Counting Markov Equivalent Directed Acyclic Graphs Consistent with Background Knowledge*

Vidya Sagar Sharma†

Abstract

We study the problem of counting the number of directed acyclic graphs in a Markov equivalence class (MEC) that are consistent with background knowledge specified in the form of the directions of some additional edges in the MEC. A polynomial-time algorithm for the special case of the problem, when no background knowledge constraints are specified, was given by Wienöbst, Bannach, and Liśkiewicz (AAAI 2021), who also showed that the general case is NP-hard (in fact, #P-hard). In this paper, we show that the problem is nevertheless tractable in an interesting class of instances, by establishing that it is “fixed-parameter tractable”: we give an algorithm that runs in time $O(k!k^2n^4)$, where $n$ is the number of nodes in the MEC and $k$ is the maximum number of nodes in any maximal clique of the MEC that participate in the specified background knowledge constraints. In particular, our algorithm runs in polynomial time in the well-studied special case of MECs of bounded tree-width or bounded maximum clique size.

1 Introduction

A graphical model is a combinatorial tool for expressing dependencies between random variables. Both directed and undirected versions have been used in the literature for modeling different kinds of dependency structures. We study graphical models represented by directed acyclic graphs (DAGs), which represent conditional independence relations and causal influences between random variables by directed edges [Pearl 2009]. Such graphical models have been used extensively for modeling causal relationships across several fields, e.g., material science [Ren et al., 2020], game theory [Kearns et al., 2001], and biology [Friedman, 2004, Finegold and Drton, 2011].

It is well known that given access only to observational data, the causal DAG underlying a system can only be determined up to its “Markov equivalence class” (MEC) [Verma and Pearl 1990, Meek 1995, Chickering 1995]. Two DAGs are said to be in the same MEC if they model exactly the same set of conditional dependence relations between the underlying random variables. Distinguishing between two DAGs in the same MEC requires the use of interventional data [Hauser and Bühlmann, 2012].

Finding the size of an MEC, therefore, becomes a question of key interest. In particular, the size of an MEC quantifies the uncertainty of the causal model given only observational data. The problem, along with a proposed algorithm, was already mentioned by Meek [Meek 1995, Section 4.1], and has since then been the focus of a long line of work [Madigan et al., 1996, He et al., 2015, He and Yu, 2016, Bernstein and Tetali, 2017, Ghassami et al., 2019, Talvitie and Koivisto, 2019, Ganian et al., 2020], which culminated in a polynomial time algorithm for the problem by Wienöbst et al. [2021].

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†Tata Institute of Fundamental Research, Mumbai. Email: vidya.sagar@tifr.res.in.
Counting with background knowledge constraints In applications, more information about the directions of edges in the underlying DAG than that encoded in the MEC may be available, for example, due to access to domain-specific knowledge. Meek [1995] referred to this as background knowledge and modeled it as a specification of the directions of some of the edges of the underlying DAG. Thus, instead of finding the size of the whole MEC, one becomes interested in counting those DAGs in the MEC that are consistent with this specified background knowledge. An algorithm for this problem can also be used as an indicator of the efficacy of a particular intervention in pinning down a DAG within an MEC, by measuring the ratio between the size of the MEC and the number of those DAGs in the MEC that are consistent with the extra background information yielded by the intervention. Wienöbst et al. [2021] showed, however, that in general, this problem is \#P-complete (i.e., as hard as counting satisfying assignments to a Boolean formula). Our goal in this paper is to circumvent this hardness result when the specified background knowledge has some special structure.

1.1 Our Contributions

We now formalize the above problem. Our input is an MEC on \( n \) nodes, and we are given also the directions of another \( s \) edges that are not directed in the MEC: we refer to the set of these edges as the background knowledge, denoted \( K \). Our goal is to count the number of DAGs in the input MEC that are consistent with the background knowledge \( K \). The above quoted result of Wienöbst et al. [2021] implies that (under the standard \( P \neq NP \) assumption) there cannot be an algorithm for solving this problem whose run-time is polynomial in both \( n \) and \( s \).

Main result The main conceptual contribution of this paper is to define the following parameter which lets us identify important special instances of the problem where we can circumvent the above hardness result. Given the set \( K \) of background knowledge edges, we define the max-clique-knowledge \( k \) of \( K \) to be the maximum number of vertices in any clique in the input MEC that are part of a background knowledge edge that lies completely inside that clique. In particular, \( k \) can be at most twice \( s \), but it can also be much smaller. Our main result (Theorem 3.2) is an algorithm that counts the number of DAGs in the MEC that are consistent with \( K \), and runs in time \( O(k! \cdot k^2 \cdot n^4) \).

Discussion and evaluation In particular, the runtime of our algorithm is polynomially bounded when the parameter \( k \) above is bounded above by a constant, even if the actual size \( s \) of the background knowledge is very large. For example, since \( k \) is bounded above by the size of the largest clique in the input MEC, it follows that our algorithm runs in polynomial time in the well-studied special case (see, e.g., Talvitie and Koivisto [2019]) when the input MEC has constant tree-width (and hence constant maximum-clique size). We provide an empirical exploration of the run-time of our algorithm, including of the phenomenon that it depends on \( K \) only through \( k \) and not through \( s \), in Section 6.

1.2 Related Work

It is well known that an MEC can be represented as a partially directed graph, known as an essential graph, with special graph theoretic properties [Verma and Pearl 1990, Meek 1995, Chickering 1995, Andersson et al. 1997]. Initial approaches to the problem of computing the size of an MEC by Meek [1995] and Madigan et al. [1996] built upon ideas underlying this characterization. More recently, He et al. [2015] evaluated a heuristic based on the partition of essential graphs into chordal components. Ghassami et al. [2019] gave an algorithm that runs
in polynomial time for constant degree graphs, but where the degree of this polynomial grows with the maximum degree of the graph.

Our algorithm can be seen as an example of a fixed parameter tractable (FPT) algorithm in the well-studied framework of parameterized complexity theory [Cygan et al., 2015]. Parameterized complexity offers an approach to attack computationally hard problems (e.g. those that are NP-hard or #P-hard) by separating the complexity of solving the problem into two pieces – a part that depends purely on the size of the input, and a part that depends only on a well-chosen “parameter” \( \rho \) of the problem. An FPT algorithm for a computationally hard problem has a runtime that is bounded above by \( f(\rho) \text{poly}(n) \), where the degree of the polynomial does not depend upon the parameter \( \rho \), but where the function \( f \) (which does not depend upon the input size \( n \)) may potentially be exponentially growing. In our setting, the underlying parameter is the max-clique-knowledge of the background knowledge \( K \).

Thus, the algorithm of Ghassami et al. [2019] cited above is not an FPT algorithm. However, Talvitie and Koivisto [2019] improved upon it by giving an FPT algorithm for computing the size of an MEC (without background knowledge): for an undirected essential graph on \( n \) nodes whose maximum clique is of size \( c \), their algorithm runs in time \( O(c!2^c c^2 n) \). Finally, Wienöbst et al. [2021] presented the first polynomial time algorithm for computing the size of any MEC (again, without background knowledge). As discussed above, they also showed that counting Markov equivalent DAGs consistent with specified background knowledge is, in general, #P-complete.

We are not aware of any progress towards circumventing this hardness result by imposing specific properties on the specified background knowledge, and to the best of our knowledge, this paper is the first to give a fixed parameter tractable algorithm for the problem. Our algorithm is motivated by the techniques developed by Wienöbst et al. [2021].

2 Preliminaries

We mostly follow the terminology and notation used by Andersson et al. [1997] and Wienöbst et al. [2021] for notions such as graph unions, chain graphs, directed and undirected graphs, skeletons, v-structures, cliques, separators, chordal graphs, undirected connected chordal graphs (which we will typically denote using the abbreviation UCCG), and clique trees. For completeness, we provide detailed definitions in the Supplementary Material.

Notations. A graph \( G \) is a pair \((V, E)\), where \( V \) is said to be the set of vertices of \( G \), and \( E \subseteq V \times V \) is said to be the set of edges of \( G \). For \( u, v \in V \), if \((u, v), (v, u) \in E \) then we say there is an undirected edge between \( u \) and \( v \), denoted as \( u \sim v \). For \( u, v \in V \), if \((u, v) \in E \), and \((v, u) \notin E \) then we say there is a directed edge from \( u \) to \( v \), denoted as \( u \to v \). For a graph \( G \), we denote \( V_G \) as the subset of vertices of \( G \), and \( E_G \) as the set of vertices of \( G \). A clique is a set of pairwise adjacent vertices. We denote the set of all maximal cliques of \( G \) by \( \Pi(G) \). For a set \( X \), we denote by \( \#X \) (and sometimes by \(|X|\)), the size of \( X \).

Markov equivalence classes. A causal DAG encodes a set of conditional independence relations between random variables represented by its vertices. Two DAGs are said to belong to the same Markov equivalence class (MEC) if both encode the same set of conditional independence relations. Verma and Pearl [1990] showed that two DAGs are in the same MEC if, and only if, both have (i) the same skeleton and (ii) the same set of v-structures. An MEC can be represented by the graph union of all DAGs in it. Andersson et al. [1997] show that a partially directed graph representing an MEC is a chain graph whose undirected connected components (i.e., undirected connected components formed after removing the directed edges) are chordal graphs. We refer to these undirected connected components as chordal components of the MEC. With a slight abuse of terminology, we equate the chain graph with chordal components which
represents an MEC with the MEC itself, and refer to both as an “MEC”.

**AMO.** Given a partially directed graph $G$, an orientation of $G$ is obtained by assigning a direction to each undirected edge of $G$. Following [Wienöbst et al. 2021], we call an orientation of $G$ an acyclic moral orientation (AMO) of $G$ if (i) it does not contain any directed cycles, and (ii) it has the same set of $v$-structures as $G$. For an MEC $G$, we denote the set of AMOs of $G$ by $\text{AMO}(G)$.

**PEO and LBFS orderings.** For an undirected graph, a linear ordering $\tau$ of its vertices is said to be a perfect elimination ordering (PEO) of the graph if for each vertex $v$, the neighbors of $v$ that occur after $v$ form a clique. A graph is chordal if, and only if, it has a PEO [Fulkerson and Gross, 1965]. Rose et al. [1976] gave a lexicographical breadth-first-search (LBFS) algorithm to find a PEO of a chordal graph (see Algorithm 1 below for a modified version of LBFS). Any ordering of vertices that can be returned by the LBFS algorithm is said to be an LBFS ordering.

**Representation of an AMO.** Given a linear ordering $\tau$ of the vertices of a graph $G$, an AMO of $G$ is said to be represented by $\tau$ if for every edge $u \rightarrow v$ in the AMO, $u$ precedes $v$ in $\tau$. Every LBFS ordering of a UCCG $G$ represents a unique AMO of $G$, and every AMO of a UCCG $G$ is represented by an LBFS ordering of $G$ (Corollary 1, and Lemma 2 of [Wienöbst et al. 2021]). For a maximal clique $C$ of $G$, we say that $C$ represents an AMO $\alpha$ of $G$ if there exists an LBFS ordering that starts with $C$ and represents $\alpha$. Similarly, for a permutation $\pi(C)$ of a maximal clique $C$ of $G$, we say $\pi(C)$ represents $\alpha$ if there exists an LBFS ordering that starts with $\pi(C)$ and represents $\alpha$. We denote by $\text{AMO}(G, \pi(C))$ and $\text{AMO}(G, C)$, the set of AMOs of $G$ that can be represented by $\pi(C)$ and $C$, respectively.

**Canonical representation of AMO.** For an AMO $\alpha$ of a UCCG $G$, [Wienöbst et al. 2021] define a unique clique that represents $\alpha$. We denote the clique as $C_\alpha$, and say that $C_\alpha$ canonically represents $\alpha$. For the purposes of this paper, we only need certain properties of the canonical representative $C_\alpha$, and these are quoted in Lemma 4.7. However, for completeness, we also give the definition of $C_\alpha$ in the Supplementary Material.

**Background Knowledge and Clique-knowledge.** For an MEC represented by a partially directed graph $G$, background knowledge $K \subseteq E_G$ Meek 1995 is specified as a set of directed edges $K \subseteq E_G$ Meek 1995. A graph $G$ is said to be consistent with $K$ if, for any edge $u \rightarrow v \in K$, $v \rightarrow u \notin E_G$ (i.e., either $u \rightarrow v \in E_G$ or $u \rightarrow v \notin E_G$). For a clique $C$ of $G$, clique-knowledge of $K$ for $C$ is defined as the number of vertices of $C$ that are part of a background knowledge edge both of whose endpoints are in $C$. Max-clique-knowledge of $K$ for $G$ is the maximum value of clique-knowledge over all cliques of $G$.

We denote the set of AMOs of $G$ consistent with background knowledge $K$ by $\text{AMO}(G, K)$. Further, for any clique $C$ and any permutation $\pi(C)$ of the vertices of $C$, we denote by $\text{AMO}(G, \pi(C), K)$ and $\text{AMO}(G, C, K)$, respectively, the set of $K$-consistent AMOs of $G$ that can be represented by $\pi(C)$ and $C$.

### 3 Main Result

[Andersson et al. 1997] show that a DAG is a member of an MEC $G$ if, and only if, it is an AMO of $G$. Thus, counting the number of DAGs in the MEC represented by $G$ is equivalent to counting AMOs of $G$. We start with a formal description of the algorithmic problem we address in this paper.

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1. Another way to represent background knowledge is by a maximally partially directed acyclic graph (MPDAG). We do not use MPDAGs in our paper because our run time depends only on the number of directed background knowledge edges that generate the MPDAG, and not on the (possibly much larger) number of directed edges in the MPDAG.
Problem 3.1 (Counting AMOs with Background Knowledge). INPUT: (a) An MEC $G$ (in the form of a chain graph with chordal undirected components), (b) Background Knowledge $\mathcal{K} \subseteq E_G$.

OUTPUT: Number of DAGs in the MEC $G$ that are consistent with $\mathcal{K}$, i.e., $\#\text{AMO}(G, \mathcal{K})$.

As discussed in the introduction, a polynomial time algorithm for the special case of this problem where $\mathcal{K}$ is empty was given by [Wienöbst et al. 2021], in the culmination of a long line of work on that case. However, as discussed in the Introduction, a hardness result proved by [Wienöbst et al. 2021] implies, under the standard $P \neq NP$ assumption, that there cannot be an algorithm for Problem 3.1 that runs in time polynomial in both $n$ and $|\mathcal{K}|$.

We, therefore, ask: what are the other interesting cases of the problem which admit an efficient solution? We answer this question with the following result.

Theorem 3.2 (Main result). There is an algorithm for Problem 3.1 which outputs $\#\text{AMO}(G, \mathcal{K})$ in time $O(k!k^2n^4)$, where $k$ is the max-clique-knowledge value of $\mathcal{K}$ for $G$, and $n$ is the number of vertices in $G$. 
In the formalism of parameterized algorithms [Cygan et al., 2015], the above result says that the problem of counting AMOs that are consistent with background knowledge is fixed parameter tractable, with the parameter being the max-clique-knowledge of the background knowledge. This contrasts with the #P-hardness result of [Wienöbst et al., 2021] for the problem.

The starting point of our algorithm is a standard reduction to the following special case of the problem.

**Problem 3.3 (Counting Background Consistent AMOs in chordal graphs).** **INPUT:** (a) An undirected connected chordal graph (UCCG) $G$, (b) Background Knowledge $K \subseteq E_G$. **OUTPUT:** Number of AMOs of $G$ that are consistent with $K$, i.e., $\#\text{AMO}(G, K)$.

**Proposition 3.4.** Let $G$ be an MEC, and let $K \subseteq E_G$ be background knowledge consistent with $G$. Then, $\#\text{AMO}(G, K) = \prod_H \#\text{AMO}(H, K[H])$, where the product ranges over all undirected connected chordal components $H$ of the MEC $G$, and $K[H] = \{u \rightarrow v : u, v \in H, \text{ and } u \rightarrow v \in K\}$ is the corresponding background knowledge for $H$.

Proposition 3.4 reduces Problem 3.1 to Problem 3.3. The proof of Proposition 3.4 follows directly from standard arguments (a similar reduction to chordal components of an MEC has been used in many previous works), and is given in the Supplementary Material.

The rest of the paper is devoted to providing an efficient algorithm for Problem 3.3. Our strategy builds upon the recursive framework developed by [Wienöbst et al., 2021]. In the first step, in Section 4, we modify the LBFS algorithm presented by [Wienöbst et al., 2021] to make it background aware. This algorithm is used to generate smaller instances of the problem recursively. Further, we modify the recursive algorithm of [Wienöbst et al., 2021] to use this new LBFS algorithm. While building upon prior work, both steps require new ideas to take care of the background information. In particular, it is a careful accounting of the background knowledge $K$ that requires the $k!$ factor in the runtime, where $k$ is the max-clique-knowledge of the background knowledge. In Section 5, we analyze the time complexity of the resulting algorithm. Finally, Section 6 shows our experimental results. Due to space constraints, proofs of many lemmas and theorems are provided in the Supplementary Material. For most of the important results, we provide the proof sketch in the main text.

**4 The Algorithm**

In this section, we give an FPT algorithm Algorithm 3 that solves Problem 3.3 using a parameter “max-clique knowledge” (Section 2). Algorithm 3 is a background aware version of Algorithm 2 of [Wienöbst et al., 2021], which solved the special case of Problem 3.3 when there is no background knowledge. Similar to their algorithm, our algorithm uses a modified LBFS algorithm, Algorithm 1 which is a background aware version of the modified LBFS algorithm presented by them. The simple Algorithm 2 which counts background knowledge consistent permutations of a clique, is the new ingredient required in our final algorithm presented in Algorithm 3.

We start with the partitioning of the AMOs. In Section 2 we saw that each AMO of a UCCG is canonically represented by a unique maximal clique of the UCCG. We use this for partitioning the AMOs.

**Lemma 4.1.** Let $G$ be a UCCG, and $K$ be a given background knowledge. Then $\#\text{AMO}(G, K)$ equals

$$\sum_{C \in \Pi(G)} |\{\alpha : \alpha \in \text{AMO}(G, K) \text{ and } C = C_\alpha\}|,$$

(1)
Here, \( \{ \alpha : \alpha \in \text{AMO}(G, K) \text{ and } C = C_\alpha \} \) is the set of \( K \)-consistent AMOs of \( G \) that are canonically represented by a maximal clique \( C \) of \( G \). To compute this, we first compute the union of AMOs of \( G \) that are represented by \( C \). The following definition concerns objects from the work of Wienöbst et al. [2021] that are relevant to construct the union graph.

**Definition 4.2** \((G^{\pi(C)}), G^C, C_G(\pi(C)) \text{ and } C_G(C), \text{Wienöbst et al. [2021], Definition 1})\). Let \( G \) be a UCCG, \( C \) a maximal clique of \( G \), and \( \pi(C) \) a permutation of \( C \). Then, \( G^C \) (respectively, \( G^{\pi(C)} \)) denotes the union of all the AMOs of \( G \) that can be represented by \( C \) (respectively, by \( \pi(C) \)). \( C_G(C) \) (respectively, \( C_G(\pi(C)) \)) denotes the undirected connected components of \( G^C[V_G \setminus C] \) (respectively, \( G^{\pi(C)}[V_G \setminus C] \)).

The structure of \( G^C \) provides us the set of directed edges in \( G^C \), which helps us to check the \( K \)-consistency of \( G^C \). Since \( G^C \) is the union of all the AMOs that can be represented by \( C \), a directed edge in \( G^C \) is a directed edge in all the AMOs that can be represented by \( C \). Thus, if any such directed edge is not \( K \)-consistent then none of the AMOs that can be represented by \( C \) can be \( K \)-consistent. And, if all the directed edges of \( G^C \) are \( K \)-consistent then we further reduce our problem into counting \( K \)-consistent AMOs for the undirected connected components of \( G^C \) (Lemma 4.13).

In order to implement the above discussion, the main insight required is the following definition.

**Definition 4.3** \((K\text{-consistency of } G^C)\). Let \( G \) be a UCCG and \( C \) a maximal clique in \( G \). Given background knowledge \( K \) about the directions of the edges of \( G \), \( G^C \) is said to be \( K \)-consistent, if there does not exist a directed edge \( u \rightarrow v \in G^C \) such that \( v \rightarrow u \in K \).

As discussed above, Definition 4.3 implies that for a maximal clique \( C \) of \( G \), if \( G^C \) is not \( K \)-consistent then there exists no \( K \)-consistent AMO of \( G \) that is represented by \( C \). In other words, if \( G^C \) is not \( K \)-consistent then

\[
\{ \alpha : \alpha \in \text{AMO}(G, K) \text{ and } C = C_\alpha \} = 0.
\]

Then, from Lemma 4.1,

\[
\#\text{AMO}(G, K) = \sum_{C: G^C \text{ is } K\text{-consistent}} |\{ \alpha : \alpha \in \text{AMO}(G, K) \text{ and } C = C_\alpha \}|.
\]

We construct Algorithm 1 to check the \( K \)-consistency of \( G^C \), for any maximal clique \( C \) of \( G \). Wienöbst et al. [2021] give a modified LBFS algorithm that for input a chordal graph \( G \), and a maximal clique \( C \) of \( G \), outputs the undirected connected components (UCCs) of \( C_G(C) \). Their algorithm outputs the UCCs of \( C_G(C) \) in such a way that by knowing the UCCs of \( C_G(C) \), we can construct \( G^C \). We use this fact and construct an LBFS algorithm Algorithm 1 which also checks the \( K \)-consistency of \( G^C \). Algorithm 1 is a background aware version of the LBFS algorithm given by Wienöbst et al. [2021].

We now describe our background-aware version of the modified LBFS algorithm: see Algorithm 1. We do not change any line from the LBFS algorithm of Wienöbst et al. [2021]. The modifications we do in their LBFS algorithm are (a) introduction of “flag”, at line 2, which is used to check the \( K \)-consistency of \( G^C \), (b) lines 11-13 which is used to update the value of “flag”, and (c) we also output the value of “flag” with \( C_G(C) \). The correctness of this modification (stated formally in Lemma 4.5) is based on the following observation which in turn uses ideas implicit in the work of Wienöbst et al. [2021].

\(^2\text{If Algorithm 1 is executed with } C = K = \emptyset, \text{ the algorithm performs a normal LBFS with corresponding traversal ordering } \tau, \text{ which is the reverse of a PEO of } G.\)
Algorithm 1: LBFS(G, C, K) (Background aware LBFS, based on the modified LBFS of Wienöbst et al. [2021])

**Input**: A UCCG G, a maximal clique C of G, and background knowledge K ⊆ E_G.

**Output**: (1, C_G(C)): if G^C is K-consistent, (0, C_G(C)): otherwise.

1. S ← sequence of sets initialized with (C, V \ C)
2. τ ← empty list, L ← empty list, flag ← 1, Y ← empty list
3. while S is non-empty do
4.   X ← first non-empty set of S
5.   v ← arbitrary vertex from X
6.   if v is neither in a set in L nor in C then
7.     Append X to the end of the list L.
8.     Append undirected connected components of G[X] to the end of Y.
9.   end
10.  Add vertex v to the end of τ.
11.  if u → v ∈ K for any u which is neither in a set in L nor in C then
12.     flag = 0;
13. end
14.  Replace the set X in the sequence S by the set X \ {v}.
15.  N(v) ← \{x|x ∉ τ and v − x ∈ E\}
16.  Denote the current S by (S_1, . . . , S_k).
17.  Replace each S_i by S_i ∩ N(v), S_i \ N(v).
18.  Remove all empty sets from S.
19. end
20. return (flag, Y)

**Observation 4.4** (Implicit in the work of Wienöbst et al. [2021]). Let G be a UCCG, K be the known background knowledge about G, and C be a maximal clique of G. For input G, C, and K, suppose that at some iteration of Algorithm 1, L = \{X_1, X_2, . . . , X_l\}. Then,

1. For any u ∈ C, and v ∉ C, if (u, v) ∈ E_G then u → v is a directed edge in G^C.
2. For u ∈ X_i, and v ∉ C ∪ X_1 ∪ X_2 ∪ . . . ∪ X_i, if (u, v) ∈ E_G then u → v is a directed edge in G^C.
3. For u, v ∈ X_i, for 1 ≤ i ≤ l, if (u, v) ∈ E_G then u − v is an undirected edge in G^C.
4. For u, v ∈ C, u − v is an undirected edge in G^C.
5. For any X_i ∈ L, every undirected connected component of G[X_i] is an element of C_G(C).

The following lemma encapsulates the correctness of Algorithm 1.

**Lemma 4.5.** Let G be a UCCG, C be a maximal clique of G, and K be the known background knowledge about G. For the input G, C, and K, if G^C is not K-consistent Algorithm 1 outputs (0, C_G(C)) on line 20; else it returns (1, C_G(C)) on line 20.

For any maximal clique C of G such that G^C is K-consistent, to compute the size of the set of K-consistent AMOs of G that are canonically represented by C, we further partition the set based on the different permutations of C. The simple Observation 4.6 below assists us in mapping each AMO of the set to a unique permutation π(C) of C.
**Observation 4.6.** Let $G$ be a UCCG, and $\alpha$ an AMO of $G$ that is represented by a maximal clique $C$ of $G$. Then, there exists a unique permutation $\pi(C)$ of $C$ that represents $\alpha$.

By slightly extending the definition of the canonical representation of an AMO by a clique, we say that an AMO is **canonically represented by** $\pi(C)$ if the AMO is represented by $\pi(C)$, and also canonically represented by the clique $C$. Then, Observation 4.6 implies that we can partition the set of $K$-consistent AMOs that are canonically represented by $C$ into $K$-consistent AMOs that are canonically represented by its permutations $\pi(C)$, i.e., $\{\alpha : \alpha \in AMO(G, \pi(C), K) \text{ and } C = C_\alpha\}$. More formally,

$$|\{\alpha : \alpha \in AMO(G, K) \text{ and } C = C_\alpha\}| = \sum_{\pi(C)} |\{\alpha : \alpha \in AMO(G, \pi(C), K) \text{ and } C = C_\alpha\}|.$$

To compute the size of $K$-consistent AMOs of $G$ that are canonically represented by $\pi(C)$, we first have to go through the necessary and sufficient conditions for a maximal clique $C$ of $G$ to become $C_\alpha$, for an AMO $\alpha$ of $G$.

**Lemma 4.7** (Claims 1, 2 and 3 of Wienöbst et al. [2021]). Let $G$ be a UCCG. Wienöbst et al. [2021] fix a rooted clique tree of $G$ to define $C_\alpha$, for any AMO $\alpha$ of $G$. Let $T = (T, R)$ be the rooted clique tree (with root $R$) of $G$ on which $C_\alpha$ is defined, for each AMO $\alpha$ of $G$. For an AMO $\alpha$ of $G$, and a maximal clique $C$ of $G$, $C = C_\alpha$ if, and only if,

1. There exists an LBFS ordering of $G$ that starts with $C$, and represents $\alpha$, and
2. If $\pi(C)$ is the permutation of $C$ that represents $\alpha$ (from Observation 4.6) then there does not exist any edge $C_i - C_j$ in the path in $T$ from $R$ to $C$ such that $\pi(C)$ has a prefix $C_i \cap C_j$.

The set $FP(C, T)$ is defined to be the set of such forbidden prefixes $C_i \cap C_j$.

**Definition 4.8** ($FP(C, T)$, Definition 3 of Wienöbst et al. [2021]). Let $G$ be a UCCG, $T = (T, R)$ a rooted clique tree of $G$, $C$ a node in $T$ and $R = C_1 - C_2 - \ldots - C_{p-1} - C_p = C$ the unique path from $R$ to $C$ in $T$. We define the set $FP(C, T)$ to contain all sets of the form $C_i \cap C_{i+1} \subseteq C$, for $1 \leq i < p$.

Based on Lemma 4.7, we define $(K, T)$-consistency for a permutation $\pi(C)$ to simplify our computation. This definition is one of the main new ingredients that let us extend the result of Wienöbst et al. [2021].

**Definition 4.9** ($(K, T)$-consistency of permutations of maximal cliques). Let $G$ be a UCCG, $C$ a maximal clique in $G$, $\pi(C)$ a permutation of $C$, $K$ be a given background knowledge, and $T = (T, R)$ a rooted clique tree of $G$ (on which $C_\alpha$ is defined). $\pi(C)$ is said to be $(K, T)$-consistent if (a) $\pi(C)$ is $K$-consistent, i.e, for any edge $u \rightarrow v \in K$, such that $u, v \in C$, $u$ occurs before $v$ in $\pi(C)$, and (b) no element of $FP(C, T)$ (Definition 4.8) is a prefix of $\pi(C)$.

If $\pi(C)$ itself is not $K$-consistent then no $K$-consistent AMO exists that is represented by $\pi(C)$. Also, if $\pi(C)$ has a prefix in $FP(C, T)$ then from Observation 4.6 and Lemma 4.7 there does not exist an AMO $\alpha$ of $G$ such that $\alpha$ is represented by $\pi(C)$, and $C = C_\alpha$. This yields the following observation.

**Observation 4.10.** If $\pi(C)$ is not $(K, T)$-consistent then there exists no $K$-consistent AMOs of $G$ that can be canonically represented by $\pi(C)$, i.e., $|\{\alpha : \alpha \in AMO(G, \pi(C), K) \text{ and } C = C_\alpha\}| = 0$. 

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We thus focus on only those permutations \( \pi(C) \) of \( C \) that are \((K,T)\)-consistent. The main ingredient towards this end is the following recursive formula.

**Lemma 4.11.** Let \( G^C \) be \( K \)-consistent. Then, for any \((K,T)\)-consistent permutation \( \pi(C) \) of \( C \), the size of the set \( \{ \alpha : \alpha \in AMO(G,\pi(C),K) \text{ and } C = C_{\alpha} \} \) is \( \prod_{H \in C_G(C)} \#AMO(H,K[H]) \).

Note that the formula obtained in Lemma 4.11 depends only upon the clique \( C \) and not on the permutation \( \pi \) of the nodes of \( C \) (as long as \( \pi \) is itself \( K \)-consistent)! This implies immediately that the number of \( K \)-consistent AMOs of \( G \) for which \( C \) is the canonical representative is given by multiplying the product \( \prod_{H \in C_G(C)} \#AMO(H,K[H]) \) with the number of \((K,T)\)-consistent permutation of \( C \).

This motivates us to count \((K,T)\)-consistent permutations of a maximal clique \( C \) of \( G \). To count the \((K,T)\)-consistent permutations of \( C \), we define the following:

**Definition 4.12.** Let \( S \) be a set of vertices, \( R = \{R_1,R_2,\ldots,R_l\} \) such that \( R_1 \subseteq R_2 \subseteq \cdots \subseteq R_l \subseteq S \), and \( K \subseteq S \times S \). \( \Phi(S,R,K) \) is the number of \( K \)-consistent permutations of \( S \) that do not have a prefix in \( R \).

**Lemma 4.13.** Let \( G \) be a UCCG, \( K \) be a given background knowledge, and \( T = (T,R) \) a rooted clique tree of \( G \) on which \( <_\alpha \) has been defined. Then \( \#AMO(G,K) \) equals

\[
\sum_C \Phi(C,FP(C,T),K[C]) \times \prod_{H \in C_G(C)} \#AMO(H,K[H]),
\]

where the sum is over those \( C \) for which \( G^C \) is \( K \)-consistent.

**Lemma 4.14 (Wienöbst et al. 2021, Lemma 7).** We can order the elements of \( FP(C,T) \) as \( X_1 \subseteq X_2 \subseteq \cdots \subseteq X_l \subseteq C \).

The precondition of \( \Phi(S,R,K) \) is preserved throughout the recursion described in the lemma. We now give a recursive method to compute \( \Phi(S,R,K) \).

**Lemma 4.15.** Let \( S \) be a clique, and \( K \subseteq S \times S \) be a set of directed edges. Let \( R = \{R_1,R_2,\ldots,R_l\} \) where \( l \geq 1 \) be such that \( R_1 \subseteq R_2 \subseteq \cdots \subseteq R_l \subseteq S \). Then,

1. \( \Phi(S,\emptyset,K) = \frac{|S|!}{|V_K|!} \times \Psi(V_K,K) \), where \( \Psi(V_K,K) \) is the number of \( K \)-consistent permutations of vertices in \( V_K \) (\( V_K \) is the set of end points of edges in \( K \)). (Example: Suppose \( S = \{1,2,3,4,5\} \), and \( K = \{1 \to 2, 2 \to 3\} \). Then, \( V_K = \{1,2,3\} \). And, there exist only one permutation, \( (1,2,3) \), of \( V_K \) that is \( K \)-consistent, i.e., \( \Psi(V_K,K) = 1 \). This implies \( \Phi(S,\emptyset,K) = 20 \).

2. If there exists an edge \( u \to v \in K \) such that \( u \in S \setminus R_l \) and \( v \in R_l \), then \( \Phi(S,R,K) = \Phi(S,R-\{R_l\},K) \).

3. If there does not exist an edge \( u \to v \in K \) such that \( u \in S \setminus R_l \) and \( v \in R_l \), then \( \Phi(S,R,K) = \Phi(S,R-\{R_l\},K) - \Phi(R_l,R-\{R_l\},K[R_l]) \times \Phi(S \setminus R_l,\emptyset,K[S \setminus R_l]) \).
Algorithm 2: Valid-Perm(S, R, K)

Input: A clique S, R = \{R_1, R_2, \ldots, R_l\} such that \( R_1 \subseteq R_2 \subset \ldots \subset R_l \subseteq S \), and background knowledge \( K \subseteq S \times S \).

Output: \( \Phi(S, R, K) \).

1. if \( R = \emptyset \) then
   2. return \(|S|! \cdot \Psi(V_K, K)\)
3. \textbf{end}

4. sum ← Valid-Perm(S, R − \{R_l\}, K)
5. if \( \{(u, v) : u \rightarrow v \in K, v \in R_l \text{ and } u \notin R_l\} \neq \emptyset \) then
   6. return sum
7. \textbf{end}
8. return sum − Valid-Perm(R_l, R − \{R_l\}, K) \times Valid-Perm(S \setminus R_l, \emptyset, K[|S \setminus R_l|])

Proof of Lemma 4.15. Proofs of items 2 and 3 follow easily from the definition of the \( \Phi \) function (Lemma 4.13), and are similar in spirit to the corresponding results of [Wienöbst et al. 2021] in the setting of no background knowledge. We provide the details of these proofs in the supplementary material and focus here on proving item 1. If \( R = \emptyset \) then \( \Phi(S, R, K) \) is the number of \( K \)-consistent permutations of \( S \). There are \(|S|! \) permutations of \( S \) consistent with any given ordering of vertices in \( V_K \). The total number of \( K \)-consistent permutations of the vertices in \( V_K \) is \( \Psi(V_K, K) \). Therefore, the number of \( K \)-consistent permutations of \( S \) equals \(|S|! \times \Psi(V_K, K)\).

Algorithm 2 implements Lemma 4.15 to compute \( \Phi(S, R, K) \), and its correctness given below, is an easy consequence of Lemma 4.15.

Observation 4.16. For input \( S, R = \{R_1, R_2, \ldots, R_l\} \), and \( K \), where \( R_1 \subseteq R_2 \subset \ldots \subset R_l \subseteq S \), and \( K \subseteq S \times S \), Algorithm 2 returns \( \Phi(S, R, K) \).

We now construct Algorithm 3 that computes \( \#AMO(G, K) \). Algorithm 3 evaluates this formula, utilizing memoization to avoid recomputations.

Theorem 4.17. For a UCCG \( G \) and background knowledge \( K \), Algorithm 3 returns \( \#AMO(G, K) \).

Proof of Theorem 4.17: We first fix a clique tree \( T = (T, R) \) (at line 4) on which we define \( <_\alpha \). Lines 5-8 deals with the base case when \( G \) is a clique. If \( G \) is not a clique, Algorithm 3 follows Lemma 4.13. The full detail is given in Supplementary Material due to lack of space.

5 Time Complexity Analysis

In this section, we analyze the run time of Algorithm 3. The proof of the following observation, which shows that despite our modifications, Algorithm 1 still runs in linear time, is given in the Supplementary Material.

Observation 5.1. For a UCCG \( G \), a maximal clique \( C \) of \( G \), and background knowledge \( K \), Algorithm 4 runs in linear time \( O(|V_G| + |E_G|) \).

Similar to Wienöbst et al.’s \textcolor{red}{count} function, our \textcolor{red}{count} function (Algorithm 3) is also recursively called at most \( 2|\Pi(G)| - 1 \) times, where \( \Pi(G) \) is the set of maximal cliques of \( G \). Our approach to compute the background aware version of \( \Phi \) (Algorithm 2) is similar to that of
Algorithm 3: count(G, K, memo) (modification of an algorithm of [Wienöbst et al. 2021])

Input : A UCCG G, background knowledge K ⊆ E_G.
Output: #AMO(G, K).
1 if G ∈ memo then
2 return memo(G)
3 end
4 \(T = (T, R)\) ← a rooted clique tree of G
5 if \(R = V_G\) then
6 memo[G] = \(\Phi(V, \emptyset, K)\)
7 return memo[G]
8 end
9 sum ← 0
10 Q ← queue with single element \(R\)
11 while Q is not empty do
12 \(C \leftarrow \text{pop}(Q)\)
13 push(Q, children(C))
14 \((\text{flag}, \mathcal{L})\) ← LBFS(G, C, K)
15 if flag = 1 then
16 prod ← 1
17 foreach H ∈ \(\mathcal{L}\) do
18 prod = prod × count(G[H], K[H], memo)
19 end
20 sum = sum + prod × \(\Phi(C, \text{FP}(C, T), K[C])\)
21 end
22 end
23 memo[G] = sum
24 return sum

[Wienöbst et al. 2021], and the difference in time complexity comes from the high time complexity of computation of \(\Phi(S, \emptyset, K)\) at item 1 (it is \(O(1)\) for \(K = \emptyset\), which is the setting considered by [Wienöbst et al. 2021]). Proof of the claims below can be found in the Supplementary Material.

Proposition 5.2. Let \(G\) be a UCCG, and \(K\) be the known background knowledge about \(G\). The number of distinct UCCG explored by the count function (as defined in Algorithm 3) is bounded by \(2|\Pi(G)| - 1\).

Lemma 5.3. For input \(S, R = \{R_1, R_2, \ldots, R_l\}\), and \(K\), Algorithm 3 can be implemented using memoization to use \(O(k! \cdot k^2 \cdot |\Pi(G)|^2)\) arithmetic operations, where \(k\) is the max-clique knowledge of \(K\) (assuming factorials of integers from 1 to \(|V_G|\) are available for free).

Theorem 5.4 (Final runtime bound of Algorithm 3). For a UCCG \(G\), and background knowledge \(K\), Algorithm 3 runs in time \(O(k!k^2n^4)\), more precisely \(O(k!k^2 \cdot |\Pi(G)|^4)\), where \(n\) is the number of nodes in \(G\), and \(k\) is the max-clique knowledge of \(K\).

Proof of Theorem 3.2. Together, Theorems 4.17 and 5.4 prove our main result, Theorem 3.2.
Experimental evaluation

In this section, we evaluate the performance of Algorithm 3 on a synthetic dataset. For each \( n \in \{500, 510, 520, \ldots, 1000\} \), we construct 50 random chordal graphs with \( n \) nodes, and for each \( k \in \{5, 6, \ldots, 13\} \), we construct a set of background knowledge edges with \( k \) as its max clique knowledge value. We then measure the running time of Algorithm 3 for each of these (graph, background knowledge) pairs, and take the mean running time over all such pairs with the same value of \( n \) and \( k \). Further details about the construction of these instances can be found in the Supplementary Material.

Validating the run-time bound

To validate the \( O(k!k^2n^4) \) run-time bound established in Section 5, we draw log-log plots of the mean run-time \( T \) against the size \( n \) of the graph, for each fixed value of \( k \) (fig. 2). As predicted by the polynomial (in \( n \)) run-time bound in our theoretical result, we get, for each value of the parameter \( k \), a roughly linear log-log plot.

The intercept of the log-log plot

While the plots in fig. 2 for \( k \in \{5, 6, 7, 8, 9, 10, 11\} \) are quite close to each other, the separation of the plots for \( k = 12 \) and \( k = 13 \) is much larger. The reason behind it is the actual time complexity of Algorithm 3 can roughly be bounded as \( \log T \leq \log a + \log(k! \cdot k^2 + b) + 4 \log n \), where \( a \) and \( b \) are constants independent of \( n \) and \( k \). The above observation then shows that until about \( k \approx 11 \), all the plots have intercepts close to each other, as the contribution of terms involving \( a, b \) and \( n \) dominates that of \( k! \cdot k^2 \) for small values of \( k \).

Effect of the size of the background knowledge

An important feature of our analysis of Algorithm 3 is that its run-time bound does not depend directly upon the actual size of the background knowledge. To validate this, we conduct the following experiment: we fix a chordal graph of size \( n \) and the max-clique knowledge value \( k \), and then construct two different sets \( \mathcal{K}_1 \) and \( \mathcal{K}_2 \) of background knowledge edges, of different sizes such that both have the same \( k \) value (the details of the construction are given in the Supplementary Material). In table 1, \( T_1 \), \( T_2 \) are the running times of Algorithm 3 with background knowledge \( \mathcal{K}_1 \) and \( \mathcal{K}_2 \) respectively. The table confirms the expectation that when the graph and \( k \) are fixed, the running time does not increase much when the size of the background-knowledge increases. More detailed data and discussion of this phenomenon are given in the Supplementary Material.
Table 1: Exploring runtime dependence on the number of background knowledge edges

| n  | k | |K₁| |K₂| T₁  | T₂  |
|----|---|-----|-----|-----|-----|-----|
| 1000 | 10 |65   |116  |370  |353  |
| 1000 | 10 |75   |137  |346  |338  |
| 1100 | 11 |55   |121  |467  |455  |
| 1100 | 11 |51   |104  |460  |453  |

7 Conclusion

Our main result shows that the max-clique-knowledge parameter we introduce plays an important role in the algorithmic complexity of counting Markov equivalent DAGs under background knowledge constraint. In particular, it leads to a polynomial time algorithm in the special case of graphs of bounded maximum-clique size. Note that an algorithm that runs in polynomial time in the general case is precluded by the \#P-hardness result of [Wienöbst et al. 2021] (unless P = NP). However, the optimal dependence of the run time on the max-clique-knowledge parameter is an interesting open problem left open by our work.

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Supplementary Material

A  Graph terminology

Graphs and graph unions. We mostly follow the graph theory terminology of [Andersson et al., 1997]. A graph is undirected if all its edges are undirected, directed if all its edges are directed, and partially directed if it contains both directed and undirected edges. A directed graph that has no directed cycle is called a directed acyclic graph (DAG). A generalization of this idea is that of chain graphs: a partially directed graph is called a chain graph if it has no cycle which contains (i) at least one directed edge, and (ii) in which all directed edges are directed in the same direction as one moves along the cycle. We denote the neighbors of a vertex \( v \) in a graph \( G \) as \( N_G(v) \), and an induced subgraph of \( G \) on a set \( X \subseteq V \) is denoted as \( G[X] \).

The graph union (which we just call “union”) \( G_1 \cup G_2 \) includes vertices and edges present in any one of \( G_1 \) or \( G_2 \), i.e., \( V_{G_1 \cup G_2} = V_{G_1} \cup V_{G_2} \), and \( E_{G_1 \cup G_2} = E_{G_1} \cup E_{G_2} \). The skeleton of a partially directed graph \( G \) is an undirected version of \( G \) which we get by ignoring the direction of all the edges: in particular, note that the skeleton of a partially directed graph is also the graph union of all the partially directed graphs with the same skeleton as \( G \). A v-structure (or unshielded collider) in a partially directed graph \( G \) is an ordered triple of vertices \((a, b, c)\) of \( G \) which induce the subgraph \( a \leftrightarrow b \leftarrow c \) in \( G \).

Clique trees, separators, chordal graphs, and UCCG. A clique is a set of pairwise adjacent vertices for a graph. For a graph \( G \), \( u \) and \( v \) are said to be pairwise adjacent to each other if \((u, v), (v, u) \in E_G \), i.e., \( u - v \in E_G \). For an undirected graph \( G \), a set \( S \subseteq V_G \) is an \( x-y \) separator for two non-adjacent vertices \( x \) and \( y \) if \( x \) and \( y \) are in two different undirected connected components of \( G[V_G \setminus S] \). \( S \) is said to be a minimal \( x-y \) separator if no proper subset of \( S \) separates \( x \) and \( y \). A set \( S \) is said to be a minimal vertex separator if there exist vertices \( x \) and \( y \) for which \( S \) is a minimal \( x-y \) separator. An undirected graph \( G \) is chordal if, for any cycle of length 4 or more of \( G \), there exist two non-adjacent vertices of the cycle which are adjacent in \( G \). We refer to an undirected connected chordal graph by the abbreviation UCCG.

Clique trees. A rooted clique tree of a UCCG \( G \) is a tuple \( T = (T, R) \), where \( T \) is a rooted tree (rooted at the node \( R \)) whose nodes are the maximal cliques of \( G \), and which is such that the set \{ \( C : v \in C \) \} is connected in \( T \), for all \( v \in V_G \). Clique trees satisfy the important clique-intersection property: if \( C_1, C_2, C \in V_T \) and \( C \) is on the (unique) path between \( C_1 \) and \( C_2 \) in the tree \( T \), then \( C_1 \cap C_2 \subseteq C \) (see, e.g., [Blair and Peyton, 1993]). Further, a set \( S \subseteq V_G \) is a minimal vertex separator in \( G \) if, and only if, there are two adjacent nodes \( C_1, C_2 \in V_T \) such that \( C_1 \cap C_2 = S \) [Blair and Peyton, 1993, Theorem 4.3]. A clique tree for a UCCG \( G \) can be constructed in polynomial time. For more details on the above results on chordal graphs and clique trees, we refer to the survey of [Blair and Peyton, 1993].

B  Proofs omitted from Section 3

Observation B.1. If \( G \) is not \( K \)-consistent then \( \#AMO(G, K) = 0 \).

Proof. If \( G \) is not \( K \)-consistent then there exists an edge \( u \rightarrow v \in K \) such that \( v \rightarrow u \in E_G \), and all the AMOs of \( G \) have the edge \( v \rightarrow u \). This shows that no AMO of \( G \) is \( K \)-consistent. \( \square \)

We can verify in polynomial time that \( G \) is \( K \)-consistent or not, by checking the existence of an edge \( u \rightarrow v \in K \) for which \( v \rightarrow u \) is a directed edge in \( G \). This is why for further discussion we assume that \( G \) is \( K \)-consistent.

[blair_peyton_1993] refer to these objects as minimal separators, but we follow here the terminology of [blair_peyton_1993, Section 2.2] for consistency.
Proposition 3.4 is a direct consequence of the following lemma.

**Lemma B.2.** Let $G$ be an MEC consistent with a given background knowledge $K$, and let $G_d$ be the directed subgraph of $G$. Then, $\alpha \in \text{AMO}(G,K)$ if, and only if, (i) for each undirected chordal component $H$ of $G$, $\alpha[V_H]$ is a $K$-consistent AMO of $H$ and (ii) $\alpha$ is a union of $G_d$ and $\bigcup_H \alpha[V_H]$.

**Proof.** If $G$ is $K$-consistent then each directed edge of $G$ is $K$-consistent, i.e., $G_d$ is $K$-consistent. [Andersson et al.] 1997 show that for an MEC $G$, an AMO of $G$ can be constructed by choosing an AMO from each one of the chordal components of $G$ and taking the union of the directed subgraph of $G$ and the chosen AMOs of the chordal components. For every undirected connected chordal component $H$ of $G$, let us pick a $K$-consistent AMO of $H$. Then, the union of all the picked AMOs and $G_d$ is a $K$-consistent AMO of $G$. Also if $\alpha$ is an AMO of $G$ then for all undirected connected chordal components $H$ of $G$, $\alpha[V_H]$ is $K$-consistent. And $\alpha$ must be a union of $G_d$ and the union of all the $\alpha[V_H]$. This proves Lemma B.2. \hfill \Box

**C ** Definition of $C_\alpha$

Here, we define $C_\alpha$. We start with defining a few preliminary terms flower, $<_\tau$, and $<_\alpha$ that we use to define $C_\alpha$.

**Definition C.1** (Flowers and bouquets, [Wienöbst et al.] 2021, Definition 4). Let $G$ be a UCCG. An $S$-flower for a minimal vertex separator $S$ of $G$ is a maximal subset $F$ of the set of maximal cliques of $G$ containing $S$ such that $\bigcup_{C \in F} C$ is connected in the induced subgraph $G[V \setminus S]$. The bouquet $B(S)$ of a minimal separator $S$ is the set of all $S$-flowers.

**Definition C.2** (The $<_\tau$ order for a rooted clique tree, Section 5 of [Wienöbst et al.] 2021). Let $G$ be a UCCG, $S$ be a minimal vertex separator of $G$, $F_1, F_2 \in B(S)$, and $T = (T, R)$ be a rooted clique tree of $G$. $F_1 <_\tau F_2$ if $F_1$ contains a node on the unique path from $R$ to $F_2$.

**Definition C.3** (The $<_\alpha$ order for an AMO $\alpha$, Section 5 of [Wienöbst et al.] 2021). Let $G$ be a UCCG, $T = (T, R)$ be a rooted clique tree of $G$, and $\alpha$ be an AMO of $G$. We use $<_\tau$ to define a partial order $<_\alpha$ on the set of maximal cliques that represent $\alpha$, as follows: $C_1 <_\alpha C_2$ if, and only if, (i) $C_1 \cap C_2 = S$ is a minimal vertex separator, (ii) $C_1$ and $C_2$ are elements of distinct $S$-flowers $F_1, F_2 \in B(S)$, respectively, and (iii) $F_1 <_\tau F_2$.

The following result of [Wienöbst et al.] 2021 establishes the requisite property of the ordering $<_\alpha$.

**Lemma C.4** ([Wienöbst et al.] 2021, Claim 1). Let $G$ be a UCCG, $\alpha$ an AMO of $G$, and $T = (T, R)$ a rooted clique tree of $G$. Consider the order $<_\alpha$ defined on the maximal cliques $T$. Then, there always exists a unique least maximal clique with respect to $<_\alpha$.

**D ** Proofs omitted from Section 4

**Proof of Lemma 4.1.** The claim follows from the fact that for each AMO $\alpha$ of $G$, $C_\alpha$ was canonically chosen from the set of maximal cliques representing $\alpha$. \hfill \Box

**Proof of Observation 4.4.** Proof of item 1. For any edge $u - v \in E_G$, if $u \in C$ and $v \notin C$ then for any AMO that is represented by an LBFS ordering that starts with $C$, $u \rightarrow v$ is a directed edge in the AMO (see “Representation of an AMO” of Section 2). This further implies for any edge $u - v \in E_G$, if $u \in C$ and $v \notin C$ then $u \rightarrow v$ is a directed edge in $G^C$, as $G^C$ is the union
of all the AMOs of $G$ that can be represented by an LBFS ordering that starts with $C$. This proves item 1.

Proof of item 2. We prove item 2 of Observation 4.4 using induction on the size of $L$.

**Base Case:** $|L| = 0$. In this case, item 2 of Observation 4.4 is vacuously true.

Let item 2 is true when $|L| = l \geq 0$. We show that item 2 is true even for $|L| = l + 1$.

Let at some iteration of Algorithm 1, $L = \{X_1, X_2, \ldots, X_l, X_{l+1}\}$. From the induction hypothesis, for an edge $u \rightarrow v \in E_G$, if $u \in X_i$ and $v \notin C \cup X_1 \cup X_2 \cup \ldots \cup X_i$ then $u \rightarrow v \in G^C$, when $i \leq l$. Let there exists an edge $u \rightarrow v \in E_G$ such that $u \in X_{l+1}$ and $v \notin C \cup X_1 \cup X_2 \cup \ldots \cup X_{l+1}$. This means there must exist a vertex $x \in C \cup X_1 \cup X_2 \cup \ldots \cup X_l$ for which $x \rightarrow u \in E_G$ and $v \rightarrow u \notin E_G$, due to which $u$ and $v$ moves to two different sets in $S$, because initially $u$ and $v$ are in the same set $V \setminus C$. From the induction hypothesis, $x \rightarrow u \in G^C$. This implies all the AMOs that are represented by $C$ have edge $x \rightarrow u$. This further implies all the AMOs that are represented by $C$ have edge $u \rightarrow v$, as $v \rightarrow u$ creates an immorality $x \rightarrow u \leftrightarrow v$ (from the definition of AMO, there cannot be a v-structure in an AMO of $G$). This proves item 2.

Proof of item 3. Suppose $u, v \in V$. Let $u \rightarrow v \in E_G$. Let there exists an AMO $\alpha$ that is represented by $C$ and has the edge $u \rightarrow v$. Let $\tau_1$ be an LBFS ordering of $G$ that starts with $C$, and represents $\alpha$. We can construct another LBFS ordering $\tau_2$ that also starts with $C$ such that while picking the vertices of $X_i$, we pick $v$ before $u$. The AMO corresponding to this LBFS ordering has the edge $v \rightarrow u$. Since $G^C$ is the union of all the AMOs of $G$ that is represented by $C$. This implies $G^C$ has the undirected edge $u \rightarrow v$. This proves item 3.

Proof of item 4. If $u, v \in C$ then $u \rightarrow v \in E_G$, because $C$ is a clique of $G$. Suppose an AMO $\alpha$ is represented by $C$ and has the edge $u \rightarrow v$. Then, $\alpha$ must be represented by an LBFS ordering $\tau_1$ that starts with a permutation $\pi_1(C)$ of $C$ such that $u$ comes before $v$ in $\pi_1(C)$. Let $\pi_2(C)$ be a permutation of $C$ such that $v$ comes before $u$ in $\pi_2(C)$. Let us construct an LBFS ordering $\tau_2$ by replacing $\pi_1(C)$ with $\pi_2(C)$ in $\tau_1$. Let $\beta$ be the AMO represented by the LBFS ordering $\tau_2$. $\beta$ also represented by $C$ and has the edge $v \rightarrow u$. Since $G^C$ is the union of all the AMOs of $G$ that is represented by $C$, this implies $u \rightarrow v$ is an undirected edge in $G^C$, because $u \rightarrow v \in \alpha$, and $v \rightarrow u \in \beta$, and both are represented by $C$. This proves item 4.

Proof of item 5. From items 1 and 2, all the edges with only one endpoint in $X_i$ are directed in $G^C$. And, from item 3, all the edges with both of the endpoints in $X_i$ are undirected in $G^C$. This further implies all the undirected connected components of $G[X_i]$ are undirected connected components of $G^C$.

**Proof of Lemma 4.5**. At first, we want to recall that Algorithm 1 is background aware version of the modified LBFS algorithm of Wienobst et al. 2021. As discussed in the main paper, we do not change any line from the LBFS algorithm of Wienobst et al. 2021, the only modifications we do to their LBFS algorithm are (a) introduction of flag, at line 2, which is used to check the $K$-consistency of $G^C$, (b) lines 11-13, which is used to update the value of flag, and (c) We also output the value of flag with $C_G(C)$. The output of Algorithm 1 has 2 components. The first component is the value of flag, and the second value is the value returned by the LBFS algorithm of Wienobst et al. 2021, which is $C_G(C)$. Thus, the only thing we need to verify is that the first component of our output, i.e., the value of flag, is 1 if $G^C$ is $K$-consistent, and 0 if $G^C$ is not $K$-consistent, which is equivalent to show that the value of flag returned by the algorithm is 0 if, and only if, $G^C$ is not $K$-consistent (since the value of flag is either 0 or 1).

Suppose $G^C$ is not $K$-consistent. Then, from the definition of $K$-consistency of $G^C$ (Definition 4.3), there must exist an edge $v \rightarrow u$ in $G^C$ such that $u \rightarrow v \in K$. From Observation 4.4, if $v \rightarrow u \in G^C$ then either (a) $v \in C$ and $u \notin C$, or (b) at some iteration, when $L = \{X_1, X_2, \ldots, X_l\}$, $v \in X_l$ and $u \notin C \cup X_1 \cup X_2 \cup \ldots \cup X_l$. In both of the cases, $v$ must be picked before $u$ at line 14, as $v$ is present in a set that comes before the set in which $u$ is
present. At the iteration when \( v \) is picked, the algorithm finds the edge \( u \rightarrow v \) that obeys the condition stated in line 11. This further sets the value of \( \text{flag} \) to 0. From the construction of the algorithm, once the value of \( \text{flag} \) sets to 0, it remains at 0. This shows that if \( G^C \) is not \( \mathcal{K} \)-consistent then the value of \( \text{flag} \) is 0.

Now suppose the \( \text{flag} \) value returned by the algorithm is 0. At line 2, the value of \( \text{flag} \) is initialized with 1. If \( \text{flag} \) value returned by the algorithm is 0 then there must exist an edge \( u \rightarrow v \in \mathcal{K} \) (found at line 11), which causes to change the value of \( \text{flag} \) to 0 at line 12. Since \( u \rightarrow v \) obeys the condition state at line 11, we can certainly say that the iteration when \( v \) is picked at the line 5 \( u \) must be neither in \( \mathcal{C} \) nor in any set of \( \mathcal{L} \). And, \( u \) must be either in \( C \), if \( \mathcal{L} = \emptyset \), or in \( X_l \), if \( \mathcal{L} = \{X_1, X_2, \ldots, X_l\} \) such that \( l \geq 1 \). From Observation 4.4, \( v \rightarrow u \) must be a directed edge in \( G^C \). This makes \( G^C \) inconsistent with \( \mathcal{K} \), as \( u \rightarrow v \in \mathcal{K} \) (Definition 4.3). This shows if the value of \( \text{flag} \) returned by the algorithm is 0 then \( G^C \) is not \( \mathcal{K} \)-consistent. This completes the proof.

**Proof of Observation 4.6** If \( \alpha \) is a member of AMO\((G, \pi_1(C))\) and AMO\((G, \pi_2(C))\) both, for two different permutations \( \pi_1(C) \) and \( \pi_2(C) \), then there must exist two vertices \( u, v \in C \) such that \( u \) comes before \( v \) in \( \pi_1(C) \), and \( v \) comes before \( u \) in \( \pi_2(C) \). Since \( u \) and \( v \) are members of the same clique, there exists an edge \( u \rightarrow v \in E_G \). And, since the AMO is a member of both AMO\((G, \pi_1(C))\), and AMO\((G, \pi_2(C))\) it should have both \( u \rightarrow v \) and \( v \rightarrow u \), which is not possible. This implies there exists a unique permutation \( \pi(C) \) of \( C \) that represents \( \alpha \).

**Proof of Lemma 4.7** Claims 1 and 2 of Wienöbst et al. [2021] translate into the “only if” part of Lemma 4.7 while Claim 3 of Wienöbst et al. [2021] translates into the “if” part of Lemma 4.7. We give details of the translation below. Given an AMO \( \alpha \), [Wienöbst et al. 2021] define a partial order \( \prec_\alpha \) (as described above) on the set of maximal cliques that represent \( \alpha \). Claim 1 of Wienöbst et al. [2021] shows that there exists a unique maximal clique representing \( \alpha \) (which we name as \( C_\alpha \)) such that for any maximal clique \( C \neq C_\alpha \) that represents \( \alpha \), \( C_\alpha \prec_\alpha C \). Claim 2 of Wienöbst et al. [2021] then translates immediately into the “only if” part of Lemma 4.7.

For the “if” part, we consider any maximal clique \( C \) representing \( \alpha \) and satisfying both the conditions of Lemma 4.7. Suppose, if possible, that \( C \neq C_\alpha \). Then, from the above discussion, \( C_\alpha \prec_\alpha C \). The proof of Claim 3 (and the definition of \( FP(C, T) \)) then shows that if \( \pi(C) \) is the permutation of \( C \) representing \( \alpha \), then there is a prefix \( S \) of \( \pi(C) \) of the form \( C_i \cap C_j \) for some two adjacent cliques on the path from \( R \) to \( C \) in \( T \). This leads to a contradiction with item 2 of Lemma 4.7 and hence shows that \( C \neq C_\alpha \) is not possible.

For the proof of Lemma 4.11, we need the following observation of Wienöbst et al. [2021].

**Observation D.1** (Wienöbst et al. [2021], Proposition 1). For each permutation \( \pi(C) \) of a maximal clique \( C \) of \( G \), all edges of \( G^\pi(C) \) coincide with the edges of \( G^C \), excluding the edges connecting the vertices in \( C \). In particular, \( C_G(\pi(C)) = C_G(C) \).

**Proof of Lemma 4.11** Let \( G^C \) be \( \mathcal{K} \)-consistent, and \( \pi(C) \) is a \((\mathcal{K}, T)\)-consistent permutation of \( C \). We show that the number of \( \mathcal{K} \)-consistent AMOs of \( G \) that are canonically represented by \( \pi(C) \), i.e., \( \{\alpha : \alpha \in \text{AMO}(G, \pi(C), \mathcal{K}) \text{ and } C = C_\alpha\} \), equals \( \Pi_{H \in \mathcal{C}_G(C)} \#\text{AMO}(H, \mathcal{K}[H]) \). To prove this, we first show that if \( \alpha \) is a \( \mathcal{K} \)-consistent AMO of \( G \) that is canonically represented by \( \pi(C) \) then for any connected component \( H \) of \( C_G(C) \), \( \alpha[H] \) is \( \mathcal{K}[H] \)-consistent AMO of \( H \). We also show that if we have a \( \mathcal{K}[H] \)-consistent AMO for each connected component \( H \) of \( C_G(C) \) then we can construct a \( \mathcal{K} \)-consistent AMO of \( G \) by combining them. This proves Lemma 4.11.

We first show the first part. Let \( \alpha \) be a \( \mathcal{K} \)-consistent AMO of \( G \) that is canonically represented by \( \pi(C) \). Then, for any connected component \( H \) of \( C_G(C) \), \( \alpha[H] \) is \( \mathcal{K}[H] \)-consistent AMO of \( H \). Otherwise, if for any connected component \( H \) of \( C_G(C) \), \( \alpha[H] \) is not \( \mathcal{K}[H] \)-consistent then
there must exist an edge \( u \to v \in K[H] \) such that \( v \to u \in \alpha[H] \). But, this implies \( \alpha \) is not \( K \)-consistent either, as if \( u \to v \in K[H] \) then \( u \to v \in K \), and if \( v \to u \in \alpha[H] \) then \( v \to u \in \alpha \).

We now show the other part. Let \( H_1, H_2, \ldots, H_l \) are the undirected connected components of \( C_G(C) \), in the same order as we get as the output of Algorithm 1 for input \( G, C \), and \( K \). For each \( H_i \in C_G(C) \), let we have a \( K[H_i] \)-consistent AMO \( D_i \), and \( \tau_i \) be an LBFS ordering of \( D_i \). Then, \( \tau = \{ \pi(C), \tau_1, \tau_2, \ldots, \tau_l \} \) is a \( K \)-consistent LBFS ordering of \( G \) starting with \( \pi(C) \) that we can get from Algorithm 1. The DAG \( \alpha \) represented by \( \tau \) is an AMO of \( G \) represented by \( \pi(C) \). And, since \( \pi(C) \) is \( (K, T) \)-consistent, from Lemma 4.7 \( C = C_\alpha \). This implies \( \alpha \) is a \( K \)-consistent AMO of \( G \) and is canonically represented by \( \pi(C) \). This gives us a one-to-one mapping between the set of \( K \)-consistent AMOs of \( G \) that is canonically represented by \( \pi(C) \), and the \( K[H] \)-consistent AMOs of the connected components \( H \) of \( C_G(C) \), which further implies the equality between the size of \( K \)-consistent AMOs of \( G \) that is canonically represented by \( \pi(C) \) and \( \Pi_{H \in C_G(C)} \# \text{AMO}(H, K[H]) \). This completes our proof.

**Proof of Lemma 4.13.** From Lemma 4.1, \( \# \text{AMO}(G, K) = \sum_{C \in \Pi(G)} \{ \alpha : \alpha \in \text{AMO}(G, K) \text{ and } C = C_\alpha \} \). In Section 4 after defining \( K \)-consistency of \( G^C \) (Definition 4.3), we show that for any maximal clique \( C \) of \( G \), if \( G^C \) is not \( K \)-consistent then \( \{ \alpha : \alpha \in \text{AMO}(G, K) \text{ and } C = C_\alpha \} = 0 \). From Lemma 4.11 for any maximal clique \( C \) of \( G \), if \( G^C \) is \( K \)-consistent then for any \( (K, T) \)-consistent permutation \( \pi(C) \) of \( C \), \( \{ \alpha : \alpha \in \text{AMO}(G, \pi(C), K) \text{ and } C = C_\alpha \} = \prod_{H \in C_G(C)} \# \text{AMO}(H, K[H]) \). And, from Observation 4.10 for any permutation \( \pi(C) \) of a maximal clique \( C \) of \( G \), if \( \pi(C) \) is not a \( (K, T) \)-consistent permutation of \( C \) then \( \{ \alpha : \alpha \in \text{AMO}(G, \pi(C), K) \text{ and } C = C_\alpha \} = 0 \). This further implies for any maximal clique \( C \) of \( G \), if \( G^C \) is \( K \)-consistent then \( \{ \alpha : \alpha \in \text{AMO}(G, K) \text{ and } C = C_\alpha \} = \Phi(C, FP(C, T), K[C]) \times \prod_{H \in C_G(C)} \# \text{AMO}(H, K[H]) \), where \( \Phi(C, FP(C, T), K[C]) \) is the number of \( (K, T) \)-consistent permutations of a maximal clique \( C \) of \( G \) (from Definitions 4.9 and 4.12). All these things further imply \( \# \text{AMO}(G, K) = \sum_{C:G^C \text{ is } K\text{-consistent}} \Phi(C, FP(C, T), K[C]) \times \prod_{H \in C_G(C)} \# \text{AMO}(H, K[H]) \). This proves the correctness of Lemma 4.13.

**Proof of Lemma 4.15.**

**Proof of item 1.** If \( R = \emptyset \), then a permutation \( \pi(S) \) of \( S \) is \( K \)-consistent if ordering of \( V_K \) in \( \pi(S) \) is \( K \)-consistent. \( \Psi(V_K, K) \) gives the number of \( K \)-consistent permutations of \( V_K \). Number of permutations of \( S \) that has the same ordering of \( V_K \) in it is \( |S|! \). This completes the proof of item 1.

**Proof of item 2.** If there exists an edge \( u \to v \in K \) such that \( u \in S \setminus R_l \) and \( v \in R_l \) then no \( K \)-consistent permutation of \( S \) exists that starts with \( R_l \).

**Proof of item 3.** If there does not exist an edge \( u \to v \in K \) such that \( u \in S \setminus R_l \) and \( v \in R_l \), then one way to compute \( \Phi(S, R, K) \) is to first compute number of \( K \)-consistent permutations of \( S \) that do not start with \( R_1, R_2, \ldots, R_{l-1} \), i.e., \( \Phi(S, R - \{R_l\}, K) \). But, \( \Phi(S, R - \{R_l\}, K) \) also counts the \( K \)-consistent permutations of \( S \) that starts with \( R_l \) but not with any \( R_i \), for \( 1 \leq i < l \). We subtract such permutations from \( \Phi(S, R - R_l, K) \). To construct a \( K \)-consistent permutation of \( S \) that starts with \( R_l \) but does not start with any \( R_i \), \( 1 \leq i < l \), we have to first construct a permutation of \( R_l \) that does not start with any \( R_i \), \( 1 \leq i < l \), and then we have to construct a \( K \)-consistent permutation of the remaining vertices of \( S \). This implies the number of \( K \)-consistent permutations of \( S \) that start with \( R_l \) and not with any \( R_i \), \( 1 \leq i < l \), is \( \Phi(R_l, R - \{R_l\}, K) \times \Phi(S \setminus R_l, \emptyset, K) \).

**Proof of Observation 4.16.** If \( R = \emptyset \) then from item 1 of Lemma 4.15, \( \Phi(S, R, K) = \frac{|S|!}{|V_K|!} \times \Psi(V_K, K) \). Line 2 of Algorithm 2 returns the same.

If \( R = \{R_1, R_2, \ldots, R_l\} \neq \emptyset \), and there exist an edge \( u \to v \in K \) such that \( u \in S \setminus R_l \) and \( v \in R_l \), then from item 2 of Lemma 4.15, \( \Phi(S, R, K) = \Phi(S, R - R_l, K) \). Line 6 of Algorithm 2 returns the same.
If \( R = \{R_1, R_2, \ldots, R_t\} \neq \emptyset \), and there does not exist an edge \( u \to v \) in \( \mathcal{K} \) such that \( u \in S \setminus R_t \) and \( v \in R_t \), then using item 3 of Lemma 4.15, we have:

\[
\Phi(S, R, \mathcal{K}) = \Phi(S, R - \{R_t\}, \mathcal{K}) - \Phi(R_t, R - \{R_t\}, \mathcal{K}[R_t]) \times \Phi(S \setminus R_t, \emptyset, \mathcal{K}[S \setminus R_t]).
\]

The line 8 of Algorithm 2 returns the same.

\[ \square \]

**Proof of Theorem 4.17.** At line 4, Algorithm 3 constructs a rooted clique tree of \( G \). Lines 5-8 deals with a special case when \( |\{\alpha : \alpha \in \text{AMO}(G, \pi(C), \mathcal{K}) \text{ and } C = C_\emptyset\}| = 0 \). This is why we skip lines 10-21 if the first component of LBFS(\( G, C, \mathcal{K} \)) (Algorithm 1) is 0. If the first component LBFS(\( G, C, \mathcal{K} \)) is 1 then \( G^C \) is \( \mathcal{K} \)-consistent. In this case, at lines 17-19, we compute \( \prod_{H \subseteq C_\emptyset} \#\text{AMO}(H, \mathcal{K}[H]) \), by recursively calling Algorithm 3. At line 20, we compute \( |\{\alpha : \alpha \in \text{AMO}(G, \mathcal{K}) \text{ and } C = C_{\emptyset}\}| \) using the discussion following Lemma 4.11. At the end of line 22, the variable \( \text{sum} \) has the value \( \sum_{C:G^C \text{ is } \mathcal{K} \text{-consistent}} \Phi(C, \mathcal{F}(C, T), \mathcal{K}[C]) \times \prod_{H \subseteq C_\emptyset} \#\text{AMO}(H, \mathcal{K}[H]) \), i.e., \( \text{sum} \) equals \( \#\text{AMO}(G, \mathcal{K}) \) (from Lemma 4.13). \( \text{memo}[G] \) stores the number of \( \mathcal{K} \)-consistent AMOs of \( G \), once it is computed. This completes the proof.

\[ \square \]

**E  Proofs omitted from Section 5**

**Proof of Observation 5.2.** The “While” loop on lines 3-19 runs at most \( |V_G| \) times. Using two additional arrays (one for checking whether \( v \) is in \( C \) or not, and another for checking whether \( v \) is in \( L \) or not) we can run lines 6-9 in \( O(1) \) time. Checking the existence of edge \( u \to v \) in \( \mathcal{K} \) at line 11 takes \( O(|\mathcal{K}|) \) time cumulatively, for all \( v \in V_G \). Finding neighbors of \( v \) at line 16 takes \( O(E_G) \) time cumulatively, for all \( v \in V_G \). Partitioning each set at line 17 also takes \( O(E_G) \) time cumulatively. Since the size of \( \mathcal{K} \) can be at most \( E_G \), this implies the overall time complexity of Algorithm 3 is \( O(|V_G| + |E_G|) \) (with the same technique that is used to implement the standard LBFS of Rose et al. [1976]).

**Proof of Proposition 5.2.** Algorithm 3 calls itself at line 18, for each \( H \in L \), when \( \text{flag} = 1 \). The value of \( \text{flag} \) is always 1 when \( \mathcal{K} = \emptyset \), and \( L = C_\emptyset \) (from Algorithm 1) does not depend on \( \mathcal{K} \). This further implies that the \( \text{count} \) function has the maximum number of distinct recursive calls to itself when \( \mathcal{K} = \emptyset \). But, for \( \mathcal{K} = \emptyset \), Algorithm 3 is the same as the Clique-Picking algorithm of Wienöbst et al. [2021], who showed that the number of these distinct recursive calls is at most \( 2|H(G)| - 1 \) times. This completes the proof.

**Proof of Lemma 5.3.** Let us denote \( \mathcal{R}_i = \{R_1, R_2, \ldots, R_i\} \). For the computation of \( \Phi(S, \mathcal{R}_1, \mathcal{K}) \), from items 2 and 3 of Lemma 4.15, we need to compute \( \Phi(S, \emptyset, \mathcal{K}), \Phi(S \setminus R_1, \emptyset, \mathcal{K}[S \setminus R_1]), \Phi(S \setminus R_2, \emptyset, \mathcal{K}[S \setminus R_2]), \ldots, \Phi(S \setminus R_l, \emptyset, \mathcal{K}[S \setminus R_l]), \Phi(S, \mathcal{R}_1, \mathcal{K}), \Phi(S, \mathcal{R}_2, \mathcal{K}), \ldots, \Phi(S, \mathcal{R}_l, \mathcal{K}) \), and for each \( 1 \leq i \leq l \), \( \Phi(R_i, \emptyset, \mathcal{K}[R_i]), \Phi(R_i \setminus R_1, \emptyset, \mathcal{K}[R_i \setminus R_1]), \ldots, \Phi(R_i \setminus R_{i-1}, \emptyset, \mathcal{K}[R_i \setminus R_{i-1}]), \Phi(R_i, \mathcal{R}_1, \mathcal{K}[R_i]), \Phi(R_i, \mathcal{R}_2, \mathcal{K}[R_i]), \ldots, \Phi(R_i, \mathcal{R}_{l-1}, \mathcal{K}[R_i]). \)

Computation of each \( \Phi(X, \phi, \mathcal{K}' = \mathcal{K}[X]) \) takes \( O(k! \cdot k^2) \) arithmetic operations. To see this, note that item 1 of Lemma 4.15 gives \( \Phi(X, \phi, \mathcal{K}') = \frac{|X|!}{|\mathcal{K}'|!} \times \Phi(V_{\mathcal{K}'}, \mathcal{K}') \). From our assumption, the factorials are already pre-computed. On the other hand, to compute \( \Psi(V_{\mathcal{K}'}, \mathcal{K}') \) we can check one-by-one the \( \mathcal{K}' \)-consistency of each permutation of \( V_{\mathcal{K}'} \). The number of permutations
of \( V_{\mathcal{K}'} \) is \( O(k!) \), since \( |V_{\mathcal{K}'}| \leq k \) (max-clique knowledge), while the verification of whether a
permutation of \( V_{\mathcal{K}'} \) is \( \mathcal{K}' \)-consistent or not takes \( O(|\mathcal{K}'|) \) time. Since \( V_{\mathcal{K}'} \leq k \), we have \( |\mathcal{K}'| \leq k^2 \). Thus, the computation of \( \Psi(V_{\mathcal{K}'}, \mathcal{K}') \) takes \( O(k^2 \cdot k!) \) arithmetic operations.

Since the number of required computations of the type \( \Phi(X, \phi, \mathcal{K}' = \mathcal{K}[X]) \) (as already listed
above) is \( O(l^2) \), their total cost is \( O(k! \cdot k^2 \cdot l^2) \). After all the values listed above of the type
\( \Phi(X, \phi, \mathcal{K}' = \mathcal{K}[X]) \) have been computed, we can implement a dynamic programming procedure
using items 2 and 3 of Lemma 4.15 (or, alternatively, a memoized version of Algorithm 2)
to compute all the required values of type \( \Phi(X, Y \neq \emptyset, \mathcal{K}[X]) \) (as listed above) using \( O(1) \)
arithmetic operations each. Since the number of required computations of the type \( \Phi(X, Y \neq \emptyset, \mathcal{K}[X]) \) (again, as already listed above) is also \( O(l^2) \), it follows that the total cost of these
computations is \( O(l^2) \). Adding the computational costs for both types of computations, we see
that the total cost is \( O(k! \cdot k^2 \cdot l^2) \) arithmetic operations.

As the value of \( l \) can be at most \( |\Pi(G)| \) (the number of nodes in the clique tree \( T \)), the
overall number of arithmetic operations we need to compute \( \Phi(S, \mathcal{R}_l, \mathcal{K}) \) is \( O(k! \cdot k^2 \cdot |\Pi(G)|^2) \).

\( \square \)

\textbf{Proof of Theorem 5.4.} Algorithm 3 is analogous to Clique-Picking Algorithm of \cite{Wien2021}. We can also say that Algorithm 3 is the background knowledge version of the Clique-Picking Algorithm of \cite{Wien2021}. At line 4, we construct a clique tree of \( G \), which takes \( O(|V_G| + |E_G|) \) time. Computing \( \Phi \) function at line 5 for a clique \( C \), takes \( O(|\Pi(G)|^2 \cdot k^2 \cdot k!) \) time (from Lemma 5.3). While loop (at lines 11-22) runs for \( O(|\Pi(G)|) \) times, as the
number of maximal cliques of \( G \) is \( |\Pi(G)| \). Running LBFS-algorithm (Algorithm 1) at line 14
takes \( O(|V| + |E|) \) time (from Observation 5.1). Computation of function \( \Phi \) at line 20 takes
\( O(k! \cdot k^2 \cdot |\Pi(G)|^2) \) time (from Lemma 5.3).

Note that it was assumed in Algorithm 2 that factorials of integers from 1 to \( |V_G| \) are
pre-computed. The pre-computation of this table can be done using \( O(|V_G|) \) arithmetic operations. From Proposition 5.2, the number of distinct calls to \texttt{count} function of Algorithm 3 is
\( O(|\Pi(G)|) \). Together, the above calculations show that the running time of Algorithm 3 is at
most \( O(k! \cdot k^2 \cdot |\Pi(G)|^4) \) or \( O(k! \cdot k^2 \cdot |V_G|^4) \), as for a chordal graph \( G \), \( |\Pi(G)| \) can be at most
\( |V_G| \).

\( \square \)

\textbf{F Detailed explanation of Experimental Results}

\textbf{Construction of chordal graphs with \( n \) vertices:} We first construct a connected \textit{Erdős-Rényi graph} \( G \) with \( n \) vertices such that each of its edges is picked with probability \( p \), where \( p \) is a random value in \( [0.1, 0.3) \). We give a unique rank to each node of the graph. We then
process the vertices in decreasing order of rank. For each vertex \( x \) of the graph, if \( u \) and \( v \) are
two neighbors of \( x \) such that \( u \) and \( v \) are not connected, and \( u \) and \( v \) both have lesser rank
than the rank of \( x \), then we put an edge between \( u \) and \( v \) in \( G \). This makes \( G \) an undirected
chordal graph, because, by construction, the decreasing order of ranks is a perfect elimination
ordering. After this, we use rejection sampling to get an undirected connected chordal graph,
i.e., if \( G \) is not a connected graph then we reject \( G \), and repeat the above process until we get
an undirected connected chordal graph \( G \).

\textbf{Construction of background knowledge edges:} For each chordal graph constructed
above, and for each \( k \in \{5, 6, \ldots, 13\} \), we construct a set of background knowledge edges such
that (i) for any maximal clique \( C \) of size greater than or equal to \( k \), the number of vertices of the
clique that are part of an edge of the background knowledge with both endpoint in \( C \) is \( k \); and (ii) for any maximal clique of size less than \( k \), the number of vertices of the clique that are
part of an edge of background knowledge equals to the size of the clique. To do this, we
Table 2: Exploring runtime dependence on the number of background knowledge edges: detailed table

| n   | k | $|K_1|$ | $|K_2|$ | $T_1$ | $T_2$ |
|-----|---|-------|-------|------|------|
| 600 | 6 | 58    | 73    | 95   | 92   |
| 600 | 6 | 52    | 65    | 192  | 190  |
| 700 | 7 | 47    | 67    | 144  | 144  |
| 700 | 7 | 49    | 74    | 132  | 128  |
| 800 | 8 | 56    | 83    | 199  | 195  |
| 800 | 8 | 55    | 85    | 200  | 195  |
| 900 | 9 | 46    | 89    | 258  | 256  |
| 900 | 9 | 39    | 68    | 257  | 252  |
| 1000| 10| 65    | 116   | 370  | 353  |
| 1000| 10| 75    | 137   | 346  | 338  |
| 1100| 11| 55    | 121   | 467  | 455  |
| 1100| 11| 51    | 104   | 460  | 453  |

pick one by one each maximal clique of $G$, and select the edges of the clique such that at most $k$ vertices are involved in the set of selected edges with both of its endpoints in that clique. For this, we construct a rooted clique tree $T = (T, R)$ of $G$. We start with $R$ and then do a depth-first search (DFS) on $T$ to cover all the maximal cliques of $G$. At the iteration when we are at a maximal clique $C$, we first compute the set of vertices of the picked edges having both of their endpoints in $C$. If the size of the set is $k$ (or $|C|$, if $|C| < k$) we move to the next maximal clique. Otherwise, we one by one pick edges of $C$ and add to the selected set of edges until the set of vertices of the picked edges having both of their endpoints in $C$ reaches $k$ (or $|C|$, if $|C| < k$). We won’t get into a situation where the set of vertices of the picked edges having both of their endpoints in $C$ exceeds $k$ (due to the clique intersection property of the clique-tree).

We write a python program for the construction of chordal graphs, background knowledge edges, and implementation of Algorithm 3. The experiments use the open source networkx (Hagberg et al. [2008]) package.

Effect of changing the size of the background knowledge while keeping $k$ fixed Here we describe the construction of the background knowledge edge sets $K_1$ and $K_2$ used in table 1. We first construct $K_1$ as above. We then construct $K_2$ by adding a few edges to $K_1$ in such a way that the value of $k$ does not change. We do this experiment for different $n$ and $k$, where $n$ is the number of nodes of the chordal graph, and $k$ is the maximum number of vertices of any clique of the chordal graph that is part of a background knowledge edge that lies completely inside that clique, as defined earlier also. Table 2 gives a more detailed version of table 1 (given in the main section of the paper) with more dataset points.

We can also see from the table that the running time decreases slightly by increasing the size of background knowledge edges. This is because as the number of background knowledge increases the number of background consistent permutations of any clique decreases.

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