^{k} InterSim(V_i) \geq \tau$ in G'. □

C.2 Proofs for Section 4

Next, we prove some simple lemmas that will be useful later on. We denote by $\mathcal{H}_{UV}$ the summary DAG where nodes U and V are contracted.

Lemma C.1. *The following holds:*

$$\pi_{\mathcal{H}_{UV}}(\mathbf{X_{UV}}) = \pi_{\mathcal{G}_{UV}}(U) \qquad \pi_{\mathcal{G}_{UV}}(V) = \pi_{\mathcal{G}_{UV}}(U) \cup \{U\} \tag{5}$$

$$\mathsf{ch}_{\mathcal{H}_{UV}}(\mathbf{X_{UV}}) = \mathsf{ch}_{\mathcal{G}_{UV}}(V) \qquad \mathsf{ch}_{\mathcal{G}_{UV}}(U) = \mathsf{ch}_{\mathcal{G}_{UV}}(V) \cup \{V\} \tag{6}$$

$$\mathsf{NDsc}_{\mathcal{H}_{UV}}(\mathbf{X_{UV}}) = \mathsf{NDsc}_{\mathcal{G}_{UV}}(U) \qquad \mathsf{NDsc}_{\mathcal{G}_{UV}}(V) = \mathsf{NDsc}_{\mathcal{G}_{UV}}(U) \cup \{U\} \tag{7}$$

Lemma C.2. *Let $T \in \mathcal{V}$ such that $T \notin \{U,V\} \cup \mathsf{ch}_{\mathcal{G}}(U) \cup \mathsf{ch}_{\mathcal{G}}(V)$. Then it holds that:*

$$\pi_{\mathcal{G}_{UV}}(T) = \pi_{\mathcal{H}_{UV}}(T) \text{ and} \tag{8}$$

$$\mathsf{NDsc}_{\mathcal{G}_{UV}}(T) \backslash \{UV\} = \mathsf{NDsc}_{\mathcal{H}}(T) \backslash \{\mathbf{X_{UV}}\} \text{ and} \tag{9}$$

$$\{U,V\} \subseteq \mathsf{NDsc}_{\mathcal{G}_{UV}}(T) \text{ if and only if } \mathbf{X_{UV}} \in \mathsf{NDsc}_{\mathcal{H}}(T) \tag{10}$$

Now, let $T \in \mathcal{V}$ such that $T \notin \{U,V\} \cup \pi_{\mathcal{G}}(U) \cup \pi_{\mathcal{G}}(V)$. Then:

$$\mathsf{ch}_{\mathcal{G}_{UV}}(T) = \mathsf{ch}_{\mathcal{H}_{UV}}(T) \text{ and} \tag{11}$$

$$\mathsf{Dsc}_{\mathcal{G}_{UV}}(T) \backslash \{U,V\} = \mathsf{Dsc}_{\mathcal{H}_{UV}}(T) \backslash \{\mathbf{X_{UV}}\} \tag{12}$$

$$\{U,V\} \subseteq \mathsf{Dsc}_{\mathcal{G}_{UV}}(T) \text{ if and only if } \mathbf{X_{UV}} \in \mathsf{Dsc}_{\mathcal{H}_{UV}}(T) \tag{13}$$

Proof of Lemma C.1. By the definition of G', it holds that $\pi_{G'}(u) = \pi_G(u) \cup \pi_G(v)$. Since $(u,v) \in \mathsf{E}(G')$, then $\pi_{G'}(v) = \pi_{G'}(u) \cup \{u\}$. Similarly, $\mathsf{ch}_{G'}(v) = \mathsf{ch}_G(u) \cup \mathsf{ch}_G(v)$, and since $(u,v) \in \mathsf{E}(G')$, then $\mathsf{ch}_{G'}(u) = \mathsf{ch}_{G'}(v) \cup \{v\}$. By definition of edge contraction, it holds that $\pi_H(X_{uv}) = \pi_G(u) \cup \pi_G(v) = \pi_{G'}(u)$, proving (5). Also, by definition of edge contraction, it holds that $\mathsf{ch}_H(X_{uv}) = \mathsf{ch}_G(u) \cup \mathsf{ch}_G(v) = \mathsf{ch}_{G'}(v)$, proving (6).

We now prove (7). Let $t \in \mathsf{NDsc}_H(X_{uv})$. If $t \notin \mathsf{NDsc}_{G'}(u)$, then $t \in \mathsf{Dsc}_{G'}(u) \backslash \{v\}$. This means that there is a directed path P from u to t in G'. Let s be the first vertex on this path (after u). Since $s \in \mathsf{ch}_{G'}(u) \backslash \{v\}$, then by the definition of G', $s \in \mathsf{ch}_G(u) \cup \mathsf{ch}_G(v)$. By the definition of edge contraction, $s \in \mathsf{ch}_H(X_{uv})$. Since $s \notin uv \cup \pi_G(u) \cup \pi_G(v)$, then every directed path starting at s in G remains a directed path in H. But this means that there is a directed path from X_{uv} to t (via s); contradicting the assumption that $t \in \mathsf{NDsc}_H(X_{uv})$. Now, let $t \in \mathsf{NDsc}_{G'}(u)$. If $t \notin \mathsf{NDsc}_H(X_{uv})$, then $t \in \mathsf{Dsc}_H(X_{uv}) \backslash \{X_{uv}\}$. This means that there is a directed path P from X_{uv} to t in H. Let s be the first vertex on this path (after X_{uv}). Since $s \in \mathsf{ch}_H(X_{uv})$, then by the definition of H, $s \in \mathsf{ch}_G(u) \cup \mathsf{ch}_G(v)$. But then, by the definition of G', it holds that $s \in \mathsf{ch}_{G'}(u)$. Since no edges are removed by the transition from G to G', there is a directed path from u to (via s) in G'; contradicting the assumption that $t \in \mathsf{NDsc}_{G'}(u)$. □

Proof of Lemma C.2. By the definition of contraction, the only vertices in G whose parent-set can potentially change following the contraction of u and v belong to the set $uv \cup \mathsf{ch}_G(u) \cup \mathsf{ch}_G(v)$. By the definition of $\mathsf{E}(G')$, the only vertices in G whose parent-set can potentially change belong to the set $uv \cup \mathsf{ch}_G(u) \cup \mathsf{ch}_G(v)$. Therefore, if $t \notin uv \cup \mathsf{ch}_G(u) \cup \mathsf{ch}_G(v)$, then $\pi_{G'}(t) = \pi_H(t) = \pi_G(t)$. This proves (8).

By the definition of contraction, the only vertices in G whose child-set can potentially change following the contraction of u and v belong to the set $uv \cup \pi_G(u) \cup \pi_G(v)$. By the definition of $\mathsf{E}(G')$, the only vertices in G whose child-set can potentially change belong to the set $uv \cup \pi_G(u) \cup \pi_G(v)$. Therefore, if $t \notin uv \cup \pi_G(u) \cup \pi_G(v)$, then $\mathsf{ch}_{G'}(t) = \mathsf{ch}_H(t) = \mathsf{ch}_G(t)$. This proves (11).

We now prove (9); Let $s \in \mathsf{NDsc}_H(t) \backslash \{X_{uv}\}$. If $s \notin \mathsf{NDsc}_{G'}(t)$, then $s \in \mathsf{Dsc}_{G'}(t)$. That is, there is a directed path P from t to s in G'. Let us assume wlog that P is the shortest directed path from t to s in G'. By this assumption, exactly one of the following holds: (1) $u, v \notin \mathsf{V}(P)$ (2) $u \in \mathsf{V}(P)$, $v \notin nodes(P)$ (3) $v \in \mathsf{V}(P)$, $u \notin nodes(P)$, or (4) $(u,v) \in \mathsf{E}(P)$. In the first case, every edge of P is also an edge of $\mathsf{E}(G)$, that does not enter or exit $\{u,v\}$. Therefore, P is a directed path in H, a contradiction. In case (2), since $\pi_{G'}(u) = \pi_H(X_{uv})$ (see (5)), and $\mathsf{ch}_{G'}(u) = \mathsf{ch}_H(X_{uv}) \backslash \{v\}$ (see (6)), then the path with nodes $X_{uv} \cup (\mathsf{V}(P) \setminus \{u\})$, is a directed path in H from s to t; a contradiction. In case (3), since $\mathsf{ch}_{G'}(v) = \mathsf{ch}_H(X_{uv})$ (see (6)), and $\pi_{G'}(v) = \pi_H(X_{uv}) \backslash \{u\}$ (see (5)), then the path with nodes $X_{uv} \cup (\mathsf{V}(P) \setminus \{v\})$, is a directed path in H from s to t; a contradiction. Finally, if $(u,v) \in \mathsf{E}(P)$, then since $\pi_{G'}(u) = \pi_H(X_{uv})$ and $\mathsf{ch}_{G'}(v) = \mathsf{ch}_H(X_{uv})$, then the path with nodes $X_{uv} \cup (\mathsf{V}(P) \backslash uv)$, is a directed path from s to t in H; a contradiction. For the other direction, let $s \in \mathsf{NDsc}_{G'}(t) \backslash uv$. If $s \notin \mathsf{NDsc}_H(t)$, then there is a directed path P from t to s in H. If $X_{uv} \notin \mathsf{V}(P)$, then $\mathsf{E}(P) \subseteq \mathsf{E}(G) \subseteq \mathsf{E}(G')$, and hence P is a directed path from t to s in G'. Otherwise, if $X_{uv} \in \mathsf{V}(P)$, then since $\pi_H(X_{uv}) = \pi_{G'}(u)$, $\mathsf{ch}_H(X_{uv}) = \mathsf{ch}_{G'}(v)$, and $(u,v) \in \mathsf{E}(G')$, then replacing X_{uv}, with the edge (u,v) results in a directed t,s-path in G'; a contradiction. □

Proof of Theorem 4.1. We first prove that $\Sigma_{\text{RB}}(G') \implies \Sigma_{\text{RB}}(H)$. We divide to cases. Let $(X_i; B_i | \pi_H(X_i)) \in \Sigma_{\text{RB}}(H)$, where $X_{uv} \notin B_i \cup \pi_H(X_i) \cup \{X_i\}$. In particular, $X_i \in \mathsf{V}(G)$, and $X_i \notin \{u,v\} \cup \mathsf{ch}_H(X_{uv}) = \{u,v\} \cup \mathsf{ch}_G(u) \cup \mathsf{ch}_G(v)$. By (9), we have that $\pi_{G'}(X_i) = \pi_H(X_i)$, and that $\mathsf{NDsc}_{G'}(X_i) \backslash uv = \mathsf{NDsc}_H(X_i) \backslash X_{uv}$. Therefore, we have that $(X_i; \mathsf{NDsc}_H(X_i) \backslash \{X_{uv}\} | \pi_{G'}(X_i))_{G'}$. Since $B_i \subseteq \mathsf{NDsc}_H(X_i) \backslash \{X_{uv}\}$, then, by decomposition, we have that $\Sigma_{\text{RB}}(G') \implies (X_i; B_i | \pi_H(X_i))$.

Now, let $(X_i; X_{uv} B_i | \pi_H(X_i)) \in \Sigma_{\text{RB}}(H)$. In this case as well $X_i \in \mathsf{V}(G)$, and $X_i \notin \{u,v\} \cup \mathsf{ch}_H(X_{uv}) = \{u,v\} \cup \mathsf{ch}_G(u) \cup \mathsf{ch}_G(v)$. By (9), we have that $\pi_{G'}(X_i) = \pi_H(X_i)$, and that $\mathsf{NDsc}_{G'}(X_i) \backslash uv = \mathsf{NDsc}_H(X_i) \backslash X_{uv}$. By , we have that $X_{uv} \in \mathsf{NDsc}_H(X_i)$ iff $uv \subseteq \mathsf{NDsc}_{G'}(X_i)$. Therefore, $B_i X_{uv} \subseteq \mathsf{NDsc}_H(X_i)$ iff $B_i uv \subseteq \mathsf{NDsc}_{G'}(X_i)$. This means that $\Sigma_{\text{RB}}(G') \implies (X_i; \mathsf{NDsc}_{G'}(X_i) | \pi_{G'}(X_i))$. By decomposition, we have that $\Sigma_{\text{RB}}(G') \implies (X_i; B_i uv | \pi_H(X_i))$ as required.

Now, suppose that $X_{uv} \in \pi_H(X_i)$, or that $X_i \in \mathsf{ch}_H(X_{uv})$. Since $X_i \in \mathsf{V}(G) \backslash \{u,v\}$, then by (6), we have that $X_i \in \mathsf{ch}_{G'}(v) \backslash \{v\}$.

Therefore, $\pi_{G'}(X_i) = \pi_H(X_i)\backslash\{X_{uv}\} \cup \{u, v\}$. By (9), we have that:

$$\begin{aligned}\mathsf{NDsc}_{G'}(X_i)\backslash\pi_{G'}(X_i) &= \mathsf{NDsc}_{G'}(X_i)\backslash(\pi_H(X_i)\backslash\{X_{uv}\} \cup uv)\\ &= (\mathsf{NDsc}_{G'}(X_i)\backslash uv)\backslash(\pi_H(X_i)\backslash\{X_{uv}\})\\ &\underbrace{=}_{(9)} (\mathsf{NDsc}_H(X_i)\backslash\{X_{uv}\})\backslash(\pi_H(X_i)\backslash\{X_{uv}\})\\ &= \mathsf{NDsc}_H(X_i)\backslash\pi_H(X_i)\end{aligned}$$

Therefore, $\Sigma_{\mathrm{RB}}(G') \implies (X_i; \mathsf{NDsc}_H(X_i)\backslash\pi_H(X_i) \mid \pi_H(X_i)\backslash\{X_{uv}\}\cup \{u, v\})$. Finally, we consider the case where $X_i = X_{uv}$. By construction of G', and by (7), it holds that:

$$\Sigma_{\mathrm{RB}}(G') \implies (u; \mathsf{NDsc}_{G'}(u)\backslash\pi_{G'}(u) \mid \pi_{G'}(u)) \tag{14}$$

$$\Sigma_{\mathrm{RB}}(G') \implies (v; \mathsf{NDsc}_{G'}(u)\backslash\pi_{G'}(u) \mid \pi_{G'}(u) \cup \{u\}) \tag{15}$$

By applying the contraction axiom on (14) and (15), we get that

$$\Sigma_{\mathrm{RB}}(G') \implies (uv; \mathsf{NDsc}_{G'}(u)\backslash\pi_{G'}(u) \mid \pi_{G'}(u)).$$

Using the fact that hat $\pi_H(X_{uv}) = \pi_{G'}(u)$ (see (5)), and that $\mathsf{NDsc}_H(X_{uv}) = \mathsf{NDsc}_{G'}(u)$ (see (7)), we get that

$$\Sigma_{\mathrm{RB}}(G') \implies (uv; \mathsf{NDsc}_H(X_{uv})\backslash\pi_H(X_{uv}) \mid \pi_H(X_{uv})).$$

Since $B_i \subseteq \mathsf{NDsc}_H(X_{uv})\backslash(\pi_H(X_{uv}) \cup \{X_{uv}\})$, this proves the claim.

Now, for the other direction. Let $(X_i; B_i \mid \pi_{G'}(X_i)) \in \Sigma_{\mathrm{RB}}(G')$. If $u, v \notin X_i \cup B_i \cup \pi_{G'}(X_i))$, then $X_i \notin \{u, v\} \cup \mathsf{ch}_G(u) \cup \mathsf{ch}_G(v)$. By (9), it holds that $\pi_H(X_i) = \pi_{G'}(X_i)$, and that $\mathsf{NDsc}_{G'}(X_i)\backslash uv = \mathsf{NDsc}_H(X_i)\backslash X_{uv}$. Since $B_i \subseteq \mathsf{NDsc}_{G'}(X_i)\backslash uv = \mathsf{NDsc}_H(X_i)\backslash X_{uv}$, then $\Sigma_{\mathrm{RB}}(H) \implies (X_i; B_i \mid \pi_{G'}(X_i))$.

If $uv \subseteq B_i$, then $u, v \notin \pi_{G'}(X_i)$, then $X_i \notin uv \cup \mathsf{ch}_G(u) \cup \mathsf{ch}_G(v)$. By (9), we have that $\pi_H(X_i) = \pi_{G'}(X_i)$, and that $\mathsf{NDsc}_H(X_i)\backslash X_{uv} = \mathsf{NDsc}_{G'}(X_i)\backslash uv$. Therefore, $B_i\backslash uv \subseteq \mathsf{NDsc}_H(X_i)$, and by (10), if $uv \subseteq B_i \subseteq \mathsf{NDsc}_{G'}(X_i)$, then $X_{uv} \in \mathsf{NDsc}_H(X_i)$. Therefore, $\Sigma_{\mathrm{RB}}(H) \implies (X_i; B_i\backslash uv \cup X_{uv} \mid \pi_{G'}(X_i))$, and since $X_{uv} = uv$, then $\Sigma_{\mathrm{RB}}(H) \implies (X_i; B_i \mid \pi_{G'}(X_i))$.

Since $(u, v) \in \mathsf{E}(G')$, we are left with two other cases. First, that $(u; B_u \mid \pi_{G'}(u))$, and second $(v; B_v \mid \pi_{G'}(v))$. By d-separation in H, the following holds:

$$\begin{aligned}\Sigma_{\mathrm{RB}}(H) &\implies (X_{uv}; \mathsf{NDsc}_H(X_{uv})\backslash\pi_H(X_{uv}) \mid \pi_H(X_{uv}))\\ &\underbrace{\implies}_{(5),\,(7)} (X_{uv}; \mathsf{NDsc}_{G'}(u)\backslash\pi_{G'}(u) \mid \pi_{G'}(u))\\ &\implies (uv; \mathsf{NDsc}_{G'}(u)\backslash\pi_{G'}(u) \mid \pi_{G'}(u))\end{aligned} \tag{16}$$

By (5), it holds that $\pi_{G'}(v) = \pi_{G'}(u) \cup \{u\}$. By (7), it holds that

$$\begin{aligned}B_v \subseteq \mathsf{NDsc}_{G'}(v)\backslash\pi_{G'}(v) &= (\mathsf{NDsc}_{G'}(u) \cup \{u\})\backslash(\pi_{G'}(u) \cup \{u\})\\ &= \mathsf{NDsc}_{G'}(u)\backslash\pi_{G'}(u)\end{aligned}$$

Therefore, $B_v \cup B_u \subseteq \mathsf{NDsc}_{G'}(u)\backslash\pi_{G'}(u)$. In other words, by (16), we have that;

$$\Sigma_{\mathrm{RB}}(H) \implies (uv; B_u \cup B_v \mid \pi_{G'}(u)) \text{ if and only if}$$

$$\Sigma_{\mathrm{RB}}(H) \implies (u; B_u \cup B_v \mid \pi_{G'}(u)), (v; B_u \cup B_v \mid \pi_{G'}(u) \cup \{u\})$$

Since $\pi_{G'}(v) = \pi_{G'}(u)\cup\{u\}$, then overall, we have that $\Sigma_{\mathrm{RB}}(H) \implies (u; B_u \mid \pi_{G'}(u))$, and $\Sigma_{\mathrm{RB}}(H) \implies (v; B_v \mid \pi_{G'}(v))$. This completes the proof. □

To prove Theorem 4.2, we first show the following lemma that establishes the connection between d-separation on the canonical causal DAG and the original causal DAG.

Lemma C.3. *Let $\mathcal{G}$ and $\mathcal{G}'$ be causal DAGs defined over the same set of nodes, i.e., $\mathsf{V}(\mathcal{G}) = \mathsf{V}(\mathcal{G}')$, where $\mathcal{G}'$ is a supergraph of $\mathcal{G}$ ($\mathsf{E}(\mathcal{G}') \supseteq \mathsf{E}(\mathcal{G})$). Then, for any three disjoint subsets $\mathbf{X}, \mathbf{Y}, \mathbf{Z} \subseteq \mathsf{V}(\mathcal{G})$, it holds that: $(\mathbf{X} \perp\!\!\!\perp_d \mathbf{Y}|\mathbf{Z})_{\mathcal{G}'} \implies (\mathbf{X} \perp\!\!\!\perp_d \mathbf{Y}|\mathbf{Z})_{\mathcal{G}}$*

Proof of Lemma C.3. Suppose that X and Y are d-separated by Z in G' (i.e., $(X; Y|Z)_{G'}$). If X and Y are d-connected by Z in G, then let P denote the unblocked path between X and Y, relative to Z. Since $\mathsf{E}(G') \supseteq \mathsf{E}(G)$, then clearly P is a path in G' as well. Consider any triple (x, w, y) on this path. If this triple has one of the forms

$$\{x \to w \to y, x \leftarrow w \leftarrow y, x \leftrightarrow w \to y, x \leftarrow w \leftrightarrow y\},$$

then since P is unblocked in G, relative to Z, then $w \notin Z$. Since $w \notin Z$, then the subpath (x, w, y) is also unblocked in G'. If the triple has one of the forms:

$$\{x \leftrightarrow w \leftarrow y, x \to w \leftrightarrow y, x \to w \leftarrow y\},$$

then since P is unblocked in G, relative to Z, then $\mathsf{Dsc}_G(w) \cap Z \neq \emptyset$. Since $\mathsf{E}(G') \supseteq \mathsf{E}(G)$, then $\mathsf{Dsc}_G(w) \subseteq \mathsf{Dsc}_{G'}(w)$. Therefore, $\mathsf{Dsc}_{G'}(w) \cap Z \neq \emptyset$. Consequently, we have, again, that the subpath (x, w, y) is unblocked in G'. Overall, we get that every triple (x, w, y) on the path P is unblocked in G', relative to Z, and hence X and Y are d-connected in G', a contradiction.

By definition, G' is compatible with G'. Therefore, if X and Y are d-connected by Z in G', then by the completeness of d-separation, there exists a probability distribution that factorizes according to G' in which the CI $(X; Y|Z)$ does not hold. This proves completeness. □

Proof of Theorem 4.2. Let $\mathcal{G}_{\mathcal{H}}$ denote the canonical causal DAG corresponding to $\mathcal{H}$. By Theorem 4.1, $\Sigma_{\mathrm{RB}}(\mathcal{H}) \equiv \Sigma_{\mathrm{RB}}(\mathcal{G}_{\mathcal{H}})$. Therefore, $(\mathbf{X} \perp\!\!\!\perp_d \mathbf{Y}|\mathbf{Z})_{\mathcal{H}} \iff (f^{-1}(\mathbf{X}) \perp\!\!\!\perp_d f^{-1}(\mathbf{Y})|f^{-1}(\mathbf{Z}))_{\mathcal{G}_{\mathcal{H}}}$ Since $\mathsf{E}(\mathcal{G}) \subseteq \mathsf{E}(\mathcal{G}_{\mathcal{H}})$, the claim immediately follows from Lemma C.3. □

C.3 Proofs for Section 6

We next show a smile lemma that will be useful for proving the soundness and completeness of do-calculus in summary graphs.

Lemma C.4. *Let G be ADMG, and let G' be an ADMG where $\mathsf{V}(G') = \mathsf{V}(G)$, and $\mathsf{E}(G') \supseteq \mathsf{E}(G)$. Let $A, B, C \subseteq \mathsf{V}(G)$ be disjoint sets of variables, and let $X, Z \subseteq \mathsf{V}(G)$. Then:*

$$(A; B|C)_{G'_{\overline{X}\underline{Z}}} \implies (A; B|C)_{G_{\overline{X}\underline{Z}}} \tag{17}$$

Corollary C.4.1. *Let G be ADMG, and let (H, f) be a summary-DAG for G. Let $A, B, C \subseteq \mathsf{V}(H)$ be disjoint sets of nodes, and let $X, Z \subseteq \mathsf{V}(H)$. Then:*

$$(A; B|C)_{H_{\overline{X}\underline{Z}}} \implies (\mathbf{A}; \mathbf{B}|\mathbf{C})_{G_{\overline{\mathbf{X}}\underline{\mathbf{Z}}}} \tag{18}$$

where for $U \subseteq \mathsf{V}(H)$, we denote $\mathbf{U} \stackrel{def}{=} f(U)$.

Theorem C.5 (Soundness of Do-Calculus in supergraphs). *Let $\mathcal{G}$ be a causal DAG encoding an interventional distribution $P(\cdot \mid do(\cdot))$. Let $\mathcal{G}'$ be a causal DAG where $\mathsf{V}(\mathcal{G}) = \mathsf{V}(\mathcal{G}')$ and $\mathsf{E}(\mathcal{G}) \subseteq \mathsf{E}(\mathcal{G}')$. For any disjoint subsets $\mathbf{X}, \mathbf{Y}, \mathbf{Z}, \mathbf{W} \subseteq \mathsf{V}(\mathcal{G})$, the following three rules hold:*

$$\mathrm{R}_1: \quad (\mathrm{Y} \perp\!\!\!\perp \mathrm{Z}|\mathrm{X}, \mathrm{W})_{\mathcal{G}'_{\overline{\mathrm{X}}}} \implies P(\mathrm{Y} \mid do(\mathrm{X}), \mathrm{Z}, \mathrm{W}) = P(\mathrm{Y} \mid do(\mathrm{X}), \mathrm{W})$$
$$\mathrm{R}_2: \quad (\mathrm{Y} \perp\!\!\!\perp \mathrm{Z}|\mathrm{X}, \mathrm{W})_{\mathcal{G}'_{\overline{\mathrm{X}}\underline{\mathrm{Z}}}} \implies P(\mathrm{Y} \mid do(\mathrm{X}), do(\mathrm{Z}), \mathrm{W}) = P(\mathrm{Y} \mid do(\mathrm{X}), \mathrm{Z}, \mathrm{W})$$
$$\mathrm{R}_3: \quad (\mathrm{Y} \perp\!\!\!\perp \mathrm{Z}|\mathrm{X}, \mathrm{W})_{\mathcal{G}'_{\overline{\mathrm{X}\mathrm{Z}(\mathrm{W})}}} \implies P(\mathrm{Y} \mid do(\mathrm{X}), do(\mathrm{Z}), \mathrm{W}) = P(\mathrm{Y} \mid do(\mathrm{X}), \mathrm{W})$$

where $\mathbf{Z}(\mathbf{W})$ *is the set of nodes in* $\mathbf{Z}$ *that are not ancestors of any node in* $\mathbf{W}$*. That is,* $\mathbf{Z}(\mathbf{W}) = \mathbf{Z} \backslash \mathsf{Ancs}_{\mathcal{G}'}(\mathbf{W})$ *where* $\mathsf{Ancs}_{\mathcal{G}'}(\mathbf{W}) \stackrel{def}{=} \bigcup_{W \in \mathbf{W}} \mathsf{Ancs}_{\mathcal{G}'}(W)$.

Theorem C.6 (Soundness of Do-Calculus in supergraphs). *Let* G *be a causal BN (CBN) encoding an interventional distributions* $P(\cdot \mid do(\cdot))$*. Let* G' *be an ADMG where* $\mathsf{E}(G) \subseteq \mathsf{E}(G')$*. For any disjoint subsets* $X, Y, Z, W \subseteq \mathsf{V}(G)$*, the following three rules hold:*

$$\mathrm{R}_1: \quad (Y; Z|X, W)_{G'_{\overline{X}}} \implies P(Y \mid do(X), Z, W) = P(Y \mid do(X), W)$$
$$\mathrm{R}_2: \quad (Y; Z|X, W)_{G'_{\overline{X}\underline{Z}}} \implies P(Y \mid do(X), do(Z), W) = P(Y \mid do(X), Z, W)$$
$$\mathrm{R}_3: \quad (Y; Z|X, W)_{G'_{\overline{XZ(W)}}} \implies P(Y \mid do(X), do(Z), W) = P(Y \mid do(X), W)$$

where $Z(W)$ *is the set of vertices in* Z *that are not ancestors of any vertex in* W*. That is,* $Z(W) = Z \backslash \mathsf{Ancs}_{G'}(W)$ *where* $\mathsf{Ancs}_{G'}(W) \stackrel{def}{=} \bigcup_{w \in W} \mathsf{Ancs}_{G'}(w)$.

Proof of Lemman C.4. We show that $\mathsf{E}(G_{\overline{X}\underline{Z}}) \subseteq \mathsf{E}(G'_{\overline{X}\underline{Z}})$, and the claim then follows from Theorem ??. Let $(u, v) \in \mathsf{E}(G_{\overline{X}\underline{Z}}) \subseteq \mathsf{E}(G) \subseteq \mathsf{E}(G')$. By definition, $u \notin Z$ and $v \notin X$. But this means that $(u, v) \in \mathsf{E}(G'_{\overline{X}\underline{Z}})$, which completes the proof. ◻

Proof of Corollary C.4.1. Let $G_{H_{\overline{X}\underline{Z}}}$ denote the grounded DAG corresponding to $H_{\overline{X}\underline{Z}}$. By Theorem 4.1, $\Sigma_{\mathrm{RB}}(H_{\overline{X}\underline{Z}}) \equiv \Sigma_{\mathrm{RB}}(G_{H_{\overline{X}\underline{Z}}})$, and hence $(A; B|C)_{H_{\overline{X}\underline{Z}}}$ if and only if $(\mathbf{A}; \mathbf{B}|\mathbf{C})_{G_{H_{\overline{X}\underline{Z}}}}$. Since $\mathsf{E}(G_H) \supseteq \mathsf{E}(G)$, then by Lemma C.4, it holds that if $(\mathbf{A}; \mathbf{B}|\mathbf{C})_{G_{H_{\overline{X}\underline{Z}}}}$, then $(\mathbf{A}; \mathbf{B}|\mathbf{C})_{G_{\overline{X}\underline{Z}}}$. Overall, we have that:

$$(A; B|C)_{H_{\overline{X}\underline{Z}}} \Leftrightarrow (\mathbf{A}; \mathbf{B}|\mathbf{C})_{G_{H_{\overline{X}\underline{Z}}}} \implies (\mathbf{A}; \mathbf{B}|\mathbf{C})_{G_{\overline{X}\underline{Z}}} \tag{19}$$

which proves the claim. ◻

Proof of Theorem C.6. If $(Y; Z|X, W)_{G'_{\overline{X}}}$, then by Lemma C.4, it holds that $(Y; Z|X, W)_{G_{\overline{X}}}$. By the soundness of do-calculus for causal BNs, we get that $P(Y \mid do(\boldsymbol{X}), \boldsymbol{Z}, \boldsymbol{W}) = P(Y \mid do(\boldsymbol{X}), \boldsymbol{W})$. If $(Y; Z|X, W)_{G'_{\overline{X}\underline{Z}}}$, then by Lemma C.4, it holds that $(Y; Z|X, W)_{G_{\overline{X}\underline{Z}}}$. By the soundness of do-calculus for causal BNs, we get that $P(Y \mid do(X), do(Z), W) = P(Y \mid do(X), Z, W)$. Finally, if $(Y; Z|X, W)_{G'_{\overline{XZ(W)}}}$, then by Lemma C.4, it holds that $(Y; Z|X, W)_{G_{\overline{XZ(W)}}}$. By the soundness of do-calculus for causal BNs, we get that $P(Y \mid do(X), do(Z), W) = P(Y \mid do(X), W)$. ◻

Proof of Theorem 6.1. If $(Y; Z|X, W)_{H_{\overline{X}}}$, then by Corollary C.4.1, it holds that $(Y; \boldsymbol{Z}|\boldsymbol{X}, \boldsymbol{W})_{G_{\overline{X}}}$. By the soundness of do-calculus for causal BNs, we get that $P(Y \mid do(\boldsymbol{X}), \boldsymbol{Z}, \boldsymbol{W}) = P(Y \mid do(\boldsymbol{X}), \boldsymbol{W})$. If $(Y; Z|X, W)_{H_{\overline{X}\underline{Z}}}$, then by Corollary C.4.1, it holds that $(Y; \boldsymbol{Z}|\boldsymbol{X}, \boldsymbol{W})_{G_{\overline{X}\underline{Z}}}$. By the soundness of do-calculus for causal BNs, we get that $P(Y \mid do(\boldsymbol{X}), do(\boldsymbol{Z}), w) = P(Y \mid do(\boldsymbol{X}), \boldsymbol{Z}, \boldsymbol{W})$. Finally, if $(Y; Z|X, W)_{H_{\overline{XZ(W)}}}$, then by Corollary C.4.1, it holds that $(Y; \boldsymbol{Z}|\boldsymbol{X}, \boldsymbol{W})_{G_{\overline{X}\underline{Z(W)}}}$. By the soundness of do-calculus for causal BNs, we get that $P(\boldsymbol{Y} \mid do(\boldsymbol{X}), do(\boldsymbol{Z}), \boldsymbol{W}) = P(\boldsymbol{Y} \mid do(\boldsymbol{X}), \boldsymbol{W})$. ◻

Proof of Theorem 6.2. Consider G_H, the grounded-DAG of (H, f), that is, by definition, compatible with H. If Y is d-connected to Z in $H_{\overline{X}}$ with respect to $X \cup W$, then by Definition 5, it holds that y is d-connected to z in $G_{H_{\overline{f(X)}}}$ with respect to $f(X \cup W)$, for every $y \in f(Y)$ and $z \in f(Z)$. Therefore, $f(Y)$ is d-connected to $f(Z)$ in $G_{H_{\overline{f(X)}}}$ with respect to $f(X \cup W)$. ◻

D HANDLING MIXED GRAPHS

While one dominant form of graph input for causal inference is a causal DAG, other graph representations are also used when a full causal DAG is not retrievable, say, by a causal discovery algorithm (e.g., [73]). Many of these graph representations are referred to as *mixed graphs* due to their inclusion of undirected, bidirected, and other types of edges [20, 74].

One commonly used of mix graph is an acyclic-directed mixed graph (ADMG), which consists of a DAG with bidirected edges. As mentioned in the introduction, all of our results apply to scenarios where the input graph is an ADMG. Subsequently, we present an extension to the CaGreS algorithm to accommodate an ADMG.

In this scenario, we modify the cost function (Algorithm 2) as follows: When we remove a bidirected edge between nodes U and V (i.e., $U \leftrightarrow V$) by merging U and V into a single node, the cost incurred is doubled compared to removing a "standard" directed edge. For instance, in line 4 of Algorithm 2, if **U** and **V** were linked by a bidirected edge, the line would be updated to:

$$cost \leftarrow cost + 2 \cdot size(\mathbf{U}) \cdot size(\mathbf{V})$$

This adjustment is necessary because losing a bidirected edge should carry a higher cost than losing a regular directed edge, given that more information is lost.