Recovering Causal Structures from Low-Order Conditional Independencies

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Abstract
One of the common obstacles for learning causal models from data is that high-order conditional independence (CI) relationships between random variables are difficult to estimate. Since CI tests with conditioning sets of low order can be performed accurately even for a small number of observations, a reasonable approach to determine causal structures is to base merely on the low-order CIs. Recent research has confirmed that, e.g. in the case of sparse true causal models, structures learned even from zero- and first-order conditional independencies yield good approximations of the models. However, a challenging task here is to provide methods that faithfully explain a given set of low-order CIs. In this paper, we propose an algorithm which, for a given set of conditional independencies of order less or equal to $k$, where $k$ is a small fixed number, computes a faithful graphical representation of the given set. Our results complete and generalize the previous work on learning from pairwise marginal independencies. Moreover, they enable to improve upon the 0-1 graph model which, e.g. is heavily used in the estimation of genome networks.

1 Introduction
Graphical models, as e.g. directed acyclic graphs (DAGs), allow an intuitive and mathematically sound approach to analyze complex causal mechanisms (Lauritzen 1996; Pearl 2009). Generally, they encode the causal links between variables of interests based on conditional independence (CI) statements between the variables (Spirtes, Glymour, and Scheines 2000). Hence, the accuracy of estimate of the CIs plays a key role in learning graphical models and consequently in causal inference from observational data.

CI testing is a challenging task, particularly in the presence of high-order independencies, where the number of variables far exceeds the number of observations (Wille and Bühlmann 2006). In such cases, estimations of CIs are usually inaccurate, potentially resulting in incorrect links between variables in the graphical model. On the other hand, CI tests with conditioning sets of low dimension can be performed accurately even for relatively small observed data sets. Thus, a natural task is to approximate the true causal

model using merely low-order CIs. Recent research in inferring genetic networks has confirmed the effectiveness of this approach when basing only on zero- and first-order independencies (Wille et al. 2004; Magwene and Kim 2004).

In this paper, we systematically study the problem to extract as much "causal knowledge" as possible from CI statements of order at most $k$, where $k \geq 0$ is a (typically small) integer. More precisely, we investigate the following task: For a set of variables $V$ and a given set $I$ of CI statements of the form $(a \perp b | Z)$, with $a, b \in V$, $Z \subseteq V$, and $|Z| \leq k$, find all DAGs $D$ which encode up to order $k$ exactly the CIs in $I$, i.e., such that for all $a, b, Z$, with $|Z| \leq k$, it is true that $a$ and $b$ are $d$-separated by $Z$ in $D$ if and only if $(a \perp b | Z)$ is in $I$. We will call such DAGs $k$-faithful to $I$ (for formal definitions, see Section 3). Figure 1 illustrates all DAGs which are 1-faithful to a single CI statement $(c \perp d | a)$ for the vertex set $V = \{a, b, c, d\}$.

We observe that this is a generalization of several problems already studied in the literature. For the simplest case $k = 0$, the CI statements are marginal independencies and the 0-faithful DAGs are called faithful to pairwise marginal independencies. The problem of deciding if a 0-faithful DAG exists for a given set of CIs of order zero, represented as an undirected graph, has been studied in (Pearl and Vermunt 1994; Textor, Idelberger, and Liškiewicz 2015).

Next, with $n$ denoting the cardinality of $V$, the problem for $k = n - 2$ was first investigated by Verma and Pearl (1992). They called such $k$-faithful DAGs just faithful ones and presented an algorithm which, for a given $I$, tests for the existence of a DAG faithful to $I$ and produces a representation of all such DAGs encoded in form of a completed partially directed acyclic graph (CPDAG) (we recall all used graphical notions in Section 2).
Note the important difference between the \( k \)-faithful and faithful DAGs. Even if \( \mathcal{I} \) consists of CI statements of order \( \leq k \), these two notions differ considerably, E.g., for the CI statements \( \mathcal{I} \) of order zero and one induced by the underlying DAG \( D \) shown in Fig. 2(a) the only 1-faithful DAG is \( D \) itself, while no faithful DAG to such \( \mathcal{I} \) exists. This is because for a 1-faithful DAG, the CIs of order \( > 1 \) are irrelevant, while a faithful DAG takes that \( (x \perp y | Z) \), for all \( x, y, \text{ and } Z \), with \( |Z| > 1 \).

We also notice that one cannot construct a \( k \)-faithful DAG just using a constraint-based structure learning algorithm, as the SGS or the PC algorithm (Spirtes, Glymour, and Scheines 2000; Kalisch and Bühlmann 2007), restricting the CI tests to independencies of order \( \leq k \). For example, for the underlying true DAG shown in Fig. 2(a) such an approach returns a structure with the skeleton given in Fig. 2(b). It is analyzed in detail in Section 4 why the superfluous edge \( a \rightarrow b \) is included in the result of classical causal structure learning algorithms and through which rule we are able to remove it.

**Previous Work.** Pearl and Wermuth (1994) investigated the problem whether a set of marginal independencies \( \mathcal{I} \) has a causal interpretation – meaning a DAG faithful to \( \mathcal{I} \). Moreover, they proposed an algorithm to construct a faithful DAG, but in their paper they did not give proofs for their theorems. Textor, Idelberger, and Liškiewicz (2015) further considered the stated problem, characterizing the DAG-representable sets by graph-theoretical properties of the marginal independence graphs (these are undirected graphs with an edge between \( a \) and \( b \) iff \( a \) and \( b \) are marginally dependent). Additionally, they proposed an algorithm which is based on the construction by Pearl and Wermuth (1994). However, they did not provide the missing proofs.

Other works have considered the more general setting which includes conditional independencies with a singleton conditioning set on top of marginal independencies. In this context, de Campos and Huete (2000) introduced the notion of a 0-1 graph. This is an undirected graph which contains an edge \( a \leftrightarrow b \) iff \((a \neq b) \land [\forall c : (a \neq b | c)]\). In other words, we obtain the graph by removing all edges between nodes for which we find an independence of order zero or one.

Wille and Bühlmann (2006) showed that – in the case of graphical Gaussian models – the 0-1 graphs are good estimators of sparse graphical models and relevant in biological applications. In particular, they have been used to model genome networks (De la Fuente et al. 2005; Magwene and Kim 2004; Wille et al. 2004). Later, Castelo and Roverato (2006) generalized the 0-1 graph and the covariance graphs (Cox and Wermuth 1993) to so called \( q \)-partial graphs.

**Our Results.** We provide a constructive solution to the problem of deciding if, for a given set \( \mathcal{I} \) of CIs of order less or equal to \( k \), there exists a DAG which is \( k \)-faithful to \( \mathcal{I} \). We propose an algorithm called LOCI (Low-Order Causal Inference) which – in case a \( k \)-faithful DAG exists – outputs all such DAGs encoded in form of a CPDAG. This extends and generalizes previously known results by Pearl and Wermuth (1994) as well as by Textor, Idelberger, and Liškiewicz (2015) who provided solutions only for sets of marginal independencies, i.e. for \( k = 0 \). Moreover, the analysis for the correctness of the construction given in this paper, fills the gaps in the proofs by Pearl and Wermuth, and by Textor, Idelberger, and Liškiewicz.

The proposed approach also improves some other methods known in the literature to learn DAGs from CIs up to a fixed order \( k \). In particular, it improves the algorithm by De Campos and Huete (2000) that presupposes knowledge of the topological sorting of nodes in the underlying DAG. In contrast, no such knowledge is assumed in our algorithm.

**Structure of the paper.** In the following section we introduce all preliminary definitions. Afterwards, in Section 3, we formally define what faithfulness to a set of CIs means. In Sections 4 and 5 we derive an algorithm for finding a compact and faithful representation of a set of low-order independencies. We experimentally compare this algorithm to previous approaches in Section 6. Finally, we discuss our results in Section 7. Auxiliary results and most proofs are moved to an appendix.

## 2 Preliminaries

We consider directed and partially directed graphs \( G = (V, E) \) with \(|V| = n\). In the latter case, a graph has both directed \( a \rightarrow b \) and undirected \( c \leftrightarrow d \) edges. Two nodes \( a \) and \( b \) are called adjacent if there is an edge between them (directed or undirected). The degree of a node \( a \) is the number of nodes adjacent to \( a \). For an edge \( a \rightarrow b \) we call \( a \) the parent of \( b \) and \( b \) the child of \( a \). A way is a sequence \( p_0, \ldots, p_t \) of nodes so that for all \( i \), with \( 0 \leq i < t \), there is an edge connecting \( p_i \) and \( p_{i+1} \). Such a sequence is called a path if \( p_t \neq p_0 \) holds for all \( i, j \), with \( 0 \leq i < j \leq t \). A path from \( p_0 \) to \( p_t \) is called causal if every edge on the path is directed from \( p_i \) towards \( p_{i+1} \). A node \( b \) is called an ancestor of \( a \) if there is a causal path from \( a \) to \( b \). \( \text{Anc}(a) \) is the set of all ancestors of \( a \) in graph \( G \). \( \text{Deg}(a) \) is the set of all descendants of \( a \) in \( G \). We use small letters for nodes and values, and capital letters for sets and random variables.

Of special importance are directed acyclic graphs (DAGs) containing only directed edges and no directed cycles, and partially directed acyclic graphs (PDAGs) that may contain both directed and undirected edges but no directed cycles. Every DAG is a PDAG. The skeleton of a PDAG \( G \) is the
undirected graph where every edge in \( G \) is substituted by an undirected edge.

Let \( P \) be a joint probability distribution over random variables \( X_i \), with \( i \in V \), and \( X, Y \) and \( Z \) stand for any subsets of variables. We use the notation \( (X \perp \!
olimits\!
oloslash\! Y \mid Z)_P \) to state that \( X \) is independent of \( Y \) given \( Z \) in \( P \). A distribution \( P \) and a DAG \( D = (V, E) \) are called compatible if \( D \) factors \( P \) as \( \prod_{i \in V} P(x_i | pa_i) \) over all realizations \( x_i \) of \( X_i \) and \( pa_i \) of variables corresponding to the parents of \( i \) in \( D \). It is possible to read CIs over \( X_i \), with \( i \in V \), off a compatible DAG through the notion of d-separation. Recall, a path \( \pi \) is said to be d-separated (or blocked) by a set of nodes \( Z \) iff (1.) \( \pi \) contains a chain \( u \rightarrow v \rightarrow w \) or \( u \leftarrow v \leftarrow w \) or a fork \( u \leftarrow v \rightarrow w \) such that the middle node \( v \) is in \( Z \), or (2.) \( \pi \) contains an inverted fork (or collider) \( u \rightarrow v \leftarrow w \) such that the middle node \( v \) is not in \( Z \) and such that no descendant of \( v \) is in \( Z \). A set \( Z \) is said to d-separate \( a \) from \( b \) iff \( Z \) blocks every path from \( a \) to \( b \). We write \( (a \perp b \mid Z)_D \) when \( a \) and \( b \) are d-separated by \( Z \) in \( D \). Whenever \( G \) and \( P \) are compatible, it holds for all \( a, b \in V \), and \( Z \subseteq V \), that \( (a \perp b \mid Z)_D \) then \( (X_a \perp X_b \mid \{X_i : i \in Z\})_P \).

An inverted fork \( u \rightarrow v \leftarrow w \) is called a v-structure if \( u \) and \( w \) are not adjacent. A pattern of a DAG \( D \) is the PDAG which has the same skeleton as \( D \) and which has an oriented edge \( a \rightarrow b \) iff there is a vertex \( c \), which is not adjacent to \( a \), such that \( c \rightarrow b \) is an edge in \( D \), too. Essentially, in the pattern of \( D \), the only directed edges are the ones which are part of a v-structure in \( D \).

A special case of PDAGs are the so called CPDAGs (Andersson, Madigan, and Perlman 1997) or completed partially directed graphs. They represent Markov equivalence classes. If two DAGs are Markov equivalent, it means that every probability distribution that is compatible with one of the DAGs is also compatible with the other (Pearl 2009). As shown by Verma and Pearl (1990) two DAGs are Markov equivalent iff they have the same skeleton and the same v-structures.

Given a DAG \( D = (V, E) \), the class of Markov equivalent graphs to \( D \), denoted as \( \{D\} \), is defined as \( \{D\} = \{D' \mid D' \text{ is Markov equivalent to } D\} \). The graph representing \( \{D\} \) is called a CPDAG and is denoted as \( D^* = (V, E^*) \), with the set of edges defined as follows: \( a \rightarrow b \) belongs to \( E^* \) if \( a \rightarrow b \) belongs to every \( D' \in \{D\} \) and \( a \rightarrow b \) is in \( E^* \) if there exist \( D', D'' \in [D] \) so that \( a \rightarrow b \) is an edge of \( D' \) and \( a \rightarrow b \) is an edge of \( D'' \). A partially directed graph \( G \) is called a CPDAG if \( G = D^* \) for some DAG \( D \).

Given a partially directed graph \( G \), a DAG \( D \) is an extension of \( G \) iff \( G \) and \( D \) have the same skeleton and if \( a \rightarrow b \) is in \( G \), then \( a \rightarrow b \) is in \( D \). An extension is called consistent if additionally \( G \) and \( D \) have the same v-structures. Due to Meek (1995, Theorem 3), we know that when starting with a pattern \( G \) of some DAG \( D \) and repeatedly executing the following three rules until none of them applies, we obtain a CPDAG \( D^* \) representing the Markov equivalent DAGs:

1. Orient \( b \leftarrow c \rightarrow a \) if there is \( a \rightarrow b \) such that \( a \) and \( c \) are nonadjacent.
2. Orient \( a \rightarrow c \rightarrow a \) if there is a chain \( a \rightarrow b \rightarrow c \).
3. Orient \( a \rightarrow b \rightarrow a \) if there are two chains \( a \rightarrow c \rightarrow b \) and \( a \rightarrow d \rightarrow b \) such that \( c \) and \( d \) are nonadjacent.

We will call these three rules the Meek rules.

We note that one obtains the CPDAG \( D^* \) by applying the rules not only when starting with the pattern of a DAG \( D \) but also, more generally, when the initial graph \( G \) is any PDAG whose consistent extensions form a Markov equivalence class \( \{D\} \). We will use this property in the correctness proof of the LOCI algorithm (Algorithm 1).

### 3 Models Faithful to CI Statements

In this section, we give a formal definition for a \( k \)-faithful DAG and – for the sake of completeness – we recall the definitions of a faithful and a \( k \)-partial graph. Next, we propose a definition for a compact representation of all \( k \)-faithful DAGs in terms of PDAGs and show that it yields a CPDAG.

Let \( V \) represent the set of variables and \( k \geq 0 \) be a fixed integer. Let \( \mathcal{I}_V \) be a set of CI statements over variables \( X_i \), with \( i \in V \), given as \( (a \perp b \mid Z) \), with \( a, b \in V \) and \( Z \subseteq V \). Analogously, let \( \mathcal{I}^k \) be a set of CI statements of order \( k \), i.e. such that \( |Z| \leq k \). For example, the set \( \mathcal{I}^k \) solely contains marginal independencies. For a more consistent notation we write \( (a \perp b \mid Z)_\mathcal{I}^k \) instead of \( (a \perp b \mid Z)_\mathcal{I}^k \) and respectively, \( (a \nmid b \mid Z)_\mathcal{I}^k \) for \( (a \perp b \mid Z) \notin \mathcal{I}^k \). We use an analogous notation for \( \mathcal{I}_V \). Additionally, in statements like e.g. \( (a \perp b \mid \{c, d\}) \), we omit the brackets and write \( (a \perp b \mid c, d) \).

**Definition 1** (Faithful Graph (Verma and Pearl 1990)). For a set \( \mathcal{I}_V \) of CIs, a DAG \( D = (V, E) \) is called faithful to \( \mathcal{I}_V \) if

\[
\forall (a, b, Z) \quad [(a \perp b \mid Z)_{\mathcal{I}_V} \iff (a \perp b \mid Z)_D].
\]

**Definition 2** \((k\text{-Partial Graph (Castelo and Roverato 2006)})\). For a set \( \mathcal{I}_V \) of CIs of order \( k \), an undirected graph \( D = (V, E) \) is called a \( k \)-partial graph with respect to \( \mathcal{I}_V \) if

\[
(\forall a, b, Z, |Z| \leq k) \quad [(a \nmid b \mid Z)_{\mathcal{I}_V} \iff (a \nmid b \mid Z)_D].
\]

We will call \( k \)-partial graphs with \( k = 1 \) also 0-1 graphs, as proposed by Wille and Bühlmann (2006) who considered such structures in the context of graphical Gaussian models.

**Definition 3** (\(k\text{-Faithful Graph})\). For a set \( \mathcal{I}_V \) of CIs of order \( k \), a DAG \( D = (V, E) \) is called \( k \)-faithful to \( \mathcal{I}_V \) if

\[
(\forall a, b, Z, |Z| \leq k) \quad [(a \nmid b \mid Z)_{\mathcal{I}_V} \iff (a \nmid b \mid Z)_D].
\]

Due to Verma and Pearl (1990), we know that, for a given set \( \mathcal{I}_V \), all DAGS faithful to \( \mathcal{I}_V \) can be represented as a CPDAG over \( V \). A representation of a \( k \)-partial graph follows straightforwardly from the definition. On the other hand, note that it is not obvious how to represent all DAGS which are \( k \)-faithful to \( \mathcal{I}_V \), like e.g. those shown in Fig. 1.

**Definition 4**. A set \( \mathcal{I}_V \) of CI statements will be termed DAG-representable if there is a DAG which is \( k \)-faithful to it. We call a DAG \( D \), which is \( k \)-faithful to \( \mathcal{I}_V \), edge maximal if there is no \( k \)-faithful DAG whose edge set is a superset of \( D \). Moreover, we denote by \( \mathcal{F}(\mathcal{I}_V) \) the set of all \( k \)-faithful DAGs to \( \mathcal{I}_V \).

For example, for \( \mathcal{I}_V = \{(a \nmid d \mid a)\} \) with \( V = \{a, b, c, d\} \), Fig. 1 shows all DAGS in \( \mathcal{F}(\mathcal{I}_V) \).
Figure 3: For the example from Fig. 1 we show the $k$-partial graph (part (a) on the left), the pattern of the edge maximal DAGs (part (b) in the middle) and the PDAG representing $\mathcal{F}(\mathcal{I}_V^k)$, with $\mathcal{I}_V^k = \{ (c \perp d \mid a) \}$ (part (c) on the right).

Below, we define a representation of a set $\mathcal{F}(\mathcal{I}_V^k)$ as a PDAG. Using our definition, the set of $k$-faithful DAGs from Fig. 1 is represented by the PDAG shown in part (c) of Fig. 3.

We say that a PDAG $G = (V, E)$ contains a set of DAGs $\{ D_i = (V, E_i) : i = 1, \ldots, t \}$ if for every DAG $D_i = (V, E_i)$ it is true that $E_i \subseteq E$. Here, we assume that an undirected edge $a \rightarrow b$ in $G$ is encoded by two directed edges $a \rightarrow b$ and $b \rightarrow a$. Obviously, a complete undirected graph over $V$ contains every set $\mathcal{F}(\mathcal{I}_V^k)$. From a causal structure learning perspective, our goal is to extract from $\mathcal{I}_V^k$ as much causal knowledge as possible. We formalize this goal as to find the minimal PDAG which contains every DAG $k$-faithful to $\mathcal{I}_V^k$. In this setting, minimality is considered in regard to the inclusion relation between the sets of edges.

**Definition 5.** A PDAG $G$ represents the set $\mathcal{F}(\mathcal{I}_V^k)$ if $G$ is a minimal graph that contains every graph in $\mathcal{F}(\mathcal{I}_V^k)$.

It is easy to see, that, according to this definition, the PDAG in part (c) of Fig. 3 represents the set of $k$-faithful DAGs from Fig. 1.

We note that a PDAG $G$ representing a set $\mathcal{F}(\mathcal{I}_V^k)$ fulfills the following conditions:
1. There is an edge $a \rightarrow b$ in $G$ iff DAGs $D, D' \in \mathcal{F}(\mathcal{I}_V^k)$ exist such that there is an edge $a \rightarrow b$ in $D$ and an edge $a \leftarrow b$ in $D'$.
2. There is an edge $a \rightarrow b$ in $G$ iff a DAG $D \in \mathcal{F}(\mathcal{I}_V^k)$ exists which contains the edge $a \rightarrow b$ and no DAG in $\mathcal{F}(\mathcal{I}_V^k)$ contains the edge $a \leftarrow b$.
3. There is no edge between $a$ and $b$ in $G$ iff no DAG in $\mathcal{F}(\mathcal{I}_V^k)$ contains an edge between $a$ and $b$.

From this perspective one can already view the representation $G$ as a generalization of the notion of a CPDAG that is used to represent Markov equivalent DAGs of the same skeleton. Note that DAGs in $\mathcal{F}(\mathcal{I}_V^k)$ can have different skeletons. Interestingly, we prove that the PDAG representing the set of $k$-faithful graphs is still a CPDAG.

**Proposition 1.** For a given set $\mathcal{I}_V^k$ of CIs, the representation $G$ of all $k$-faithful DAGs $\mathcal{F}(\mathcal{I}_V^k)$ is a CPDAG. Moreover, any consistent extension of $G$ is a DAG $k$-faithful to $\mathcal{I}_V^k$.

In particular, this means that the representation $G$ is itself a faithful model of all CIs up to order $k$.

### 4 Determining the Skeleton

For a given set $\mathcal{I}_V^k$ of conditional independence statements up to order $k$, our goal is to find the representation of the set of $k$-faithful DAGs $\mathcal{F}(\mathcal{I}_V^k)$. By definition, this is the minimal graph which contains every $k$-faithful DAG. Thus, our strategy is the following. Starting with the complete graph, we want to remove all edges which do not belong to any $k$-faithful DAG and, vice versa, keep all edges which are in at least one $k$-faithful DAG. This is in line with the paradigm of constraint-based causal structure learning.

In this section, we characterize all pairs of nodes which are nonadjacent in every $k$-faithful DAG. These pairs of nodes are exactly the ones which are nonadjacent in the representation as well. This means that, by finding them, we can construct the skeleton of the representation. We will explore how edges are oriented in the subsequent section.

One setting in which two nodes have to be nonadjacent is quite obvious. If we have a statement $(a \perp b \mid Z)$, it follows trivially that there cannot be an edge between $a$ and $b$ in any $k$-faithful DAG. However, as we will see, though this condition is necessary, it is not sufficient for the nonadjacency of vertices in $k$-faithful DAGs. As the main result of this section, we provide a property between two nodes (we call it incompatibility) and using this property we formulate a criterion for non-adjacency which is both necessary and sufficient (Proposition 2). The incompatibility between two nodes $a$ and $b$ expresses some higher order conditional independencies which can be derived from CI statements up to order $k$.

**Derivation of Higher-Order CI Statements**

When having access to all conditional independencies without a restriction on the order, removing edges corresponding to these known CIs is sufficient for learning the skeleton of the underlying causal structure. For example, the SGS and the PC algorithm (Spirtes, Glymour, and Scheines 2000) work exactly in this fashion. However, only removing these edges is not sufficient even for obtaining the skeleton of the representation (or the skeleton of a $k$-faithful DAG) when we consider order-bounded sets of independencies. We will now investigate why this is the case and show how this obstacle can be overcome.

The outlined problem is illustrated in Fig. 4, for the CI statements of order 0 or 1 induced by the underlying DAG
D shown in Fig. 2(a), i.e. for the set \(I_1^k = \{(u \perp c), (u \perp d), (u \perp b), (u \perp v), (a \perp v), (c \perp v), (d \perp v), (c \perp d), (u \perp c \mid v), \ldots \}\) of all zero- and first-order independencies found in this DAG. Choosing the value \(k = 1\) allows us a comparison with 0-1 graphs, but such an example can be constructed for all \(0 \leq k < n - 2\). In part (a) we show the corresponding 0-1 graph. This is constructed using the simple strategy of removing an edge if a zero- or first-order independence is a large obstacle for practical applicability. DAG and they did not classify these edges. Requiring the edges relied on the topological ordering in the underlying structure of their paper. However, their method for deleting such edges is flawed. In the second stage (lines 2 to 6), directed edges are removed according to the rule in Lemma 1. Recall that an undirected edge \(u \leftrightarrow v\) is represented as a pair \(u \rightarrow v\) and \(v \leftarrow u\). Thus, removing only the edge \(u \rightarrow v\) means the orientation of \(u \rightarrow v\) into \(u \leftarrow v\). Obviously, removing both
Algorithm 1: The LOCI algorithm computes the representation $G$ for a DAG-representable set of CIs up to order $k$. Note that we represent an undirected edge $a \sim b$ as a pair $a \rightarrow b$ and $a \leftarrow b$.

1. Form the graph $G$ on the vertex set $V$ which has an undirected edge $a \sim b$ if for every subset $Z$ of $V$, with $|Z| \leq k$, it is true $(a \nmid b \mid Z)_{\mathcal{I}_V^k}$.

2. For each $CI (a \nmid b \mid Z)_{\mathcal{I}_V^k}$ and every $c \in V \setminus \{a, b\}$ do
   - Remove $a \leftarrow c$ and $c \rightarrow b$ from $G$.

3. Repeat the Meek rules until no rule can be applied.
   - $a \rightarrow b \sim c \Rightarrow a \rightarrow b \rightarrow c$
   - $a \rightarrow b \sim c \Rightarrow a \rightarrow b \leftarrow c$
   - $a \leftarrow c \rightarrow b \sim d \Rightarrow a \leftarrow c \leftarrow d \rightarrow b$

4. Output: CPDAG $G$ representing $\mathcal{F}(\mathcal{I}_V^k)$ of CIs with order $\leq k$.

The algorithm also involves further steps, which are not directed edges. The aim of the second stage is (1) to remove the remaining undirected edges which do not satisfy the criterion in Proposition 2, i.e., the edges $u \sim v$ between incompatible nodes, and (2) to determine all $v$-structures. We note that in this stage, the algorithm also orients some further edges, which are not involved in $v$-structures.

To prove the correctness, we make use of the fact that we have such a causal explanation as, if this were the case, the graph obtained after completing stage two already characterizes a Markov equivalence class, as the skeleton and the $v$-structures are determined. In order to obtain the representation, we have to maximally extend it into a CPDAG. This is why we are able to apply the Meek rules.

Before stating the main results, we illustrate how the LOCI algorithm works using an example instance the zero- and first-order independencies $\mathcal{I}_V^k = \{(c \nmid d \mid a)\}$ over $V = \{a, b, c, d\}$, that have been discussed in Fig. 1 and 3. In (a), (b) and (c) of Fig. 3 the graph $G$ is shown after completing stage one, two, and three, respectively. Thus, in (a) there is no edge between $c$ and $d$ as we have the independence $(c \nmid d \mid a)_{\mathcal{I}_V^k}$, while all other edges are present. In (b) we see that the edges $c \rightarrow b$ and $d \rightarrow b$ are oriented. Essentially, there can be no edge $c \leftarrow b$ (or $d \leftarrow b$) as in that case $(c \nmid d \mid a)_{\mathcal{I}_V^k}$ cannot hold without a collider at node $b$. In this regard, stage two is similar to the orientation of $v$-structures in the SGS or PC algorithm (Spirtes, Glymour, and Scheines 2000). The difference is, however, as emphasized before, that in the LOCI algorithm further nodes can be separated during this stage.

Some ingredients of the proof of this theorem have already been stated in this and the previous section. The complete proof can be found in the appendix.

The result enables us to decide whether a given set $\mathcal{I}_V^k$ has a causal explanation. This is possible through the following approach: We can apply the LOCI algorithm to $\mathcal{I}_V^k$ and check whether the resulting graph is a $k$-faithful CPDAG. If it is, clearly there is a causal explanation of $\mathcal{I}_V^k$, namely the produced graph (Proposition 1). If it is not, then $\mathcal{I}_V^k$ cannot have such a causal explanation as, if this were the case, $G$ would be the representation (Theorem 1) and, therefore, as argued above, a faithful model. Thus, we conclude:

Proposition 3. There exists an algorithm which for a given set $\mathcal{I}_V^k$ of CIs tests if the set is DAG-representable.

6 Experimental Analysis

The representation $G$ of a set $\mathcal{I}_V^k$ is in itself a very useful graph as it faithfully models the CIs of order $\leq k$. But apart from this, it can also be used as an approximation of the true underlying causal structure. It can even be argued that it is the best approximation obtained through the given conditional independence information. Because of the minimality
also have access to the underlying true DAG dependencies in the 0-1 graph. From this DAG we can read off all zero- and first-order independencies (meaning the number of edges in the skeleton) in the 0-1 graph. For this, we compare the number of adjacencies in both graphs. This enables us, in particular, to estimate the influence of removing edges between incompatible nodes. Additionally, we investigate how many v-structures from the true DAG can already be found in the CPDAG $G$, giving us an indication how well the edge orientations are captured in the representation.

We begin the analysis by exploring how close $G$ is to the true causal structure. It can be seen that, in particular for larger graphs, we are only able to reasonably estimate the underlying structure up to expected degree 3. For example for $n = 100$ and $d = 4$, the representation $G$ contains almost three times as many adjacencies as $D$. For $n = 100$ and $d = 2$, the estimation is very close to the true DAG and even for $d = 3$ the ratio between the number of adjacencies in $G$ and $D$ is quite reasonable, being well below two. Notably, in the latter setting the improvement over the 0-1 graphs is significant. Actually, the difference in the number of adjacencies is larger between the 0-1 graph and $G$ than between $G$ and $D$. More generally, we see that for larger graphs the gap between the 0-1 graph and $G$ is substantial, meaning there is a great number of incompatible nodes. This underlines the importance of removing edges between such nodes in order to find a graphical model which is $k$-faithful to $I^*_V$. We can conclude that it is possible to estimate the true causal structure reasonably well, given that it is sparse. Moreover, it is crucial to remove the edges between incompatible nodes. But, apart from the adjacencies (or in other words the skeleton), the representation also contains directed edges and, thus, also v-structures. Therefore, it is interesting to investigate how many v-structures from the true DAG can already be found in $G$. These numbers are presented in Table 2. Here, we show the number of v-structures in $D$, in $G$ and those which are in both $D$ and $G$. For better readability, the numbers are normalized by the number of nodes $n$. We consider the same setting as above.

We investigate first how many v-structures are in both $G$ and $D$ compared to the number of v-structures in $D$. This

| $n$ | $d$ | Number of edges |
|-----|-----|-----------------|
| 20  | 2   | 27.21           |
| 20  | 3   | 57.88           |
| 20  | 4   | 96.57           |
| 20  | 5   | 126.73          |
| 60  | 2   | 77.85           |
| 60  | 3   | 226.03          |
| 60  | 4   | 512.89          |
| 60  | 5   | 820.69          |
| 100 | 2   | 125.87          |
| 100 | 3   | 413.68          |
| 100 | 4   | 1,061.39        |
| 100 | 5   | 1,905.20        |

| $n$ | $d$ | Number of v-s per node |
|-----|-----|------------------------|
| 20  | 2   | 1.427                  |
| 20  | 3   | 5.276                  |
| 20  | 4   | 10.784                 |
| 20  | 5   | 13.556                 |
| 60  | 2   | 1.445                  |
| 60  | 3   | 10.904                 |
| 60  | 4   | 42.979                 |
| 60  | 5   | 90.279                 |
| 100 | 2   | 1.383                  |
| 100 | 3   | 12.982                 |
| 100 | 4   | 59.859                 |
| 100 | 5   | 161.390                |

Table 1: We consider random DAGs with $n$ nodes and expected node degree $d$. This means each edge is present with probability $d/(n-1)$. We present the number of edges in the 0-1 graph, the skeleton of representation $G$ and the skeleton of the true DAG $D$. All values are the means of 100 independent trials.
shows how many of the v-structures of the true underlying DAG the LOCI algorithm is able to detect. We can see that almost all v-structures are found even for larger expected node degrees 4 or 5. E.g. for \( n = 100 \) and \( d = 5 \), the LOCI algorithm discovers 3.504 out of 3.872 v-structures per node.

While the LOCI algorithm finds most of the v-structures in \( D \), we can see that there are many more additional v-structures in the representation \( G \). While this is in reasonable limits for sparse graphs (for \( d = 2 \) we see roughly a doubling of the number of v-structures), the difference is much more extreme in denser graphs. In particular, for \( n = 100 \) and \( d = 5 \) there are 161.39 v-structures per node in \( G \) and only 3.872 in \( D \). This is due to the fact that, as we have seen in Table 1, there are many more edges in \( G \). At first glance, however, the increase in v-structures is much more extreme (a factor more than forty) than the increase in edges (a factor slightly less than five). But recall that these additional edges have an important property. As we know that \( G \) is a \( k \)-faithful CPDAG, both \( G \) and \( D \) contain the same zero- and first-order CIs. Therefore, all additional edges in \( G \) lead to no further dependencies of order zero or one. It is reasonable to assume that these additional edges are, thus, part of a disproportionate number of v-structures as they do not create new paths and thereby new dependencies.

7 Discussion

This paper has investigated the problems of determining how, for a given set of CI statements of order up to \( k \), all DAGs \( k \)-faithful to the set can be represented and how such a representation can be computed. We solve both problems showing that such faithful DAGs can be represented in a compact way as a CPDAG \( G \) and then proving that the representation \( G \) can be computed efficiently.

The experimental results show that, for small values of \( k \), this graphical representation is also useful as a good estimator of the underlying true causal structure in case of sparse models. It is considerably better than the \( k \)-partial graph because further edges are removed due to the concept of incompatible nodes which allows us to infer the existence of higher-order independencies. An additional advantage over \( k \)-partial graphs is that we also obtain edge orientations and can, through this, recover a large portion of the v-structures in the true DAG.

Our experiments are conducted in the oracle model where we assume all CI statements up to order \( k \) are known. This has the reason that, in this model, we are able to estimate best how many incompatible edges are removed. In future work, it would be interesting to analyze how the proposed algorithm performs if one would use statistical tests to find the independence statements. Another interesting topic for future research is to extend our algorithmic technique to compute the \( k \)-faithful representation, or a good approximation of it, by asking conditional independence queries in such a way that the number of queries is significantly smaller than the number of all CI statements of order up to \( k \). This would be interesting both in the oracle model and when using statistical tests to estimate independencies.

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Appendix

A Proof of Correctness of Algorithm 1

In this section we rigorously prove Theorem 1 which states that the graph resulting from Algorithm 1 is the representation of the set of k-faithful DAGs to $I_V \cup$. This theorem is the main result of the paper. During the proof we, moreover, obtain further results. A few of them were already stated in the main paper. In particular, as stated below in more detail, Proposition 1 follows immediately from Corollary 3 and Theorem 1, and Proposition 2 follows from Proposition 4.

In the proof, we will at first consider the PDAG obtained from Algorithm 1 at line 6 (after the for loop) before applying the Meek rules. Throughout this whole section we will refer to this PDAG as $G_{ep}$ while we will refer to the output graph of Algorithm 1 as $G$. Considering $G_{ep}$ instead of $G$ will simplify some proofs and we will show the correctness of the three Meek rules afterwards.

Before we begin, we prove the following lemma. It can be viewed as a stronger version of Lemma 1 in the main paper.

**Lemma 2.** Given a set of CIs $I_V \cup$. If we have $(u \perp b | Z)_{I_V \cup}$, $(u \perp b | Z)_{I_V ^k} = (u \perp b | Z)_{I_V \cup}$ and $a \not\in Z$, then no DAG k-faithful to $I_V \cup$ contains a causal path from $a$ to $b$.

**Proof.** Assume, for the sake of contradiction, that there is a k-faithful DAG $D$ which contains a causal path from $a$ to $b$ even though the stated conditions hold. It follows from $(u \perp b | Z)_{I_V \cup}$ and the k-faithfulness of $D$ that there is a path from $u$ to $a$ which is not blocked by $Z$. But as $u$ is supposed to be independent of $b$ given $Z$, some node on the causal path from $a$ to $b$ (we call this node $n$) has to be in $Z$ blocking this path. Moreover, we know that there is a path from $a$ to $b$ not blocked by $Z$ as $(u \perp b | Z)_{I_V \cup}$ has to hold. Thus, there has to be a collider at node $a$ (because of $a \not\in Z$) blocking this possible path from $u$ to $b$. But this collider would be unblocked by node $n$ as it is a successor of $a$ and in $Z$. It follows that $(u \perp b | Z)_{I_V \cup}$ does not hold. A contradiction.

The following statement follows directly (as Corollary 1 did):

**Corollary 2.** Assume $I_V \cup$ is a set of CIs. If the nodes $a$ and $b$ are incompatible, no DAG k-faithful to $I_V \cup$ contains a causal path between $a$ and $b$.

We begin the proof that $G$ is the representation with the statement that every DAG k-faithful to a set of independencies $I_V \cup$ is a subgraph of $G_{ep}$.

**Lemma 3.** $G_{ep}$ contains every DAG in $F(I_V \cup)$.

**Proof.** Every $k$-faithful DAG is contained in the graph formed in line 1 of Algorithm 1. Moreover, for every edge $a \rightarrow b$ removed in line 4 the following holds:

$\exists Z \subseteq V$ with $|Z| \leq k \\ \exists w \in V$

$[(u \perp b | Z)_{I_V \cup}, (u \perp a | Z)_{I_V \cup}, (a \perp b | Z)_{I_V \cup}, a \not\in Z]$

By Lemma 1 the edge $a \rightarrow b$ is not part of any $k$-faithful DAG.

Our goal is to show that the edge maximal DAGs have the same skeleton as $G_{ep}$. We have already shown with Lemma 3 that all pairs of nodes, which are adjacent in an edge maximal $k$-faithful DAG, are also adjacent in $G_{ep}$ because every $k$-faithful DAG is contained in $G_{ep}$. It remains to show that all pairs of nodes which are adjacent in $G_{ep}$ are also adjacent in an edge maximal DAG.

We begin with the following technical lemma which is necessary for the proof of Proposition 5 below.

**Lemma 4.** Given a DAG $D \in F(I_V \cup)$, two nodes $a, b \in V$ and a set $Z$ with $|Z| \leq k$ such that the following holds:

$(a \perp b | Z)_{I_V \cup}, (a \perp b | Z \cup \text{De}(b))_{I_V \cup}$ and $a \not\in \text{De}(b).$ Then there is a path d-connecting $a$ and $b$ in $D$ given $Z$ which ends with $\rightarrow b$.

**Proof.** Assume, for the sake of contradiction, that there is no path d-connecting $a$ and $b$ given $Z$ ending with $\rightarrow b$ in $D$. This means every path ends with the edge $\leftarrow b$. Moreover, we know that there cannot be a causal path from $b$ to $a$ because $a \not\in \text{De}(b)$. Then, it is clear that every path $p$ which d-connects $a$ and $b$ given $Z$ in $D$ contains at least one collider. We also note that on $p$ every node unblocking the collider closest to $b$ is a descendant of $b$. We will now consider the set $Z' = Z \setminus \text{De}(b)$ meaning we remove all nodes from $Z$ which are a descendant of $b$. We will show that there can be no path d-connecting $a$ and $b$ given $Z'$. This will contradict the assumption that $(a \perp b | Z')_{I_V \cup}$ holds for $Z' = Z \setminus \text{De}(b)$.

Every path d-connecting $a$ and $b$ given $Z'$ contains a node $x \in \text{De}(b)$. If this were not the case and there actually is such a path which contains no node in $\text{De}(b)$, then this path would d-connect $a$ and $b$ given $Z$ as well. Moreover, this path would have to end with the edge $\rightarrow b$ (else the node preceding $b$ on the path is a descendant of $b$). But we have assumed above, for the sake of contradiction, that there is no path d-connecting $a$ and $b$ given $Z$ in $D$ ending with $\rightarrow b$.

We will consider a path $p'$ d-connecting $a$ and $b$ given $Z'$ which contains a node $x \in \text{De}(b)$. This node cannot be a collider to $x \leftarrow x$ in $p'$, because $x$ is not in $Z'$ and neither is any descendant $y$ of $x$, as $y$ is by transitivity a descendant of $b$ as well. Thus, the collider $x \leftarrow x$ would be unblocked. It follows that in $p'$ there is an edge $\leftarrow x$ or an edge $x \rightarrow$. We investigate these two cases which are also displayed in Figure 5:

1. Consider the edge $\leftarrow x$ in $p'$. This case is shown in part (a) of Figure 5. We denote the subpath between $a$ and $x$ of $p'$ as $p'_a \rightarrow x$. This subpath cannot be causal from $x$ to $a$ as then there would be a causal path from $b$ to $a$ because $x$ is a descendant of $b$. But we required that $a \not\in \text{De}(b)$ holds.
We have seen that there cannot be a path $d$-connecting $b$ to $x$. In (a) there is an edge $\rightarrow$ and $\rightarrow$ between $a$ and $b$. A causal path from $a$ to $b$ (dotted line) is impossible because then there would be a causal path from $b$ to $a$. We show that the collider $c_1$ is unblocked. In (b) the edge $\rightarrow$ is part of the path between $a$ and $b$. A causal path from $x$ to $b$ (dotted line) is impossible because this would imply a cycle. We show that the collider $c_2$ is unblocked.

This means that there has to be a collider on $p'_{x-b}$. We will look at the collider $c_1$ closest to $x$. The collider $c_1$, however, cannot be unblocked by a node $d_1$ in $Z'$. This is because $d_1$ would be a descendant of $b$.

2. Consider the edge $\rightarrow$ in $p'$. This case is shown in part (b) of Figure 5. We denote the subpath between $x$ and $b$ of $p'$ as $p'_{x-b}$. This subpath cannot be causal from $x$ to $b$ as then there would be a cycle because $x$ is a descendant of $b$.

It follows that there is a collider on the subpath $p'_{x-b}$. We look at the collider $c_2$ closest to $x$. This collider cannot be unblocked by a node $d_2$ in $Z'$ because $d_2$ would be a descendant of $b$.

We have seen that there cannot be a path $d$-connecting $a$ and $b$ given $Z'$ in $D$. This is a contradiction to the requirement that $(a \perp b \mid Z')_{Z''}$ holds for $Z'' = Z \setminus \text{De}(b)$. Therefore, we conclude that indeed there is a path $d$-connecting $a$ and $b$ given $Z$ ending with $\rightarrow b$ in $D$.

The following lemma is of central importance for this section. We show that every edge in $G_{ep}$ can be added to a $k$-faithful DAG $D$ iff this does not produce a cycle. This is an important step towards showing that the edge maximal DAGs $k$-faithful to $\mathcal{I}_V^k$ have the same skeleton as $G_{ep}$.

**Lemma 5.** Given a DAG $D \in \mathcal{F}(\mathcal{I}_V^k)$ and $a, b \in V$ nonadjacent in $D$. The DAG $D' = D \cup \{a \rightarrow b\}$ is $k$-faithful to $\mathcal{I}_V^k$ iff $a \notin \text{De}_D(b)$ and $a \rightarrow b \in G_{ep}$ hold.

**Proof.** We show two directions. We begin by showing that if the DAG $D' = D \cup \{a \rightarrow b\}$ is $k$-faithful to $\mathcal{I}_V^k$, then $a \notin \text{De}_D(b)$ and $a \rightarrow b \in G_{ep}$ hold. Clearly, $a$ cannot be in $\text{De}_D(b)$ as then there would be a cycle in $D'$. Moreover, every $k$-faithful DAG is contained in $G_{ep}$ (Lemma 3) and because $D'$ is $k$-faithful it follows that $a \rightarrow b$ is in $G_{ep}$.

We will now show the more interesting direction that if $a \notin \text{De}_D(b)$ and $a \rightarrow b \in G_{ep}$ are satisfied, the DAG $D' = D \cup \{a \rightarrow b\}$ is $k$-faithful to $\mathcal{I}_V^k$. We prove this by showing that the following holds:

$$\forall Z \subseteq V \text{ with } |Z| \leq k \quad \forall u, v \in V \quad [(u \perp v \mid Z)_{D'} \iff (u \perp v \mid Z)_D]$$

We show two directions. We begin with the direction $(u \perp v \mid Z)_{D'} \implies (u \perp v \mid Z)_D$. Every conditional independence of order $\leq k$ in $D'$ is also in $D$ because $D$ is a subgraph of $D'$. The second direction $(u \not\perp v \mid Z)_{D'} \implies (u \not\perp v \mid Z)_D$ is more intricate. We will prove that every conditional dependence of order $\leq k$ in $D'$ is also in $D$ by considering a path $p'$ which $d$-connects $u$ and $v$ given a set $Z$ in $D'$. Then we show that there will also be a path $p$ in $D$ not blocked by $Z$.

There are two cases to consider displayed in Figure 6. The case (a) describes the situation when the edge $a \rightarrow b$ is on the path $p'$ $d$-connecting $u$ and $v$ given $Z$ in $D'$. The case (b) appears when a collider $c$ on the path $p'$ is unblocked by the descendant $x$ which is in $Z$ and the edge $a \rightarrow b$ is on the causal path from $c$ to $x$. The nodes $d$ and $d'$ as well as the red arrows and boxes visualize later parts of the proof and can be ignored for now. It is clear that any further occurrence of the edge $a \rightarrow b$ in $p'$ would be redundant. Moreover, it is obvious that if none of the two cases applies and the edge is neither present in $p'$ nor takes part in unblocking a collider, the same path $p'$ will also exist in $D$.

We prove that for the two cases in Figure 6 there is a path $p$ $d$-connecting $u$ and $v$ given $Z$ in $D$. We do this by showing that a way $w_{u-b}$ connecting $u$ and $b$ given $Z$ exists which does not contain the edge $a \rightarrow b$, but is still ending with $\rightarrow b$. We will first argue that if such a way $w_{u-b}$ exists, then there will be a path $p$ $d$-connecting $u$ and $v$ given $Z$ in $D$. Afterwards, we prove the existence of $w_{u-b}$.

In both cases illustrated in Figure 6 we can construct the desired path $p$. In case (a) we have a way $w$ which is the concatenation of the way $w_{u-b}$ and the path $p'_{x-b}$ which is the subpath between $b$ and $v$ of path $p'$. The concatenation of $w_{u-b}$ and $p'_{x-b}$ is valid because $w_{u-b}$ ends with $\rightarrow b$ just as $p'_{x-b}$ did and because of the fact that $p'$ is a valid path. If $b$ is no collider in $p'$, it will also not be a collider in $w$ and, vice versa, if it is an unblocked collider in $p'$, then it is also an unblocked collider in $w$. In case (b) the way $w$ is the concatenation of the way $w_{u-b}$ and $w_{u-b}$ (we see below that this way exists as well by symmetry) as the node $x$ unblocks the collider at node $b$. Finally, we know that the existence of a way which $d$-connects $u$ and $v$ given $Z$ implies the existence of a path with the same property. This means we are able to obtain the desired path $p$ in both cases and it follows that $(u \not\perp v \mid Z)_D$ holds.

Thus, it remains to find a way $w_{u-b}$ $d$-connecting $u$ and $b$ given $Z$ in $D$ which ends with $\rightarrow b$ under the assumption
that there is a path \( p'_{u-b} : u = v_1, v_2, \ldots, v_{l-1} = a, v_l = b \) of length \( l \) which d-connects \( u \) and \( b \) given \( Z \) in \( D' \) and ends with the edge \( a \rightarrow b \). Let \( d = v_l \) be the node with the minimal \( i \) such that \( b \in \text{De}_{D'}(v_l) \) holds. Then either \( d = u \) or we have \( v_{l-1} \leftarrow d \) on \( p'_{u-b} \). We will use this fact below to argue that there can be no collider at node \( d \).

Moreover, \( v_j \notin Z \) holds for \( i \leq j < l \), because the path from \( d = v_i \) to \( b \) is causal and we assumed that \( p'_{u-b} \) is a valid path d-connecting \( u \) and \( b \) given \( Z \). In particular, \( a \notin Z \) follows as \( i \leq i = 1 \) holds for \( d \). We will show that there is a path \( q_{d-b} \) d-connecting \( d \) and \( b \) in \( D \) which ends with \( b \). Concatenating the subpath \( p'_{u-d} \) with this path \( q_{d-b} \) will result in the required way \( w_{u-b} \) because there can be no collider at node \( d \) and \( d \notin Z \) holds.

The path \( q_{d-b} \) exists in \( D \) because of the following argument: The node \( d \) cannot be a descendant of \( b \) because then with \( a \) being a descendant of \( d \), it would follow that \( a \) is a descendant of \( b \) contradicting our assumption that \( a \notin \text{De}_D(b) \).

Moreover every node \( v_j \) with \( j \geq i \) is not in \( Z \) as seen above. Then the statement \((d \not\perp b | Z')_D \) holds for every subset \( Z' \) of \( Z \) because \((d \not\perp b | Z')_D \) would imply the following contradiction: We know that \((a \perp b | Z')_D \) (this holds for every \( Z' \) with \( |Z'| \leq k \) because the edge \( a \rightarrow b \) is in \( G \)) and also \((d \not\perp a | Z')_D \) hold (because of the fact that no node \( v_j \) with \( j \geq i \) is in \( Z \) meaning the same follows for \( Z' \) as it is a subset and because there is a causal path from \( d \) to \( a \) by definition of \( d \)). Note that because of the \( k \)-faithfulness of \( D \), the same statements hold according to \( \mathcal{I}_V^k \) as well. With \( a \notin Z \) (and therefore also \( a \notin Z' \)) the edge \( a \rightarrow b \) would have been removed from \( G_{ep} \) because these are exactly the conditions checked in line 3 of Algorithm 1. However, this would mean that we are not able to add the edge \( a \rightarrow b \) to \( D' \). A contradiction. This means that \((d \not\perp b | Z')_D \) holds for every subset \( Z' \) of \( Z \) and therefore in particular for \( Z' = Z \backslash \text{De}(b) \). With Lemma 4 it follows that there is a path \( q_{d-b} \) d-connecting \( d \) and \( b \) given \( Z \) ending with \( b \). 

In addition to Lemma 5, we need the following Lemma for the proof of Theorem 4 below.

**Lemma 6.** If \( a \leftarrow b \in G_{ep} \) and \( a \rightarrow b \notin G_{ep} \), it follows that \( b \notin \text{De}_D(a) \) holds for every DAG \( D \in \mathcal{F}(\mathcal{I}_V^k) \).

**Proof.** Having the edge \( a \leftarrow b \) in \( G_{ep} \) but not the edge \( a \rightarrow b \) implies that the following holds:

\[
\exists Z \subseteq V \text{ with } |Z| \leq k \quad \exists u \in V \\
[(u \perp b | Z)_{\mathcal{I}_V^k}, (u \not\perp a | Z)_{\mathcal{I}_V^k}, (a \not\perp b | Z)_{\mathcal{I}_V^k}, a \notin Z]
\]

This is because these are exactly the conditions required to remove the edge \( a \rightarrow b \) in line 4 of algorithm 1. From Lemma 2 we know that these conditions mean that no \( k \)-faithful DAG contains a causal path from \( a \) to \( b \). Thus, \( b \notin \text{De}_D(a) \) holds. 

We obtain one of the main results of this section that the edge maximal \( k \)-faithful DAGs have same skeleton as \( G_{ep} \).

**Proposition 4.** The edge maximal DAGs \( k \)-faithful to \( \mathcal{I}_V^k \) have the same skeleton as \( G_{ep} \).
Proof. We show two directions. If \( a \) and \( b \) are adjacent in an edge maximal \( k \)-faithful DAG \( D \), they are also adjacent in \( G_{ep} \). This follows from Lemma 3 because every \( k \)-faithful DAG is contained in \( G_{ep} \).

The second direction is more intricate. We show that if \( a \) and \( b \) are adjacent in \( G_{ep} \), they are also adjacent in any edge maximal \( k \)-faithful DAG \( D \). Assume, for the sake of contradiction, that \( a \) and \( b \) are not adjacent in an edge maximal \( k \)-faithful DAG \( D \). We consider three cases:

1. The edges \( a \to b \) and \( a \leftarrow b \) are in \( G_{ep} \). From Lemma 5 we know that the edge \( a \to b \) can be added to \( D \) if \( a \notin \text{De}_D(b) \). If on the other hand \( a \in \text{De}_D(b) \) holds, then the edge \( a \leftarrow b \) can be added, because in this case \( b \notin \text{De}_D(a) \) has to hold (else there would be a cycle in \( D \)). Thus, \( D \) is not edge maximal. A contradiction.
2. The edge \( a \leftarrow b \) is in \( G_{ep} \) and the edge \( a \to b \) is not. From Lemma 6 it follows that \( b \notin \text{De}_D(a) \) holds for every \( k \)-faithful DAG. Thus, as shown in Lemma 5 the edge \( a \leftarrow b \) can be added to \( D \). This means that \( D \) is not edge maximal. A contradiction.
3. The edge \( a \to b \) is in \( G_{ep} \) and the edge \( a \leftarrow b \) is not. This case is symmetrical to case 2 above.

\( \square \)

From this, we can immediately conclude Proposition 2 given in the main paper. This is due to the fact that the two points stated there are the exact reasons two nodes are non-adjacent in \( G_{ep} \) and by Proposition 4 in the edge maximal \( k \)-faithful DAGs. These all have the same skeleton which is precisely the skeleton of the representation.

Of all DAGs \( k \)-faithful to \( I_k \), the edge maximal DAGs possess another very unique property. We will prove that these DAGs form a Markov equivalence class. This result has far reaching consequences. In order to show this, we state that the edge maximal \( k \)-faithful DAGs not only have the same skeleton, but also the same set of v-structures as \( G_{ep} \).

**Proposition 5.** For all \( a, b, c \in V \) it is true: \( a \to c \leftarrow b \) is a v-structure in an edge maximal DAG \( D \in \mathcal{F}(I_k) \) iff \( a \to c \leftarrow b \) is a v-structure in \( G_{ep} \).

**Proof.** We begin by showing that if a v-structure \( a \to c \leftarrow b \) is in \( D \), it will also be in \( G_{ep} \). We note that, because \( a \) and \( c \) as well as \( c \) and \( b \) are adjacent in the \( k \)-faithful DAG \( D \), the following holds:

\[
\forall Z \text{ with } |Z| \leq k \quad (a \not\perp c \mid Z)_{I_k} \text{ and } (c \not\perp b \mid Z)_{I_k}
\]

The nodes \( a \) and \( b \) are not adjacent in \( D \) and as \( D \) is edge maximal, it follows from the fact that \( G_{ep} \) and \( D \) have the same skeleton (Proposition 4) that they will not be adjacent in \( G_{ep} \) either. We will now show that the edges \( a \leftarrow c \) and \( c \to b \) are not in \( G_{ep} \). Then we can conclude from the fact that every \( k \)-faithful DAG is contained in \( G_{ep} \) (Lemma 3) that the v-structure \( a \to c \leftarrow b \) is in \( G_{ep} \).

If the nodes \( a \) and \( b \) are not adjacent in \( G_{ep} \) there are two possible reasons for this:

\[
(u \not\perp a \mid Z)_D \quad (b \not\perp v \mid Z')_D
\]

\[
\begin{align*}
(a \not\perp b \mid Z)_{I_k} \quad (a \not\perp c \mid Z)_{I_k} \quad (c \not\perp b \mid Z)_{I_k}
\end{align*}
\]

Figure 7: Case 2 of the proof of Proposition 5. The v-structure \( a \to c \leftarrow b \) is in \( D \) and there exist \( Z \) and \( Z' \) such that \( (u \not\perp a \mid Z)_D \) and \( (b \not\perp v \mid Z')_D \) hold. We argue that \( (u \not\perp c \mid Z)_D, (v \not\perp c \mid Z')_D, c \notin Z \) and \( c \notin Z' \) hold as well.

1. The edge \( a \leftarrow b \) was not added to \( G_{ep} \) in line 1 because of an independence \( (a \not\perp b \mid Z)_{I_k} \). Moreover, because we have \( a \to c \leftarrow b \) in the \( k \)-faithful DAG \( D \), it follows that \( c \notin Z \) has to hold. This means that the edges are directed \( a \to c \leftarrow b \) in \( G_{ep} \) because the conditions in line 3 of Algorithm 1 are met

\[
(a \not\perp b \mid Z)_{I_k}, (a \not\perp c \mid Z)_{I_k}, (c \not\perp b \mid Z)_{I_k}, c \notin Z
\]

and therefore the edges \( a \leftarrow c \) and \( c \to b \) were removed from \( G_{ep} \).

2. The edges \( a \to b \) and \( a \leftarrow b \) were removed in line 4. This case is displayed in Figure 7.

This means we have nodes \( u \) and \( v \) and sets \( Z \) and \( Z' \) such that

\[
(u \not\perp b \mid Z)_{I_k} \quad (a \not\perp a \mid Z)_{I_k} \quad (a \not\perp b \mid Z)_{I_k} \quad a \notin Z
\]

and

\[
(v \not\perp a \mid Z')_{I_k} \quad (v \not\perp b \mid Z')_{I_k} \quad (b \not\perp a \mid Z')_{I_k} \quad b \notin Z'
\]

hold. Then \( (u \not\perp c \mid Z)_{I_k} \) and \( (v \not\perp c \mid Z')_{I_k} \) hold as well because of \( a \notin Z \) and \( b \notin Z' \) and the fact that with the edges \( a \to c \) and \( b \to c \) in the \( k \)-faithful DAG \( D \) there is neither a collider at node \( a \) nor at node \( b \). On the other hand there is a collider at node \( c \) (one the path from \( u \) to \( b \) as well as from \( v \) to \( a \)) and therefore \( c \notin Z \) and \( c \notin Z' \) hold. Then with \( (c \not\perp b \mid Z)_{I_k} \) (with the edge \( c \leftarrow b \) in \( D \) there cannot be any independence) and \( (u \not\perp b \mid Z)_{I_k} \) the edge \( c \to b \) is removed from \( G \) because the conditions in line 3 of Algorithm 1 are met. The edge \( a \leftarrow c \) is removed, too, as additional to \( (v \not\perp c \mid Z')_{I_k} \) and \( c \notin Z' \) the statements \( (v \not\perp c \mid Z')_{I_k} \) and \( (v \not\perp a \mid Z')_{I_k} \) hold. Therefore we have the v-structure \( a \to c \leftarrow b \) in \( G \) as well.

Now we show that a v-structure in \( G_{ep} \) will be present in \( D \) as well. It follows from Lemma 3 that if we have \( a \to c \leftarrow b \) in \( G_{ep} \), \( D \) can neither contain an edge between \( a \) and \( b \) nor the edges \( a \leftarrow c \) or \( c \to b \). Moreover because of the edge maximality of \( D \) and the fact that \( D \) and \( G_{ep} \) have the same skeleton (Proposition 4) that the edges \( a \to c \leftarrow b \) will be present in \( D \).

\( \square \)

We will now include the Meek rules in our argument in order to show the following important result which shows a way to obtain \( k \)-faithful DAGs from the graph \( G \) which is the final result of Algorithm 1.
Corollary 3. The set of edge maximal DAGs $k$-faithful to $\mathcal{I}_V^k$ is the Markov equivalence class formed by all consistent extensions of the CPDAG $G$.

Proof. Proposition 4 states that the edge maximal DAGs have the same skeleton and Proposition 5 states that they have the same set of $v$-structures as $G_{ep}$. Thus, these DAGs form a Markov equivalence class which is exactly the set of all consistent extensions of $G_{ep}$. It immediately follows that the graph $G$ which results from applying the Meek rules to $G_{ep}$ is a CPDAG. Moreover, by correctness of the Meek rules (these rules neither create a new $v$-structure nor a cycle (Meek 1995)) $G$ has the same set of consistent extensions as $G_{ep}$.

Finally, it becomes clear why we can apply the Meek rules to $G_{ep}$ in Algorithm 1. As shown by Meek (1995) these rules maximally extend a PDAG whose consistent extensions form a Markov equivalence class into a CPDAG and the edge maximal DAGs are the Markov equivalence class formed by the consistent extensions of $G_{ep}$. If an edge $a \to b$ gets directed by one of the Meek rules, this means that it is in every consistent extension (while the edge $a \leftarrow b$ is in no consistent extension). That the application of these three rules is correct for all $k$-faithful DAGs — not only the edge maximal ones — will be argued in the following proof of the main result of the paper, the correctness of Algorithm 1 (Theorem 1).

Proof of Theorem 1. A representation of the set $\mathcal{F}(\mathcal{I}_V^k)$ is a minimal graph that contains every graph in $\mathcal{F}(\mathcal{I}_V^k)$. We begin by proving that $G$ indeed contains every DAG $k$-faithful to $\mathcal{I}_V^k$. We do this by showing that every $k$-faithful DAG is a subgraph of a consistent extension of $G$. Consider the $k$-faithful DAG $D \in \mathcal{F}(\mathcal{I}_V^k)$. The DAG $D$ has to be a subgraph of some edge maximal $k$-faithful DAG. We know from Corollary 3 that every edge maximal DAG is a consistent extension of $G$. Thus, $D$ is a subgraph of a consistent extension of $G$.

We show now that $G$ is indeed minimal. This holds as deleting or directing an edge in $G$ would immediately violate the condition that $G$ contains every $k$-faithful DAG. This follows as we know that $G$ is a CPDAG representing a Markov equivalence class of $k$-faithful DAGs, namely the edge maximal ones.

From the above theorems we can deduce an interesting fact. Lemma 5 holds for $G_{ep}$ and not only for $G$ and the only constraint we impose on adding edges is that they do not produce a cycle. Thus, if we have an edge $a \to b$ in $G_{ep}$, an edge $a \to b$ in $G$ (meaning the edge $a \to b$ has been directed by one of the Meek rules) and a DAG $D \in \mathcal{F}(\mathcal{I}_V^k)$, it follows that either $a \to b$ is in $D$ or there is a causal path from $a$ to $b$.

Finally, we are able to derive Proposition 1. This follows immediately from Corollary 3 and Theorem 1. It shows that the notion of a representation is a generalization of the notion of a CPDAG. More precisely, for every $k$ there is a subclass of CPDAGs (let us call these $k$-CPDAGs) which are the representation of a set of DAGs $k$-faithful to a set $\mathcal{I}_V^k$ for a fixed $|V| = n$. In particular, the set of $l$-CPDAGs is a subset of the set of $l + 1$-CPDAGs and the set of $n - 2$-CPDAGs is the set of all CPDAGs. Further investigations of these structures might be interesting, for example, for the open question of counting the number of Markov equivalence classes (which is equal to the number of CPDAGs) for a given number $n$ of nodes (Radhakrishnan, Solus, and Uhler 2017). Notably, Textor et al. (2015) analyzed the number of $0$-CPDAGs (they use a different representation termed SMIG).

B Additional proofs for the case of $k = 0$

All results in the previous section hold for the setting of marginal independencies as well. But for this special case, there already existed an algorithm (Textor, Idelberger, and Liškiewicz 2015; Pearl and Wermuth 1994) whose formal proof of correctness was, to our knowledge, never published. We recall this algorithm as Algorithm 2.

input : Vertex set $V$, a DAG-representable set $\mathcal{I}_V^0$ of marginal independence statements
output: CPDAG $H$ which contains every faithful DAG and whose extensions are faithful

1. Form the graph $H$ on the vertex set $V$ and empty edge set and the graph $U$ which has an edge $a \leftarrow b$ if $(a \perp b)_{\mathcal{I}_V^0}$.
2. foreach edge $u \leftarrow v$ in $U$ do
3. Add the edge $u \rightarrow v$ to $H$ if $\text{Bd}_U(u) \subset \text{Bd}_U(v)$.
4. Add the edge $u \leftarrow v$ to $H$ if $\text{Bd}_U(u) \supset \text{Bd}_U(v)$.
5. Add the edge $u \leftarrow v$ to $H$ if $\text{Bd}_U(u) = \text{Bd}_U(v)$.
6. end
7. Return $H$

Algorithm 2: Algorithm from Textor et al. to find faithful DAGs for sets of marginal independencies (Textor, Idelberger, and Liškiewicz 2015).

We note that the boundary $\text{Bd}(i)$ is defined as the neighborhood of node $i$ including $i$: $\text{Bd}(i) = N(i) \cup \{i\}$ with the neighborhood $N(i)$ being the set of all nodes adjacent to $i$.

By showing that Algorithm 2 produces the same result as Algorithm 1 with parameter $k = 0$, we formally prove the correctness of the former algorithm (and prove all additional properties, e.g. that the result is a CPDAG) and thereby give the proof which has been missing from the literature. Note that this section does not produce new results, but gives only the missing correctness proof. We include it for the sake of completeness.

Theorem 2. For every set $\mathcal{I}_V^0$ of marginal independencies Algorithm 1 produces the same PDAG as Algorithm 2.

Proof. In this proof we denote the PDAG produced by Algorithm 2 as $H$ and the one produced by Algorithm 1 as $G$. We have to show that $G = H$. But before, we show that $G_{ep} = H$ holds.

We will begin our proof by analyzing under which conditions a directed edge $u \leftarrow v$ is removed from $G_{ep}$ in the for-loop from line 2 to 6. We describe this through properties of the graph which was formed in line 1. We call this
4. There is no edge between $u$ and $v$ is removed if we have a node $w$ which is a neighbor of $v$, but not a neighbor of $u$ in $\mathcal{U}$. Because then we have $u \rightarrow v \leftarrow w$ with $u$ and $w$ nonadjacent and in particular the edge $u \leftarrow v$ is removed.

Formally, the edge $u \leftarrow v$ (in case we have $(u \perp v)_{\mathcal{T}_V^0}$) is removed from $G_{ep}$ if the following condition holds:

$$(\exists w)(w \not\in Bd_{\mathcal{U}}(u) \land w \in Bd_{\mathcal{U}}(v))$$

(1)

We will also consider under which condition an edge $u \rightarrow v$ is not removed from $G_{ep}$. This happens if condition 1 does not hold and by negation we get:

$$(\forall w)(w \not\in Bd_{\mathcal{U}}(u) \land w \in Bd_{\mathcal{U}}(v))$$

(2)

$$\iff (\forall w)(w \in Bd_{\mathcal{U}}(v) \implies x \in Bd_{\mathcal{U}}(u))$$

(3)

Now we can show that $H$ and $G_{ep}$ are identical. We note that both graphs have the same vertex set. Thus, it is left to prove that all edges are identical. To do this we consider all possible edge states (undirected, directed or missing) between two node $u$ and $v$ in the following case study.

1. There is no edge between $u$ and $v$ in $G_{ep}$ and $(u \perp v)_{\mathcal{T}_V^0}$ holds. Then, in the first line of both algorithms the edge was not added to $\mathcal{U}$ and thus is neither part of $H$ nor $G_{ep}$.

2. The directed edge $u \rightarrow v$ is in $G_{ep}$. From above considerations it follows that:

$$(\exists w)(w \not\in Bd_{\mathcal{U}}(u) \land w \in Bd_{\mathcal{U}}(v))$$

and

$$(\forall w)(w \in Bd_{\mathcal{U}}(u) \implies w \in Bd_{\mathcal{U}}(v))$$

hold. This is because we require that the edge $u \leftarrow v$ was removed from $G_{ep}$ while $u \rightarrow v$ was not. Only then we have the directed edge $u \rightarrow v$ in $G_{ep}$. Moreover, it is clear that the edge between $u$ and $v$ is present in $\mathcal{U}$ in both algorithms. We can see that the two conditions above are equivalent to $Bd_{\mathcal{U}}(u) \subseteq Bd_{\mathcal{U}}(v)$ which is exactly the condition in line 3 in Algorithm 2 for adding an edge $u \rightarrow v$ to $H$.

3. The directed edge $u \leftarrow v$ is in $G_{ep}$. This case can be dealt with in the same way as $u \rightarrow v$ in case 2.

4. There is no edge between $u$ and $v$ in $G_{ep}$ and $(u \perp v)_{\mathcal{T}_V^0}$. In Algorithm 1 this case occurs if the edges $u \rightarrow v$ and $u \leftarrow v$ are removed from $G_{ep}$ in different iterations in line 4. Thus, the following two conditions hold:

$$(\exists w)(w \not\in Bd_{\mathcal{U}}(u) \land w \in Bd_{\mathcal{U}}(v))$$

and

$$(\exists x)(x \in Bd_{\mathcal{U}}(u) \land x \not\in Bd_{\mathcal{U}}(v)).$$

This means that none of the three cases from line 3 to 5 in Algorithm 2 apply as $Bd_{\mathcal{U}}(u)$ and $Bd_{\mathcal{U}}(v)$ are not equal nor is one a subset of the other. This means that no edge is added to $H$. We note here that the opposite direction holds as well, meaning that if none of the three cases apply it follows that the two statements above concerning the existence of $w$ and $x$ are valid. Moreover, the nodes $u$ and $v$ are incompatible as $(w \perp u)_{\mathcal{T}_V^0}, (w \perp v)_{\mathcal{T}_V^0}, (v \perp u)_{\mathcal{T}_V^0}, (x \perp v)_{\mathcal{T}_V^0}$ and $(x \perp u)_{\mathcal{T}_V^0}$ hold.

5. There is an edge $u \rightarrow v$ in $G_{ep}$. This can only occur in Algorithm 1 if neither $u \rightarrow v$ nor $u \leftarrow v$ get removed. But this means as reasoned above that

$$(\forall x)(x \in Bd_{\mathcal{U}}(u) \implies x \in Bd_{\mathcal{U}}(v))$$

and

$$(\forall x)(x \in Bd_{\mathcal{U}}(v) \implies x \in Bd_{\mathcal{U}}(u))$$

hold. It immediately follows that $Bd_{\mathcal{U}}(u) = Bd_{\mathcal{U}}(v)$ and therefore the edge $u \rightarrow v$ is added to $H$ in line 5 of Algorithm 2.

We can conclude that $G_{ep} = H$ holds. We will show now that the Meek rules which are applied to $G_{ep}$ will not direct further edges.

1. The first Meek rule states that an edge $b \rightarrow c$ is oriented as $b \rightarrow c$ if we have $a \rightarrow b \rightarrow c$ with $a$ and $c$ nonadjacent. An analysis similar to the one made in the proof of Proposition 5 yields that whenever two nodes $a$ and $c$ are nonadjacent in $G_{ep}$, every possible chain $a \rightarrow x \rightarrow c$ is directed as either $a \rightarrow x \leftarrow c$ or $a \leftarrow x \rightarrow c$. Therefore the structure $a \rightarrow b \rightarrow c$ can never appear. Note that this holds only for sets of marginal independencies $\mathcal{T}_V^0$.

2. The second Meek rule states that an edge $a \rightarrow c$ is oriented as $a \rightarrow c$ if we have $a \rightarrow b \rightarrow c$. In $H$ (and thereby also in $G_{ep}$ as these graphs are identical) we have an edge $a \rightarrow b$ iff $Bd_{\mathcal{U}}(a) \subset Bd_{\mathcal{U}}(b)$ and $b \rightarrow c$ iff $Bd_{\mathcal{U}}(b) \subset Bd_{\mathcal{U}}(c)$. It follows that $Bd_{\mathcal{U}}(a) \subset Bd_{\mathcal{U}}(c)$ holds as well meaning the edge between $a$ and $c$ is already oriented $a \rightarrow c$.

3. The third Meek rule states that an edge $a \leftarrow b$ is oriented into $a \rightarrow b$ whenever there are two chains $a \rightarrow c \leftarrow b$ and $a \leftrightharpoons b$ such that $c$ and $d$ are nonadjacent. We know from the analysis of the first Meek rule that a structure $c \rightarrow a \leftarrow d$ with $c$ and $d$ nonadjacent will never occur in $G_{ep}$. Thus, the third Meek rule will never be applied as well.

It follows that $G = G_{ep} = H$. □