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On the completeness of orientation rules for causal discovery in the presence of latent confounders and selection bias

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ABSTRACT

Causal discovery becomes especially challenging when the possibility of latent confounding and/or selection bias is not assumed away. For this task, ancestral graph models are particularly useful in that they can represent the presence of latent confounding and selection effect, without explicitly invoking unobserved variables. Based on the machinery of ancestral graphs, there is a provably sound causal discovery algorithm, known as the FCI algorithm, that allows the possibility of latent confounders and selection bias. However, the orientation rules used in the algorithm are not complete. In this paper, we provide additional orientation rules, augmented by which the FCI algorithm is shown to be complete, in the sense that it can, under standard assumptions, discover all aspects of the causal structure that are uniquely determined by facts of probabilistic dependence and independence. The result is useful for developing any causal discovery and reasoning system based on ancestral graph models.

1. Introduction

Directed acyclic graphs (DAGs) are now widely used both as statistical models and as causal models. This double interpretation of DAGs, better known as (causal) Bayesian networks in the AI literature, is the springboard for much of the research on automated causal discovery and reasoning [12,20,25]. Given a set of variables $\mathbf{V}$, if the causal structure of $\mathbf{V}$ can be properly represented by a DAG, one can try to learn the causal structure from data by exploiting the statistical implications DAGs have as statistical models. In general the causal structure is underdetermined, as multiple DAGs may be equally compatible with the correlational pattern suggested by data. But these DAGs usually share common features, which constitute the aspects of the causal structure that are not underdetermined and are in principle learnable from observational data. To develop algorithms for inferring these learnable causal features from correlational patterns is an important goal in the project of automated causal discovery.

Assuming no confounding or selection effect due to unobserved variables, there are causal discovery algorithms that are provably sound and complete, under some plausible assumptions relating causal structure to probability distribution [7,17,25,32]. However, the assumption of no latent confounding or selection effect is seldom appropriate, and it is desirable and even necessary in many situations to relax it. Unfortunately, the problem becomes much more difficult when we drop the assumption, due to the fact that the causal structure may not be properly representable by a DAG unless latent variables are explicitly invoked. Not only are DAG models with latent variables hard to handle statistically [5,11], they make an infinite search space unless we seriously constrain the number of latent variables or the topology of the unknown causal network.

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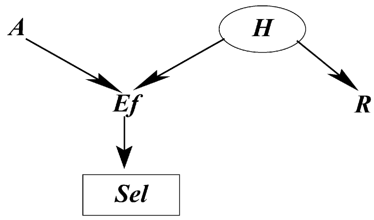

Fig. 1. A causal mechanism with latent and selection variables.

One way around this is to represent such models without explicitly introducing latent variables, especially if we are not interested in the latent variables *per se*. A class of graphical models developed for this purpose is known as ancestral graph models [23]. As we will describe in more detail, a major virtue of ancestral graphs is that for any DAG with latent confounding and selection variables, there is a unique maximal ancestral graph (MAG) over the observed variables alone that represents the conditional independence relations and causal relations entailed by the original DAG. Instead of directly targeting the causal DAG, which for all we know might involve any number of latent variables, a more tractable goal for causal discovery is to learn as many features of the causal MAG as possible.

There is a provably sound procedure for this purpose, known as the FCI algorithm [26].[1] Whether it is complete—that is, whether it can in principle discover all causal information that is not underdetermined—has been an open problem [18,25].[2] In fact, as we will explain later, the algorithm is not complete as it stands. In this paper, we provide additional orientation rules (i.e., rules for inferring edge marks), and show that the augmented FCI algorithm is complete. The result amounts to a constructive characterization of common features shared by an equivalence class of MAGs, which should be useful in any system of causal discovery and reasoning based on ancestral graph models. In this regard, our result generalizes Meek's characterization of commonalities shared by Markov equivalent DAGs [17], and builds directly on some earlier results established in [2].

Causal discovery aside, this paper should be of interest to anyone interested in ancestral graph models, which have drawn attention from both statisticians and computer scientists [1,2,9,10,23,30,37]. We also suspect that the results of this paper (and especially some lemmas in Appendix A) will be useful in providing a characterization of equivalence classes of MAGs in the style of Andersson et al.'s characterization of equivalence classes of DAGs [4].

The rest of the paper is organized as follows. Section 2 introduces the relevant background on ancestral graphs. In Section 3, we describe the FCI algorithm and report an important step made in [2] towards the completeness result. We then present additional orientation rules in Section 4, with which we show that the augmented FCI algorithm is complete. We conclude in Section 5. Most proofs are postponed to the appendices.

2. Ancestral graphs and their interpretations

The following example attributed to Chris Meek in [22] illustrates nicely the primary motivation behind ancestral graphs:

> The graph [Fig. 1] represents a randomized trial of an ineffective drug with unpleasant side-effects. Patients are randomly assigned to the treatment or control group (A). Those in the treatment group suffer unpleasant side-effects (Ef), the severity of which is influenced by the patient's general level of health (H), with sicker patients suffering worse side-effects. Those patients who suffer sufficiently severe side-effects are likely to drop out of the study. The selection variable (Sel) records whether or not a patient remains in the study, thus for all those remaining in the study $Sel = StayIn$. Since unhealthy patients who are taking the drug are more likely to drop out, those patients in the treatment group who remain in the study tend to be healthier than those in the control group. Finally health status (H) influences how rapidly the patient recovers (R) [22, p. 234].

This simple case shows how the presence of latent confounders and selection variables matters. The variables of primary interest, A and R, are observed to be correlated, even though the supposed causal mechanism entails independence between them. This correlation is not due to sample variation, but rather corresponds to genuine probabilistic association induced by design—only the subjects that eventually stay in the study are considered. The observed correlation is in effect a correlation *conditional* on the selection variable Sel, a canonical example of *selection effect*. On the other hand, H is a familiar latent confounder that contributes to "spurious correlation".

[1] FCI stands for *fast causal inference*, which is probably an overly optimistic name.

[2] These authors raised the problem with regard to an older version of the algorithm designed based on a representation called *inducing path graphs*. There is a very close relationship between inducing path graphs and MAGs, which is explained in detail in the appendix of [34]. It suffices to note here that the completeness problem addressed in this paper is an even harder problem than the completeness problem formulated in terms of inducing path graphs. Also, the FCI algorithm is sometimes claimed to be complete [28], but only in a much weaker sense than what we consider in this paper.

A main attraction of ancestral graphs is that, without explicitly including latent variables, they can represent conditional independence relations and causal relations among observed variables when the underlying data generating process involves latent confounders and/or selection variables. This of course requires a richer syntax than that of DAGs.

2.1. Ancestral graphs

A **mixed graph** is a vertex-edge graph that can contain three kinds of edges: directed ($\rightarrow$), bi-directed ($\leftrightarrow$) and undirected ($-$), and at most one edge between any two vertices. The two ends of an edge we call **marks** or **orientations**. The two marks of a bi-directed edge are both **arrowheads** ($>$), the two marks of an undirected edge are both **tails** ($-$), and a directed edge has one of each. We say an edge is **into** (or **out of**) a vertex if the edge mark at the vertex is an arrowhead (or a tail).

Two vertices are said to be **adjacent** in a mixed graph if there is an edge (of any kind) between them. Given a mixed graph $\mathcal{G}$ and two adjacent vertices A, B therein, A is a **parent** of B and B is a **child** of A if $A \rightarrow B$ is in $\mathcal{G}$; A is called a **spouse** of B (and B a spouse of A) if $A \leftrightarrow B$ is in $\mathcal{G}$; A is called a **neighbor** of B (and B a neighbor of A) if $A-B$ is in $\mathcal{G}$. A **path** in $\mathcal{G}$ is a sequence of distinct vertices $\langle V_0, \ldots, V_n \rangle$ such that for $0 \leqslant i \leqslant n-1$, V_i and V_{i+1} are adjacent in $\mathcal{G}$. A **directed path from** V_0 **to** V_n in $\mathcal{G}$ is a sequence of distinct vertices $\langle V_0, \ldots, V_n \rangle$ such that for $0 \leqslant i \leqslant n-1$, V_i is a parent of V_{i+1} in $\mathcal{G}$. A is called an **ancestor** of B and B a **descendant** of A if $A = B$ or there is a directed path from A to B. Let $\mathbf{An}_{\mathcal{G}}(B)$ denote the set of ancestors of B in $\mathcal{G}$. A **directed cycle** occurs in $\mathcal{G}$ when $B \rightarrow A$ is in $\mathcal{G}$ and $A \in \mathbf{An}_{\mathcal{G}}(B)$. An **almost directed cycle** occurs when $B \leftrightarrow A$ is in $\mathcal{G}$ and $A \in \mathbf{An}_{\mathcal{G}}(B)$.

Definition 1. A mixed graph is **ancestral** if the following three conditions hold:

(a1) there is no directed cycle;
(a2) there is no almost directed cycle;
(a3) for any undirected edge V_1-V_2, V_1 and V_2 have no parents or spouses.

Obviously DAGs are special cases of ancestral graphs. The first condition in Definition 1 is just the familiar one for DAGs. Together with the second condition, they define a nice connotation of arrowheads in ancestral graphs: an arrowhead implies non-ancestorship. The third condition requires that there be no edge into any vertex in the *undirected* component of an ancestral graph. This property simplifies parameterization and fitting of ancestral graphs [9,23], but still allows selection effect to be properly represented.

2.2. Probabilistic interpretation of ancestral graphs

As a statistical model, the vertices of an ancestral graph represent random variables, and the graph is interpreted as encoding a set of conditional independence[3] relations by a graphical criterion, called *m-separation*, which generalizes the well known d-separation criterion for DAGs [19]. Given a path p in a mixed graph, a non-endpoint vertex V on p is called a **collider** if the two edges incident to V on p are both into V; otherwise V is called a **non-collider** on p. In Fig. 2(a), for example, B is a collider on the path $\langle A, B, D \rangle$, but is a non-collider on the path $\langle C, B, D \rangle$.

Definition 2 *(m-separation).* In a mixed graph, a path p between vertices X and Y is **active** (**m-connecting**) relative to a (possibly empty) set of vertices $\mathbf{Z}$ ($X, Y \notin \mathbf{Z}$) if

(i) every non-collider on p is not a member of $\mathbf{Z}$;
(ii) every collider on p has a descendant in $\mathbf{Z}$.

$\mathbf{X}$ and $\mathbf{Y}$ are said to be **m-separated** by $\mathbf{Z}$ if there is no active path between any vertex in $\mathbf{X}$ and any vertex in $\mathbf{Y}$ relative to $\mathbf{Z}$.

The probabilistic interpretation of ancestral graphs is given by its (global) *Markov property*: if $\mathbf{X}$ and $\mathbf{Y}$ are m-separated by $\mathbf{Z}$, then $\mathbf{X}$ and $\mathbf{Y}$ are probabilistically independent conditional on $\mathbf{Z}$. This interpretation is obviously consistent with that of DAGs, for m-separation reduces to d-separation in the case of DAGs.

The following property is true of DAGs: if two vertices are not adjacent, then there is a subset of other vertices that m-separates (d-separates) the two. This, however, is not always true of ancestral graphs. For example, the graph (a) in Fig. 2 is an ancestral graph that fails this condition: C and D are not adjacent, but no subset of $\{A, B\}$ m-separates them.

This motivates the following definition:

[3] We refer to the standard notion of conditional independence in probability theory.

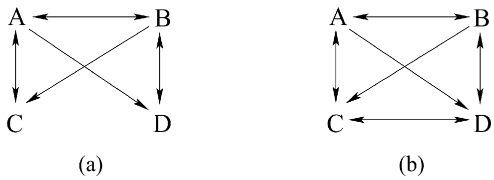

Fig. 2. (a) An ancestral graph that is not maximal; (b) a maximal ancestral graph.

Definition 3 *(maximality).* An ancestral graph is said to be **maximal** if for any two non-adjacent vertices, there is a set of vertices that m-separates them.

DAGs are all maximal. In fact, maximality corresponds to the so-called *pairwise Markov property*: every missing edge corresponds to a conditional independence relation, which is the basis for inferring the adjacency skeleton of the unknown causal graph in many causal discovery procedures, including the FCI algorithm we will discuss later.

Maximality is closely related to the notion of inducing path. The definition of the latter is quite convoluted, but the basic motivation is the following question. Partition the set of vertices into $\mathbf{V} = \mathbf{O} \cup \mathbf{L} \cup \mathbf{S}$, and consider m-separation relations of the form: X and Y are m-separated by $\mathbf{Z} \cup \mathbf{S}$, for $X, Y \in \mathbf{O}$ and $\mathbf{Z} \subseteq \mathbf{O}\backslash\{X, Y\}$.[4] When is it true that X and Y are *not* m-separated by $\mathbf{Z} \cup \mathbf{S}$ for any $\mathbf{Z} \subseteq \mathbf{O}\backslash\{X, Y\}$? The answer is given by the notion of inducing path.

Definition 4 *(inducing path).* In an ancestral graph, let X, Y be any two vertices, and $\mathbf{L}$, $\mathbf{S}$ be two disjoint sets of vertices not containing X, Y. A path p between X and Y is called an **inducing path relative to** $\langle \mathbf{L}, \mathbf{S} \rangle$ if every non-endpoint vertex on p is either in $\mathbf{L}$ or a collider, and every collider on p is an ancestor of either X, Y, or a member of $\mathbf{S}$.

When $\mathbf{L} = \mathbf{S} = \emptyset$, p is called a **primitive inducing path** between X and Y.

An important fact established by Richardson and Spirtes [23, Theorem 4.2] is that X and Y are not m-separated by $\mathbf{Z} \cup \mathbf{S}$ for any $\mathbf{Z} \subseteq \mathbf{V}\backslash(\mathbf{L} \cup \mathbf{S} \cup \{X, Y\})$ if and only if there is an inducing path between X and Y relative to $\langle \mathbf{L}, \mathbf{S} \rangle$. For example, in Fig. 1 the path $\langle A, Ef, H, R \rangle$ is an inducing path relative to $\langle \{H\}, \{Sel\} \rangle$, and A is not m-separated from R by either $\{Ef, Sel\}$ or $\{Sel\}$. This fact plays an important role below in constructing a MAG that represents a given DAG.

As a special case of this fact, the presence of a primitive inducing path is sufficient and necessary for two vertices not to be m-separated by any set of other variables in an ancestral graph, which is obviously connected to maximality.

Proposition 1. *An ancestral graph is maximal if and only if there is no primitive inducing path between any two non-adjacent vertices in the graph.*

For example, in Fig. 2(a), the path $\langle C, A, B, D \rangle$ is a primitive inducing path between C and D, so the graph is not maximal. It is shown in [23, Theorem 5.1] that every non-maximal ancestral graph has a unique supergraph that is ancestral and maximal, and every non-maximal ancestral graph can be transformed into the maximal supergraph by a series of additions of bi-directed edges. For example, in Fig. 2, (b) is the unique maximal supergraph of (a), which has an extra bi-directed edge between C and D. From now on, we focus on maximal ancestral graphs (MAGs).

2.3. Causal interpretation of maximal ancestral graphs

The simple motivating example in Fig. 1 suggests that the correlational structure of a set of observed variables can be misleading about causal structure for at least two reasons. First, there may be unobserved common causes or confounders that contribute to the observed association. Second, the samples are representative of but a subpopulation of the population of interest. The subpopulation, in particular, is characterized by a set of unobserved selection or conditioning variables such that units in the subpopulation share values of the selection variables. Hence any observed association or independence is *de facto* conditional on the selection variables.

One can formally represent such a situation by a causal DAG over the union of three disjoint sets of variables, $\mathbf{V} = \mathbf{O} \cup \mathbf{L} \cup \mathbf{S}$, where $\mathbf{O}$ denotes a set of observed variables, $\mathbf{L}$ denotes a set of latent or unobserved variables, and $\mathbf{S}$ denotes a set of unobserved selection variables to be conditioned upon. The DAG entails a set of conditional independence constraints among $\mathbf{V}$. Among these constraints, what are in principle observable or testable are ones of the form $\mathbf{A} \perp\!\!\!\perp \mathbf{B} | \mathbf{C} \cup \mathbf{S}$,[5] where $\mathbf{A}, \mathbf{B}, \mathbf{C} \subseteq \mathbf{O}$ are disjoint sets of observed variables.

[4] These m-separation relations are particularly interesting because **L** is intended to be a set of latent variables which are marginalized in the observable distribution, and **S** is intended to be a set of selection variables upon which the observable distribution conditions.

[5] $\perp\!\!\!\perp$ is a symbol that denotes probabilistic independence introduced by Dawid [8]. The vertical bar | denotes conditioning. Strictly speaking, we are conditioning on a specific value or vector of values of **S**, so it is more accurate to write $\mathbf{A} \perp\!\!\!\perp \mathbf{B} | \mathbf{C} \cup \mathbf{S} = s$.

A distinctive virtue of MAGs is that they can represent such in-principle-testable constraints without explicitly introducing $\mathbf{L}$ and $\mathbf{S}$. Given any DAG $\mathcal{G}$ over $\mathbf{V} = \mathbf{O} \cup \mathbf{L} \cup \mathbf{S}$, there exists a MAG over $\mathbf{O}$ alone such that for any three disjoint sets of variables $\mathbf{A}, \mathbf{B}, \mathbf{C} \subseteq \mathbf{O}$, $\mathbf{A}$ and $\mathbf{B}$ are entailed to be independent conditional on $\mathbf{C} \cup \mathbf{S}$ by $\mathcal{G}$ if and only if $\mathbf{A}$ and $\mathbf{B}$ are entailed to be independent conditional on $\mathbf{C}$ by the MAG. When this is the case, we say the MAG *probabilistically represents* the DAG. The following construction gives us such a MAG:

Input: a DAG $\mathcal{G}$ over $\mathbf{V} = \mathbf{O} \cup \mathbf{L} \cup \mathbf{S}$

Output: a MAG $\mathcal{M}_{\mathcal{G}}$ over $\mathbf{O}$

(1) for each pair of variables $A, B \in \mathbf{O}$, A and B are adjacent in $\mathcal{M}_{\mathcal{G}}$ if and only if there is an inducing path relative to $\langle \mathbf{L}, \mathbf{S} \rangle$ between them in $\mathcal{G}$;
(2) for each pair of adjacent vertices A, B in $\mathcal{M}_{\mathcal{G}}$, orient the edge between them as follows:
  (a) orient it as $A \to B$ in $\mathcal{M}_{\mathcal{G}}$ if $A \in \mathbf{An}_{\mathcal{G}}(B \cup \mathbf{S})$ and $B \notin \mathbf{An}_{\mathcal{G}}(A \cup \mathbf{S})$;
  (b) orient it as $A \leftarrow B$ in $\mathcal{M}_{\mathcal{G}}$ if $B \in \mathbf{An}_{\mathcal{G}}(A \cup \mathbf{S})$ and $A \notin \mathbf{An}_{\mathcal{G}}(B \cup \mathbf{S})$;
  (c) orient it as $A \leftrightarrow B$ in $\mathcal{M}_{\mathcal{G}}$ if $A \notin \mathbf{An}_{\mathcal{G}}(B \cup \mathbf{S})$ and $B \notin \mathbf{An}_{\mathcal{G}}(A \cup \mathbf{S})$;
  (d) orient it as $A - B$ in $\mathcal{M}_{\mathcal{G}}$ if $A \in \mathbf{An}_{\mathcal{G}}(B \cup \mathbf{S})$ and $B \in \mathbf{An}_{\mathcal{G}}(A \cup \mathbf{S})$.

It can be shown that $\mathcal{M}_{\mathcal{G}}$ is indeed a MAG and probabilistically represents $\mathcal{G}$—it follows from Theorem 4.18 of [23]. Moreover, it is easy to see that $\mathcal{M}_{\mathcal{G}}$ also *causally represents* $\mathcal{G}$ in that it retains ancestral relationships in $\mathcal{G}$. So, if $\mathcal{G}$ represents the causal structure for $\mathbf{V}$, it is fair to call $\mathcal{M}_{\mathcal{G}}$ the *causal MAG* for $\mathbf{O}$, in which edges encode causal information about the presence or absence of causal pathway in the underlying structure. Specifically,

- $A \to B$ means that A is a cause of B or of some selection variable, but B is not a cause of A or of any selection variable;[6]
- $A \leftrightarrow B$ means that A is not a cause of B or of any selection variable, and B is not a cause of A or of any selection variable;[7]
- $A - B$ means that A is a cause of B or of some selection variable, and B is a cause of A or of some selection variable.[8]

Put more simply, the edge marks in a causal MAG represent qualitative causal information: arrowheads represent negative causal information about "non-cause", and tails represent positive causal information about "cause". The positive causal information is admittedly less informative than one would wish, when the possibility of selection bias is allowed. This reflects the fact that the presence of selection bias seriously limits the possibility of inferring useful causal information from observations. If the only worry is confounding but not selection bias, $A \to B$ can be read unambiguously as "A is a cause of B". Of course even the disjunctive information may be combined with other information to deduce more useful facts.[9] Detailed exploration of how to use the causal information carried by ancestral graphs in causal reasoning is beyond the scope of this paper.[10] Our present concern is to what extent can such information be discovered from the correlational pattern. It is limited by Markov equivalence.

2.4. Markov equivalence

Two different MAGs carry different causal information, but may share the exact same m-separation structure, and hence entail the same set of conditional independence constraints. Such MAGs are not distinguishable by correlational pattern alone.

Definition 5 *(Markov equivalence).* Two MAGs $\mathcal{G}_1, \mathcal{G}_2$ (with the same set of vertices) are **Markov equivalent** if for any three disjoint sets of vertices $\mathbf{X}, \mathbf{Y}, \mathbf{Z}$, $\mathbf{X}$ and $\mathbf{Y}$ are m-separated by $\mathbf{Z}$ in $\mathcal{G}_1$ if and only if $\mathbf{X}$ and $\mathbf{Y}$ are m-separated by $\mathbf{Z}$ in $\mathcal{G}_2$.

Several characterizations of the Markov equivalence between MAGs are available [1,27,35,37]. We will rely on the characterization of [27] in this paper.

Definition 6 *(unshielded path).* In a MAG, a path consisting of a triple of vertices $\langle X, Y, Z \rangle$ is said to be **unshielded** if X and Z are not adjacent. The triple is called an **unshielded collider** if both the edge between X and Y and the edge between Y and Z are into Y.

[6] By saying A is (or is not) a cause of B, all we mean is that there is (or is not) a directed path from A to B in the underlying causal structure.

[7] This, together with the adjacency of A and B in the MAG, implies that there is a latent common cause of A and B.

[8] Due to the assumed acyclicity of causal structure, this is equivalent to saying that A is a cause of some selection variable, and B is a cause of some selection variable.

[9] For example, if there is $A \to B$ in a MAG, and also another edge into A, then it can be deduced that A is not a cause of any selection variable, but a cause of B.

[10] Some relevant results can be found in [24] and [34].

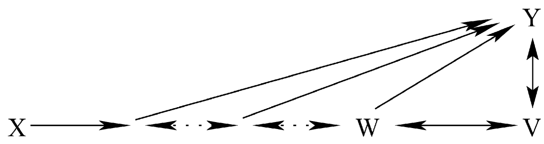

Fig. 3. A discriminating path between X and Y for V.

It is well known that two DAGs are Markov equivalent if and only if they have the same adjacencies and the same unshielded colliders [32]. These conditions are still necessary for Markov equivalence between MAGs, but are not sufficient. For two MAGs to be Markov equivalent, some shielded colliders may have to be present in both or neither of the graphs. The next definition is related to this.

Definition 7 *(discriminating path).* In a MAG, a path between X and Y, $p = \langle X, \ldots, W, V, Y\rangle$, is a **discriminating path** for V if

(i) p includes at least three edges;
(ii) V is a non-endpoint vertex on p, and is adjacent to Y on p; and
(iii) X is not adjacent to Y, and every vertex between X and V is a collider on p and is a parent of Y.

A canonical depiction of an discriminating path is given in Fig. 3. Note that we write a discriminating path in such a form $p = \langle X, \ldots, W, V, Y\rangle$; that is, we specify the endpoints and the vertices adjacent to V, the vertex being *discriminated*. The ellipsis therein designates any number (possibly zero) of other vertices.

The following proposition is proved by Spirtes and Richardson [27].

Proposition 2. *Two MAGs over the same set of vertices are Markov equivalent if and only if*

(e1) *They have the same adjacencies*;
(e2) *They have the same unshielded colliders*;
(e3) *If a path p is a discriminating path for a vertex V in both graphs, then V is a collider on the path in one graph if and only if it is a collider on the path in the other.*

Given an MAG $\mathcal{G}$, we denote its Markov equivalence class, the set of MAGs Markov equivalent to $\mathcal{G}$, by $[\mathcal{G}]$. According to Proposition 2, all members of $[\mathcal{G}]$ have the same adjacencies. But between two adjacent vertices, the edge, and hence one or both of the marks on the edge, may be different in different members of $[\mathcal{G}]$. We call a mark in $\mathcal{G}$ **invariant** if the mark is the same in all members of $[\mathcal{G}]$. It is the adjacencies and the invariant marks of the unknown causal MAG that we can hope to discover from the correlational pattern.

3. The FCI algorithm and arrowhead completeness

The MAG representation gives us a relatively tractable problem of causal discovery in the presence of latent confounders and selection variables: to infer features of the causal MAG from data. In the case of learning causal DAGs (assuming no latent confounders and selection variables), two assumptions are commonly adopted, known as the Causal Markov Condition and the Causal Faithfulness Condition. These two conditions amount to assuming that conditional independence relations that hold in the population distribution are precisely the conditional independence relations entailed by the causal DAG by d-separation.[11] If we assume these two conditions for the underlying causal DAG with latent variables, it follows that there is an exact correspondence between the observable conditional independence relations among the observed variables and m-separation relations in the causal MAG, because the causal MAG probabilistically represents the causal DAG.

Under these two assumptions, therefore, one can learn what the m-separation relations are in the causal MAG from the correlational pattern—facts of conditional independence and dependence. The correlational pattern, in turn, is built based on statistical tests of conditional independence. The constraint-based approach to causal discovery seeks to employ these conditional independence or m-separation constraints to recover features of the causal MAG.

In this paper we will sidestep the statistical problem of inferring genuine conditional independence from data, and focus on the problem of inferring causal information from facts of conditional independence. As an idealization, we will suppose that a perfect oracle for conditional independence is available, which of course can only be approximated in practice.[12]

[11] For detailed exposition and discussion of the two conditions, see [20] and [25]. The causal Markov condition generalizes the familiar principle of the common cause, and as such has been a subject of philosophical debate [3,6,13,15]. Recent reflections on the causal Faithfulness condition include [29] and [36]. In this paper, we assume the two conditions and explore the consequence.

[12] There are of course important practical issues that require further investigations, such as developing more powerful and robust statistical tests of conditional independence, quantifying uncertainty, and handling inconsistency arising from an imperfect oracle.

For any query about conditional independence among the given observed variables, the oracle supplies a correct answer regarding whether the conditional independence in question holds or not. Moreover, given the causal Markov and Faithfulness assumptions mentioned above, the unknown true causal MAG should be perfectly consistent with the oracle, in the sense that the true conditional independence relations as judged by the oracle are precisely the conditional independence relations entailed by the MAG.

Such an oracle would supply information about the m-separation relations in the true causal MAG, which we denote by $\mathcal{G}_T$. In general, however, the m-separation relations do not uniquely determine a MAG, but a Markov equivalence class of MAGs, which we denote by $[\mathcal{G}_T]$. So the causal information that is in principle identifiable given the oracle corresponds to the invariant features of the true causal MAG, i.e., features shared by all MAGs in $[\mathcal{G}_T]$. The question is how to recover these features from the oracle.

A provably sound algorithm for this task is known as the FCI algorithm, whose latest version was presented in [26].[13] The algorithm consists mainly of two stages. In the first stage, the algorithm determines the adjacencies in the causal MAG. The inference of adjacencies is based on the fact that two variables are adjacent in a MAG if and only if they are not m-separated by any set of other variables in the MAG. So the basic idea is to search, for every pair of variables, a set of other variables that renders them conditionally independent. They are not adjacent if and only if such a set is found. The FCI algorithm uses several tricks to make this search efficient, the details of which shall not concern us here. Suffice it to know that it is proved in [26] that given a reliable oracle of conditional independence, the FCI algorithm finds the correct adjacencies.[14]

Our concern is with the second stage, the stage of inferring edge marks. In this stage, the algorithm executes a set of orientation rules (i.e., mark inference rules) to introduce arrowheads or tails, with circles ($\circ$) representing undetermined edge marks. The output of the algorithm is referred to as a *partial ancestral graph*, or a PAG for short.[15] It is intended to be a representation of the Markov equivalence class determined by the oracle of conditional independence.

Definition 8 *(partial ancestral graph).* Let $[\mathcal{G}]$ be the Markov equivalence class of a MAG $\mathcal{G}$. A **partial ancestral graph (PAG)** for $[\mathcal{G}]$ is a graph $\mathcal{P}$ with possibly three kinds of marks (and hence six kinds of edges: $-$, $\rightarrow$, $\leftrightarrow$, $\circ\!-\!\!-$, $\circ\!-\!\!-\!\circ$, $\circ\!\!\rightarrow$), such that (1) $\mathcal{P}$ has the same adjacencies as $\mathcal{G}$ (and any member of $[\mathcal{G}]$) does; and (2) every non-circle mark in $\mathcal{P}$ is an invariant mark in $[\mathcal{G}]$.

If it is furthermore true that (3) every circle in $\mathcal{P}$ corresponds to a variant mark in $[\mathcal{G}]$, $\mathcal{P}$ is called the **maximally informative PAG** for $[\mathcal{G}]$.

It is known that the FCI algorithm is sound, which means that given a perfect oracle of conditional independence, the algorithm outputs a PAG for $[\mathcal{G}_T]$, the Markov equivalence class of the true causal MAG. Whether it is also complete is a matter of whether the output is the maximally informative PAG for $[\mathcal{G}_T]$.

We now describe (an equivalent version of) the FCI algorithm from [26], omitting the details of the adjacency stage. (In stating the orientation rules, a meta-symbol, asterisk ($*$), is used as a wildcard that denotes any of the three marks.[16] More specifically, if "$*$" appears in the antecedent of a rule, that means it does not matter whether the mark at that place is an arrowhead, a tail, or a circle. If "$*$" appears in the consequent of a rule, that means the mark at that place remains what it was before the firing of the rule. Greek letters are used to denote generic variables/vertices.)

FCI algorithm

F1 Form a complete graph $\mathcal{U}$ on the set of variables, in which there is an edge $\circ\!-\!\!-\!\circ$ between every pair of variables;

F2 For every pair of variables α and β, search *in some clever way* for a set of other variables that render the two independent. If such as set **S** is found, remove the edge between α and β in $\mathcal{U}$, and record **S** as $Sepset(\alpha, \beta)$;

F3 Let $\mathcal{P}$ be the graph resulting from step F2. Execute the orientation rule:

$\mathcal{R}0$ For each unshielded triple $\langle\alpha, \gamma, \beta\rangle$ in $\mathcal{P}$, orient it as a collider $\alpha{*}\!\!\rightarrow \gamma \leftarrow\!\!{*}\beta$ if and only if γ is not in $Sepset(\alpha, \beta)$.

F4 Execute the following mark inference rules until none of them applies:

$\mathcal{R}1$ If $\alpha{*}\!\!\rightarrow \beta\circ\!\!-\!\!-{*}\,\gamma$, and α and γ are not adjacent, then orient the triple as $\alpha{*}\!\!\rightarrow \beta \rightarrow \gamma$.

$\mathcal{R}2$ If $\alpha \rightarrow \beta{*}\!\!\rightarrow \gamma$ or $\alpha{*}\!\!\rightarrow \beta \rightarrow \gamma$, and $\alpha \,{*}\!\!-\!\!\circ\, \gamma$, then orient $\alpha \,{*}\!\!-\!\!\circ\, \gamma$ as $\alpha{*}\!\!\rightarrow \gamma$.

$\mathcal{R}3$ If $\alpha{*}\!\!\rightarrow \beta \leftarrow\!\!{*}\gamma$, $\alpha \,{*}\!\!-\!\!\circ\, \theta \,\circ\!\!-\!\!{*}\, \gamma$, α and γ are not adjacent, and $\theta \,{*}\!\!-\!\!\circ\, \beta$, then orient $\theta \,{*}\!\!-\!\!\circ\, \beta$ as $\theta{*}\!\!\rightarrow \beta$.

13 The algorithm was initially designed based on what is called inducing path graphs [25], and was then reinterpreted in terms of (partial) ancestral graphs. Not only are ancestral graph models more amenable to statistical analysis than inducing path graphs, causal discovery based on the former can in principle reveal more causal information than causal discovery based on the latter, for reasons elaborated in [33, Appendix].

14 There is an ambiguity in the original formulation of the algorithm in [25], which, if not interpreted in the right way, suggests a flaw in the algorithm [16]. But when interpreted as intended, the algorithm is provably correct.

15 PAGs were first invented by Richardson [21] in the context of learning causal models with feedback. They were then reinterpreted to represent the output from the FCI procedure, and to represent a Markov equivalence class of MAGs.

16 By this we mean the rule in question applies no matter which of the three marks actually appears in the position of $*$. It does not imply that all three marks *can* appear in that position.

$\mathcal{R}4$ If $u = \langle\theta, \ldots, \alpha, \beta, \gamma\rangle$ is a discriminating path between θ and γ for β, and $\beta\circ\!\!-\!\!* \gamma$; then if $\beta \in Sepset(\theta, \gamma)$, orient $\beta\circ\!\!-\!\!*\gamma$ as $\beta \to \gamma$; otherwise orient the triple $\langle\alpha, \beta, \gamma\rangle$ as $\alpha \leftrightarrow \beta \leftrightarrow \gamma$.[17]

$\mathcal{R}0$–$\mathcal{R}3$ are essentially (with slight generalization) the inference rules used in the context of learning causal DAGs, and are shown to be sound and complete for that purpose [17]. $\mathcal{R}4$ is peculiar to MAGs with bi-directed edges. It is motivated by condition (e3) for Markov equivalence in Proposition 2 (Section 2.4), and justified by the fact that discriminating paths behave similarly to unshielded triples in the following way: if a path between X and Y is discriminating for V, then V is a collider on the path if and only if every set that m-separates X and Y does not contain V; and V is a non-collider on the path if and only if every set that m-separates X and Y contains V. For a proof of this fact and the soundness of $\mathcal{R}0$–$\mathcal{R}4$ (and of the FCI algorithm), see [26].

To establish completeness, we need to show that the PAG returned by FCI is also maximally informative; that is, every circle in the PAG corresponds to a variant mark in $[\mathcal{G}_T]$. In other words, we need to show that for every circle in the PAG, there is a MAG perfectly consistent with the oracle of conditional independence and hence Markov equivalent to $\mathcal{G}_T$, in which the circle is oriented as a tail; and there is such a MAG in which the circle is oriented as an arrowhead.

This turns out to be a highly non-trivial problem. An important step was made by Ali et al. [2]. Their result amounted to showing that $\mathcal{R}0$–$\mathcal{R}4$ are complete with respect to invariant arrowheads.[18] In other words, for every circle in the PAG output by FCI, there is a MAG Markov equivalent to $\mathcal{G}_T$ in which the circle is marked as a tail.

The present paper aims to establish the full completeness result. The FCI algorithm, as it stands, is not yet complete. There could be invariant tails that fail to be picked up by $\mathcal{R}0$–$\mathcal{R}4$, as we will illustrate by a simple example shortly. In the next section we provide extra tail inference rules that we show are able to pick up all (remaining) invariant tails. The demonstration, unfortunately, is even more difficult than that of arrowhead-completeness.

4. Extra orientation rules and tail completeness

To introduce the extra tail inference rules, we need to note a couple of special paths. In the definitions below, we call a graph that can contain three kinds of edge marks—arrowhead, tail and circle—a *partial mixed graph* (PMG).

Definition 9 *(uncovered path).* In a PMG, a path $p = \langle V_0, \ldots, V_n\rangle$ is said to be **uncovered** if for every $1 \leqslant i \leqslant n-1$, V_{i-1} and V_{i+1} are not adjacent, i.e., if every consecutive triple on the path is unshielded.

A distinctive property of uncovered path is of course that after $\mathcal{R}0$ is executed, every consecutive triple on the path has a definite status either as a collider or as a non-collider.

Definition 10 *(potentially directed path).* In a PMG, a path $p = \langle V_0, \ldots, V_n\rangle$ is said to be **potentially directed** (abbreviated as **p.d.**) from V_0 to V_n if for every $0 \leqslant i \leqslant n-1$, the edge between V_i and V_{i+1} is not into V_i or out of V_{i+1}.

Intuitively, a p.d. path is one that could be oriented into a directed path by changing the circles on the path into appropriate tails or arrowheads. As we shall see, uncovered p.d. paths play an important role in locating invariant tails. A special case of a p.d. path is where every edge on the path is of the form $\circ\!\!-\!\!\circ$; we call such a path a **circle path**.

Here is the first block of additional rules:

$\mathcal{R}5$ For every (remaining) $\alpha\circ\!\!-\!\!\circ\beta$, if there is an uncovered circle path $p = \langle\alpha, \gamma, \ldots, \theta, \beta\rangle$ between α and β s.t. α, θ are not adjacent and β, γ are not adjacent, then orient $\alpha\circ\!\!-\!\!\circ\beta$ and every edge on p as undirected edges ($-$).

$\mathcal{R}6$ If $\alpha-\beta\circ\!\!-\!\!*\gamma$ (α and γ may or may not be adjacent), then orient $\beta\circ\!\!-\!\!*\gamma$ as $\beta -\!\!* \gamma$.

$\mathcal{R}7$ If $\alpha -\!\!\circ\, \beta\circ\!\!-\!\!*\gamma$, and α, γ are not adjacent, then orient $\beta\circ\!\!-\!\!*\gamma$ as $\beta -\!\!*\gamma$.

A pictorial illustration of $\mathcal{R}5$–$\mathcal{R}7$ is given in Fig. 4. These rules are obviously related to undirected edges. $\mathcal{R}5$ lead to undirected edges, and $\mathcal{R}6$ depend on undirected edges. So if it is known that the true casual MAG does not contain undirected edges—for example, in those cases where selection bias is known to be absent—these two are not needed. In that case, moreover, $\mathcal{R}7$ will not get triggered at all, because neither $\mathcal{R}0$–$\mathcal{R}4$ introduced earlier nor $\mathcal{R}8$–$\mathcal{R}10$ to be introduced shortly can lead to $-\!\!\circ$ edges, which are in the antecedent of $\mathcal{R}7$.

[17] See [2] for an alternative and perhaps more efficient formulation of this rule that takes on a special kind of discriminating paths.

[18] Ali et al. [2] employed a slightly different graphical object, called *Joined Graphs*, to represent Markov equivalence classes of MAGs. The difference between Joined Graphs and PAGs is just that the former only represent invariant arrowheads, and do not distinguish between tails and circles. This makes Joined Graphs syntactically simpler, at the price of losing information about invariant tails. Our result in this paper can also be seen as an attempt to distinguish between real tails and pseudo tails in joined graphs.

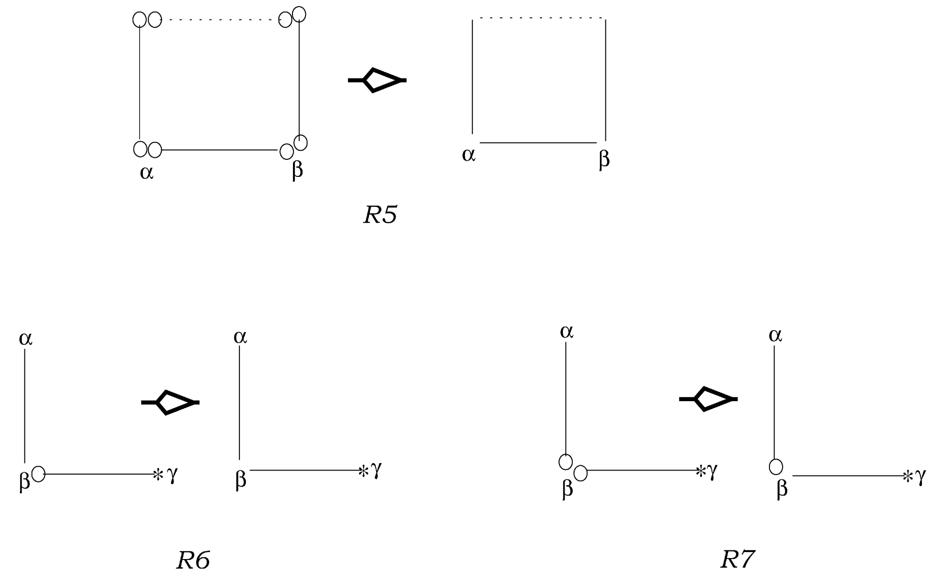

Fig. 4. Graphical illustrations of $\mathcal{R}5$–$\mathcal{R}7$.

That is why we introduce these three rules as a block. If there is no issue of selection bias, we would only consider MAGs with directed and bi-directed edges, in which case $\mathcal{R}5$–$\mathcal{R}7$ can be ignored in principle.[19] The next block of rules, by contrast, may still be applicable.

- $\mathcal{R}8$ If $\alpha \to \beta \to \gamma$ or $\alpha \!-\!\!\circ \beta \to \gamma$, and $\alpha \circ\!\!\to \gamma$, orient $\alpha \circ\!\!\to \gamma$ as $\alpha \to \gamma$.
- $\mathcal{R}9$ If $\alpha \circ\!\!\to \gamma$, and $p = \langle \alpha, \beta, \theta, \ldots, \gamma \rangle$ is an uncovered p.d. path from α to γ such that γ and β are not adjacent, then orient $\alpha \circ\!\!\to \gamma$ as $\alpha \to \gamma$.
- $\mathcal{R}10$ Suppose $\alpha \circ\!\!\to \gamma$, $\beta \to \gamma \leftarrow \theta$, p_1 is an uncovered p.d. path from α to β, and p_2 is an uncovered p.d. path from α to θ. Let μ be the vertex adjacent to α on p_1 (μ could be β), and ω be the vertex adjacent to α on p_2 (ω could be θ). If μ and ω are distinct, and are not adjacent, then orient $\alpha \circ\!\!\to \gamma$ as $\alpha \to \gamma$.

These rules are visualized in Fig. 5. All of them are about turning partially directed edges $\circ\!\!\to$ into directed ones $\to$, which are valuable because $\leftrightarrow$ and $\to$ represent very different causal information.

Call the FCI algorithm supplemented with these rules the Augmented FCI (AFCI) algorithm.[20] We first show that these rules are sound.

Theorem 1. *Let $\mathcal{P}_{FCI}$ be the output of the FCI algorithm, and $\mathcal{P}_{AFCI}$ the graph resulting from applying $\mathcal{R}5$–$\mathcal{R}10$ to $\mathcal{P}_{FCI}$ until none of them applies. The extra tails introduced in $\mathcal{P}_{AFCI}$ are invariant.*

Proof. For each rule, we just need to show that any mixed graph that violates the rule does not belong to $[\mathcal{G}_T]$, i.e., is either not a MAG or not Markov equivalent to $\mathcal{G}_T$. The theorem then follows by a simple induction.

$\mathcal{R}5$: The antecedent of this rule implies that $\langle \alpha, \gamma, \ldots, \theta, \beta, \alpha \rangle$ forms an uncovered cycle that consists of $\circ\!\!-\!\!\circ$ edges. Suppose a mixed graph, contrary to what the rule requires, has an arrowhead on this cycle. In light of $\mathcal{R}1$, the cycle must be oriented as a directed cycle to avoid unshielded colliders not in $\mathcal{G}_T$. But then the graph is not ancestral.

$\mathcal{R}6$: if any graph, contrary to what the rule requires, contains $\alpha - \beta \leftarrow\!\!* \gamma$, the graph is not ancestral.

$\mathcal{R}7$: Suppose a mixed graph, contrary to what the rule requires, has an arrowhead at β on the edge between β and γ. Then either $\alpha - \beta \leftarrow\!\!* \gamma$ is present, in which case the graph is not ancestral; or $\alpha \to \beta \leftarrow\!\!* \gamma$ is present, in which case the graph contains an unshielded collider not in $\mathcal{G}_T$.

$\mathcal{R}8$: This rule is analogous to $\mathcal{R}2$. Obviously if a mixed graph, contrary to what the rule requires, contains $\alpha \leftrightarrow \gamma$, then either an almost directed cycle is present or there is an arrowhead into an undirected edge, and hence the graph is not ancestral.

[19] We add "in principle" here to caution that this is only true with a prefect conditional independence oracle. In practice, there may be occasions where $\mathcal{R}5$ and $\mathcal{R}7$ are applicable even though in theory they should never be invoked.

[20] We will not worry about implementation here. Note that the antecedent of each rule that involves checking the presence of a certain kind of paths, like that of $\mathcal{R}4$, can be checked in $O(mn)$ with a generic algorithm for checking 'reachability', with m being the number of edges and n being the number of vertices in the graph. So in big O notation, the time complexity of the AFCI algorithm is the same as that of the FCI algorithm [26].

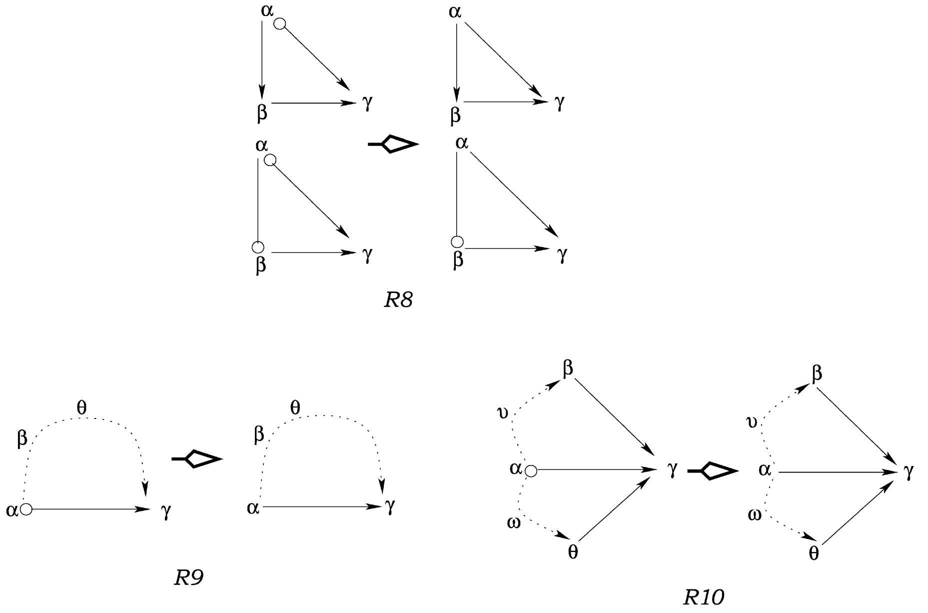

Fig. 5. Graphical illustrations of $\mathcal{R}8$–$\mathcal{R}10$.

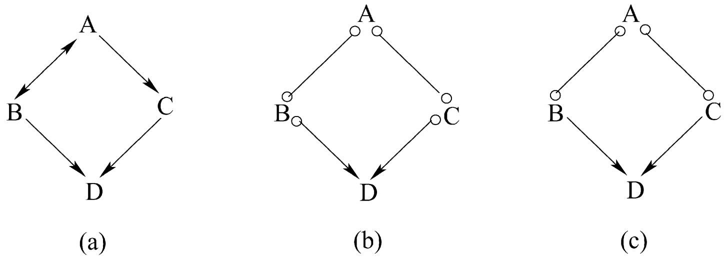

Fig. 6. An example where $\mathcal{R}9$ is needed. (a) is the (unknown) causal MAG. (b) gives the FCI output, to which $\mathcal{R}9$ can be applied (twice) to yield (c).

$\mathcal{R}9$: The essentially same argument for the soundness of $\mathcal{R}5$ applies here.

$\mathcal{R}10$: The antecedent of the rule implies that the triple $\langle \mu, \alpha, \omega \rangle$ is not a collider in $\mathcal{G}_T$, which means at least one of the two edges involved in the triple is out of α in any MAG in $[\mathcal{G}_T]$. Suppose a graph in $[\mathcal{G}_T]$, contrary to what the rule requires, contains $\alpha \leftrightarrow \gamma$. Then the edge(s) out of α must be a directed edge for the graph to be ancestral. It follows that either p_1 or p_2 is a directed path in the graph to avoid unshielded colliders not in $\mathcal{G}_T$. In either case, α is an ancestor of γ, and hence the graph is not ancestral; a contradiction. $\square$

Here is a simple example in which $\mathcal{R}9$ is needed. Suppose the true causal MAG is the one in Fig. 6(a). Given an oracle consistent with this MAG, the FCI algorithm (with $\mathcal{R}0$–$\mathcal{R}4$) gives us the graph in 6(b), to which we can further apply $\mathcal{R}9$ to get more tails, as shown in 6(c) ($B \to D$ and $C \to D$). Given the soundness of $\mathcal{R}9$, we know the additional tails are invariant. So the FCI algorithm with just $\mathcal{R}0$–$\mathcal{R}4$ is not yet complete. In fact, it is not hard to construct cases to show that all the orientation rules given above except possibly $\mathcal{R}8$ are independent. We do not yet know if $\mathcal{R}8$ is independent—we can neither construct a case in which only $\mathcal{R}8$ is applicable, nor derive $\mathcal{R}8$ from other rules—but the current proof of completeness uses $\mathcal{R}8$.

The main result to be established is that $\mathcal{R}5$–$\mathcal{R}10$ are also sufficient for picking up all remaining invariant tails. Let $\mathcal{P}_{AFCI}$ denote the output of the AFCI algorithm. We need to demonstrate that for every circle in $\mathcal{P}_{AFCI}$, there is a MAG in $[\mathcal{G}_T]$ in which the corresponding mark is an arrowhead. As we shall see, the main difficulty of proving this fact lies with circles on the $\circ\!\!\rightarrow$ edges. For circles on the other two kinds of edges, $\circ\!\!-\!\!-$ and $\circ\!\!-\!\!-\!\!\circ$, the argument is quite analogous to the argument for arrowhead completeness given in [2] or [33]. We will deal with these two first in Section 4.1, and then take up the more difficult task in Section 4.2 to show that no circle on $\circ\!\!\rightarrow$ edges in $\mathcal{P}_{AFCI}$ hides an invariant tail.

4.1. Circles on $\circ\!\!-\!\!-$ and $\circ\!\!-\!\!-\!\!\circ$ edges

Since $\mathcal{P}_{AFCI}$ is sound, any MAG in $[\mathcal{G}_T]$ is a further orientation of $\mathcal{P}_{AFCI}$; that is, all the unambiguous edge marks (arrowheads and tails) already in $\mathcal{P}_{AFCI}$ will be retained in the MAG, and the circles in $\mathcal{P}_{AFCI}$ are turned into appropriate arrowheads or tails in the MAG. Let us call the subgraph of $\mathcal{P}_{AFCI}$ consisting of all the $\circ\!\!-\!\!\circ$ edges in $\mathcal{P}_{AFCI}$ the *circle component* of $\mathcal{P}_{AFCI}$, and denote it by $\mathcal{P}^C_{AFCI}$. The first thing to note is that $\mathcal{P}^C_{AFCI}$ has the following property:

Lemma 4.1. *For every edge $A \circ\!\!-\!\!\circ B$ in $\mathcal{P}^C_{AFCI}$, $\mathcal{P}^C_{AFCI}$ can be oriented into a DAG with no unshielded colliders in which $A \to B$ appears, and can also be oriented into a DAG with no unshielded colliders in which $A \leftarrow B$ appears.*

The proof is given in Appendix A, which makes use of Lemma 5 in Meek (1995). This fact is relevant because of the following theorem:

Theorem 2. *Let $\mathcal{H}$ be the graph resulting from the following procedure applied to $\mathcal{P}_{AFCI}$:*

(1) *orient the circles on $\circ\!\!\to$ edges in $\mathcal{P}_{AFCI}$ as tails, and orient the circles on $-\!\!\circ$ edges in $\mathcal{P}_{AFCI}$ as arrowheads (that is, turn all $\circ\!\!\to$ edges and all $-\!\!\circ$ edges into directed edges $\to$); and*
(2) *orient $\mathcal{P}^C_{AFCI}$ into a DAG with no unshielded colliders.*

Then $\mathcal{H}$ is a member of $[\mathcal{G}_T]$.

The proof of this theorem is given in Appendix A. The theorem has a couple of important implications. First, it suggests a way to turn $\mathcal{P}_{AFCI}$, a representation of a Markov equivalence class of MAGs, into a representative MAG. What is special about this construction is that no extra undirected edges or bi-directed edges are introduced. So the outcome is a representative member of the Markov equivalence class with the fewest undirected edges and bi-directed edges. Such a representative is conceivably easier to fit and score than other members in the class, in light of the fact that UGs are in general harder to fit than DAGs and the results presented in [10] suggesting that it is better to have fewer bi-directed edges in fitting a MAG model. If so, it will be particularly useful for developing score-based causal discovery algorithm based on MAGs.

More importantly for our present purpose, Theorem 2 together with Lemma 4.1 entail that for every circle on a $-\!\!\circ$ edge or a $\circ\!\!-\!\!\circ$ edge in $\mathcal{P}_{AFCI}$, there is a member in $[\mathcal{G}_T]$ in which the corresponding mark is an arrowhead. In other words, no circle on $-\!\!\circ$ or $\circ\!\!-\!\!\circ$ edges in $\mathcal{P}_{AFCI}$ corresponds to an invariant tail. Therefore, what is left to show in order to establish completeness is just that circles on $\circ\!\!\to$ edges in $\mathcal{P}_{AFCI}$ do not hide invariant tails.

4.2. Circles on $\circ\!\!\to$ edges

This last task, however, turns out to be the most difficult to fulfill. Unlike circles on the $-\!\!\circ$ edges of $\mathcal{P}_{AFCI}$, which can be simultaneously turned into arrowheads as we saw in Theorem 2, circles on the $\circ\!\!\to$ edges in general cannot be turned into arrowheads simultaneously in order to make a MAG in $[\mathcal{G}_T]$. The simplest example is $X \leftarrow\!\!\circ Y \circ\!\!\to Z$, an unshielded path that can appear in $\mathcal{P}_{AFCI}$. If we turn both of the circles into arrowheads, a new unshielded collider is created, and the resulting graph will not belong to $[\mathcal{G}_T]$. By contrast, an unshielded triple such as $X -\!\!\circ Y \circ\!\!- Z$ will not appear in $\mathcal{P}_{AFCI}$ in light of $\mathcal{R}7$. So we cannot handle $\circ\!\!\to$ edges in a wholesale manner.

Let $J \circ\!\!\to K$ denote an arbitrary $\circ\!\!\to$ edge in $\mathcal{P}_{AFCI}$. We need to show that there is a MAG in $[\mathcal{G}_T]$ in which the edge appears as $J \leftrightarrow K$. Our argument consists of two major steps. In the first step, we show that we can orient $\mathcal{P}^C_{AFCI}$—the circle component of $\mathcal{P}_{AFCI}$—into a DAG with no unshielded colliders *that satisfies certain conditions relative to $J \circ\!\!\to K$*. This DAG orientation of $\mathcal{P}^C_{AFCI}$ together with operation (1) in Theorem 2 yield a MAG in $[\mathcal{G}_T]$.

This MAG is not yet what we want, because $J \circ\!\!\to K$ is oriented as $J \to K$ rather than $J \leftrightarrow K$ by operation (1) in Theorem 2. In the second step of our argument, we make use of a result on equivalence-preserving mark changes given in [30] and [35], and prove that the MAG constructed in the first step can be transformed into a MAG containing $J \leftrightarrow K$ through a sequence of equivalence-preserving changes of $\to$ into $\leftrightarrow$. It then follows that the resulting MAG with $J \leftrightarrow K$ is also Markov equivalent to $\mathcal{G}_T$, which is what we need.

The following definitions specify the conditions we want a DAG orientation of $\mathcal{P}^C_{AFCI}$ to satisfy.

Definition 11 *(Relevance).* Let $J \circ\!\!\to K$ be an arbitrary $\circ\!\!\to$ edge in $\mathcal{P}_{AFCI}$. For any $A \circ\!\!\to B$ in $\mathcal{P}_{AFCI}$, it is said to be **relevant** to $J \circ\!\!\to K$ if

(i) $A = J$ or there is a p.d. path from J to A in $\mathcal{P}_{AFCI}$ such that no vertex on the path (including the endpoints) is a parent of K; and
(ii) $B = K$ or B is a parent of K (namely $B \to K$) in $\mathcal{P}_{AFCI}$.

If $A \circ\!\!\to B$ is relevant to $J \circ\!\!\to K$, we say that A is **circle-relevant** to $J \circ\!\!\to K$, and B is **arrowhead-relevant** to $J \circ\!\!\to K$.

Intuitively, relevant edges are those that may have to be turned into bi-directed edges ($\leftrightarrow$) in order for $J \circ\!\!\to K$ to be so oriented, on pain of creating almost directed cycles. This is most obvious in Fig. 7(a), in which if $J \circ\!\!\to B$ is oriented as $J \to B$, then $J \circ\!\!\to K$ cannot be oriented as $J \leftrightarrow K$, lest an almost directed cycle be created.

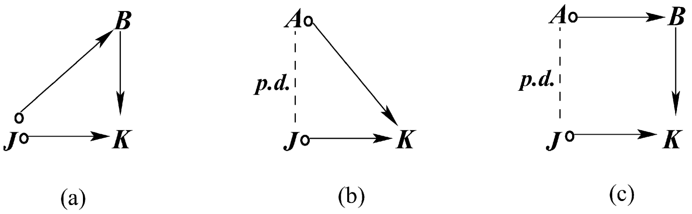

Fig. 7. Configurations of relevance. (a) $J \circ\!\!\rightarrow B$ is relevant to $J \circ\!\!\rightarrow K$, because B is a parent of K; (b) $A \circ\!\!\rightarrow K$ is relevant to $J \circ\!\!\rightarrow K$, because there is a p.d. path from J to A (with no parent of K on the path); (c) $A \circ\!\!\rightarrow B$ is relevant to $J \circ\!\!\rightarrow K$, because there is a p.d. path from J to A (with no parent of K on the path) and B is a parent of K.

Let $\mathbf{REL}(J \circ\!\!\rightarrow K)$ denote the set of $\circ\!\!\rightarrow$ edges relevant to $J \circ\!\!\rightarrow K$ in $\mathcal{P}_{AFCI}$. Notice that $J \circ\!\!\rightarrow K$ itself belongs to this set, and we will eventually show that all edges in $\mathbf{REL}(J \circ\!\!\rightarrow K)$, and so $J \circ\!\!\rightarrow K$ in particular, can be turned into bi-directed edges simultaneously. For easy reference, let us denote the set of circle-relevant vertices by $\mathbf{CR}(J \circ\!\!\rightarrow K)$, and the set of arrow-relevant vertices by $\mathbf{AR}(J \circ\!\!\rightarrow K)$.

Definition 12 *(Agreeable orientation).* A DAG orientation of $\mathcal{P}^{C}_{AFCI}$—the circle component of $\mathcal{P}_{AFCI}$—is said to be **agreeable** to $J \circ\!\!\rightarrow K$ if the following three conditions hold:

- $\mathbf{C_1}$ For every $A \circ\!\!\rightarrow B \circ\!\!-\!\!\circ C$ in $\mathcal{P}_{AFCI}$ such that $A \circ\!\!\rightarrow B \in \mathbf{REL}(J \circ\!\!\rightarrow K)$ and $C \notin \mathbf{AR}(J \circ\!\!\rightarrow K)$, $B \circ\!\!-\!\!\circ C$ is oriented as $B \rightarrow C$ in the DAG;
- $\mathbf{C_2}$ For every $C \circ\!\!-\!\!\circ A \circ\!\!\rightarrow B$ in $\mathcal{P}_{AFCI}$ such that $A \circ\!\!\rightarrow B \in \mathbf{REL}(J \circ\!\!\rightarrow K)$ and C is a parent of B (namely $C \rightarrow B$) in $\mathcal{P}_{AFCI}$, $C \circ\!\!-\!\!\circ A$ is oriented as $C \rightarrow A$ in the DAG;
- $\mathbf{C_3}$ For every $C \circ\!\!-\!\!\circ A \circ\!\!\rightarrow B$ in $\mathcal{P}_{AFCI}$ such that $A \circ\!\!\rightarrow B \in \mathbf{REL}(J \circ\!\!\rightarrow K)$ and C is not adjacent to B in $\mathcal{P}_{AFCI}$, $C \circ\!\!-\!\!\circ A$ is oriented as $C \leftarrow A$ in the DAG.

Roughly speaking, $\mathbf{C_1}$–$\mathbf{C_3}$ are motivated as necessary conditions for orienting a $\circ\!\!\rightarrow$ edge (relevant to $J \circ\!\!\rightarrow K$) into a bi-directed edge. This is especially clear for $\mathbf{C_2}$ and $\mathbf{C_3}$. Regarding a relevant edge $A \circ\!\!\rightarrow B$, if $\mathbf{C_2}$ is violated, then $A \circ\!\!\rightarrow B$ cannot be turned into a bi-directed edge, on pain of creating an almost directed cycle; similarly if $\mathbf{C_3}$ is violated, on pain of creating a new unshielded collider. The rationale behind $\mathbf{C_1}$ is less obvious, but is basically along the same line, and will be revealed in the proof of Theorem 3.

The first question is whether we can orient $\mathcal{P}^{C}_{AFCI}$ into a DAG with no unshielded colliders that is also agreeable to $J \circ\!\!\rightarrow K$. As the proof for Lemma 4.1 goes (in Appendix A), the reason why $\mathcal{P}^{C}_{AFCI}$ can be oriented into a DAG with no unshielded colliders is because $\mathcal{P}^{C}_{AFCI}$ is chordal (a.k.a triangulated). One way to orient a chordal graph into a DAG free of unshielded colliders is due to Meek [17]:

Meek's Algorithm
Input: a chordal unoriented graph $\mathcal{U}$
Output: a DAG orientation of $\mathcal{U}$ (with no unshielded colliders)

Repeat

(1) choose a yet unoriented edge $A \circ\!\!-\!\!\circ B$ in $\mathcal{U}$;
(2) orient the edge into $A \rightarrow B$ (or $A \leftarrow B$), and close orientations under the following rules:[21]
  $\mathbf{UR}_1$ If $A \rightarrow B \circ\!\!-\!\!\circ C$, A and C are not adjacent, orient as $B \rightarrow C$.
  $\mathbf{UR}_2$ If $A \rightarrow B \rightarrow C$ and $A \circ\!\!-\!\!\circ C$, orient as $A \rightarrow C$.
  $\mathbf{UR}_3$ If $A \rightarrow B \rightarrow C$, $A \circ\!\!-\!\!\circ D \circ\!\!-\!\!\circ C$, $B \circ\!\!-\!\!\circ D$, and A and C are not adjacent, orient $D \circ\!\!-\!\!\circ C$ as $D \rightarrow C$.

Until every edge is oriented in $\mathcal{H}$.

So the idea is very simple. In each round, choose an arbitrary unoriented edge to orient in any direction, and propagate the orientation using the three rules. Then repeat this until every edge is oriented. We now adapt the algorithm to fit our purpose. Given an edge $J \circ\!\!\rightarrow K$ in $\mathcal{P}_{AFCI}$, let $\mathbf{E}_i$ ($i = 1, 2, 3$) be the set of $\circ\!\!-\!\!\circ$ edges in $\mathcal{P}_{AFCI}$ whose orientations are required by condition $\mathbf{C}_i$ in Definition 12. (Note that $\mathbf{E}_i$'s are not necessarily disjoint.)

[21] There is another rule in [17]. However, the antecedent of that rule involves an unshielded collider, which will not be triggered in orienting a chordal graph into a DAG *with no unshielded colliders*. So we need not include that one here.

Orientation algorithm for the circle component of $\mathcal{P}_{AFCI}$
Input: $\mathcal{P}^C_{AFCI}$, $\mathcal{P}_{AFCI}$, and an edge $J \circ\!\!\rightarrow K$ therein
Output: a DAG orientation of $\mathcal{P}^C_{AFCI}$ with no unshielded colliders

Let $\mathcal{D} = \mathcal{P}^C_{AFCI}$
Repeat

If some edge in $\mathbf{E_1}$ is not yet oriented in $\mathcal{D}$
(a) choose such an edge $A \circ\!\!-\!\!\circ B \in \mathbf{E_1}$, and orient it as condition $\mathbf{C_1}$ requires;
(b) close orientations under $\mathbf{UR}_1, \mathbf{UR}_2, \mathbf{UR}_3$.
Else If some edge in $\mathbf{E_2}$ is not yet oriented in $\mathcal{D}$;
(a) choose such an edge $A \circ\!\!-\!\!\circ B \in \mathbf{E_2}$, and orient it as condition $\mathbf{C_2}$ requires;
(b) close orientations under $\mathbf{UR}_1, \mathbf{UR}_2, \mathbf{UR}_3$.
Else If some edge in $\mathbf{E_3}$ is not yet oriented in $\mathcal{D}$;
(a) choose such an edge $A \circ\!\!-\!\!\circ B \in \mathbf{E_3}$, and orient it as condition $\mathbf{C_3}$ requires;
(b) close orientations under $\mathbf{UR}_1, \mathbf{UR}_2, \mathbf{UR}_3$.
Else
(a) choose a yet unoriented edge $A \circ\!\!-\!\!\circ B$ in $\mathcal{D}$;
(b) orient the edge into $A \rightarrow B$ and close orientations under $\mathbf{UR}_1, \mathbf{UR}_2, \mathbf{UR}_3$.

Until every edge is oriented in $\mathcal{D}$
Return $\mathcal{D}$

This is just a more restricted version of Meek's algorithm. Therefore, given the correctness of Meek's algorithm, this Orientation Algorithm obviously returns a DAG orientation of $\mathcal{P}^C_{AFCI}$ with no unshielded colliders. Moreover, we can show that it is agreeable to $J \circ\!\!\rightarrow K$.

Lemma 4.2. *Let $\mathcal{D}_{J\circ\to K}$ be the DAG output of the* **Orientation Algorithm**. *$\mathcal{D}_{J\circ\to K}$ is a DAG orientation of $\mathcal{P}^C_{AFCI}$ free of unshielded colliders and agreeable to $J \circ\!\!\rightarrow K$.*

This lemma is the most difficult to establish in the whole argument, and a proof is given in Appendix B. The reason to take the trouble is that Lemma 4.2 enables us to prove the following fact.

Theorem 3. *Let $J \circ\!\!\rightarrow K$ be a $\circ\!\!\rightarrow$ edge in $\mathcal{P}_{AFCI}$. Construct $\mathcal{H}$ from $\mathcal{P}_{AFCI}$ by the following procedure:*

(1) *orient $\circ\!\!\rightarrow$ edges in* $\mathbf{REL}(J \circ\!\!\rightarrow K)$ *as $\leftrightarrow$, and orient other $\circ\!\!\rightarrow$ edges as $\rightarrow$;*
(2) *orient $-\!\!\circ$ edges in $\mathcal{P}_{AFCI}$ as $\rightarrow$;*
(3) *orient $\mathcal{P}^C_{AFCI}$ into $\mathcal{D}_{J\circ\to K}$ with the Orientation Algorithm.*

Then $\mathcal{H}$ is a member of $[\mathcal{G}_T]$.

See Appendix B for the proof. As hinted above, the basic idea of the proof is to start with a MAG constructed via the procedure in Theorem 2, and then show that the MAG can be transformed into the graph constructed here by a sequence of equivalence-preserving changes of $\rightarrow$ into $\leftrightarrow$.

The main theorem of this paper readily follows:

Theorem 4 *(Completeness). The Augmented FCI algorithm (with the additional tail inference rules $\mathcal{R}5$–$\mathcal{R}10$) is complete, in the sense that given a perfect conditional independence oracle, the algorithm returns the maximally informative PAG for the true causal MAG.*

Proof. Theorem 2 implies that for every circle on $\circ\!\!-\!\!\circ$ and $-\!\!\circ$ edges in the AFCI output, there is a MAG Markov equivalent to the true causal MAG in which the circle is marked as an arrowhead; Theorem 3 implies that this is also the case for every circle on $\circ\!\!\rightarrow$ edges. Hence, no circle in the AFCI output can be an invariant tail. Together with the arrowhead-completeness result, we have shown that the AFCI algorithm is complete. $\square$

5. Conclusion

Causal discovery from data becomes especially challenging when the possibility of latent confounding and selection bias cannot be ruled out. Maximal ancestral graphs provide a neat representation of such causal systems without explicitly introducing unobserved variables, which facilitates automated search over (classes of) causal structures based on correlational information. We have established a completeness result in this framework, concerning the extent to which causal information can be extracted from facts of probabilistic independence and dependence, under the standard causal Markov and Faithfulness assumptions.

Although we presented the result in the context of the FCI algorithm, its significance goes beyond this particular algorithm, because we have in effect shown that the orientation rules $\mathcal{R}0$–$\mathcal{R}10$ provide a complete characterization of invariant marks in a Markov equivalence class of MAGs. In particular, given an arbitrary MAG, these orientation rules can be used to identify its invariant marks. This will be useful in any causal discovery algorithm or causal reasoning system based on MAGs.

The orientation rules fall naturally into three independent blocks. $\mathcal{R}0$–$\mathcal{R}4$ are arrowhead complete. $\mathcal{R}5$–$\mathcal{R}7$ are relevant only when selection bias may be present. In fact, it is more common in the literature to consider latent confounding without selection bias, in which case $\mathcal{R}5$–$\mathcal{R}7$ may be either ignored or serve as a check of the assumption of no selection bias. Moreover, when there is no selection bias, a directed edge in the causal MAG carries especially clear qualitative causal information. $\mathcal{R}8$–$\mathcal{R}10$ are then particularly valuable, as they can pick up directed edges missed by $\mathcal{R}0$–$\mathcal{R}4$.

Besides the constraint-based approach to causal discovery, of which the FCI algorithm is a representative, there is also the score-based or Bayesian approach to causal discovery in the literature [7,14]. It is an ongoing project to develop a score-based causal discovery procedure based on MAGs. Not only are the orientation rules relevant to this problem, Theorem 2 in Section 4.1 is probably also useful for the purpose of scoring an equivalence class of MAGs, in that it gives a procedure for constructing a representative MAG with the fewest undirected edges and bi-directed edges.

We close by noting two related open problems. First, we have implicitly assumed that no substantial background causal knowledge is available, and so the causal MAG can only be determined up to Markov equivalence. When prior causal knowledge or limited experimental control is available, it is possible to discriminate between some Markov equivalent MAGs, and hence more edge marks than the invariant ones of the true causal MAG may be identifiable. How to adapt the AFCI algorithm to handle such background knowledge and whether the adapted algorithm is complete are worth investigating.

Second, it should be emphasized that our completeness result is in regard to causal information that can be inferred from probabilistic independence and dependence facts. But there may be other kind of probabilistic facts that are informative about causation. In fact, it is well known that causal DAGs with latent variables can entail testable constraints on the marginal probability of observed variables that do not take the form of conditional independence (see [31] for an illuminating discussion). Such constraints are not retained in the MAG representation of the underlying causal structure. This is a limitation of the MAG framework, and how to effectively employ non-independence constraints in automated causal discovery remains an intriguing open question.

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Appendix A. Proof of Lemma 4.1 and Theorem 2

We need some utility lemmas about $\mathcal{P}_{AFCI}$.

Lemma A.1. *In $\mathcal{P}_{AFCI}$, the following property holds*:

P1 *for any three vertices A, B, C, if $A{*}\!\!\rightarrow B\circ\!\!-\!\!* C$, then there is an edge between A and C with an arrowhead at C, namely, $A{*}\!\!\rightarrow C$. Furthermore, if the edge between A and B is $A \rightarrow B$, then the edge between A and C is either $A \rightarrow C$ or $A\circ\!\!\rightarrow C$ (i.e., it is not $A \leftrightarrow C$).*

This is a key lemma for proving arrowhead completeness, and only concerns $\mathcal{R}0$–$\mathcal{R}4$, because the extra inference rules do not supply arrowheads. See the proof of Lemma 4.1 in [2], which is formulated in a different but equivalent way. We omit details for interest of space.

Lemma A.2. *In $\mathcal{P}_{AFCI}$, the following property holds*:

P2 *For any two vertices A, B, if $A -\!\!\circ B$, then there is no edge into A or B.*

Proof. By **P**1, for any $A -\!\!\circ B$ in $\mathcal{P}_{AFCI}$, if there is an edge $C{*}\!\!\rightarrow B$, there is also an edge $C{*}\!\!\rightarrow A$. So it suffices to prove that there is no edge into A. Let $\mathbf{E} = \{X -\!\!\circ Y \text{ in } \mathcal{P}_{AFCI} \mid \exists Z \text{ s.t. } Z{*}\!\!\rightarrow X \text{ is in } \mathcal{P}_{AFCI}\}$. We need to show that $\mathbf{E}$ is empty. Suppose that it is not empty. Let $X_0 -\!\!\circ Y_0 \in \mathbf{E}$ be the first member of $\mathbf{E}$ that gets so oriented—i.e., the tail marks on other edges in $\mathbf{E}$, if any, get oriented after $X_0\circ\!\!-\!\!\circ Y_0$ is oriented as $X_0 -\!\!\circ Y_0$. Choose any Z_0 such that $Z_0{*}\!\!\rightarrow X_0$ is in $\mathcal{P}_{AFCI}$. Since $X_0\circ\!\!-\!\!\circ Y_0$ is oriented as $X_0 -\!\!\circ Y_0$ either by $\mathcal{R}6$ or $\mathcal{R}7$, we consider the two cases one by one:

Case 1: It is oriented by $\mathcal{R}6$. That means there is a vertex W such that $W - X_0$ is in $\mathcal{P}_{AFCI}$. But then $Z_0{*}\!\!\rightarrow X_0 - W$ violates (a3) in the definition of ancestral graphs, which contradicts the soundness of $\mathcal{P}_{AFCI}$.

Case 2: It is oriented by $\mathcal{R}7$. That means, at the time of the orientation, there is a vertex W such that W, Y_0 are not adjacent, and there is an edge $W \mathrel{-\!\!\circ} X_0$ between them. This implies that either $W \mathrel{-\!\!\circ} X_0$ or $W - X_0$ appears in $\mathcal{P}_{AFCI}$ (as no arrowhead is added by any of $\mathcal{R}5$–$\mathcal{R}10$). The latter case is again ruled out by (a3) in the definition of ancestral graphs. In the former case, since $Z_0 \mathrel{*\!\!\rightarrow} X_0$ is in $\mathcal{P}_{AFCI}$, by **P**1, $Z_0 \mathrel{*\!\!\rightarrow} W$ is also in $\mathcal{P}_{AFCI}$. But then $W \mathrel{-\!\!\circ} X_0$ is in **E** and gets oriented before $X_0 \mathrel{-\!\!\circ} Y_0$ does, which contradicts our choice of $X_0 \mathrel{-\!\!\circ} Y_0$.

Hence the supposition that **E** is not empty is false. **CP**2 holds of $\mathcal{P}_{AFCI}$. □

Call $\langle V_0, \ldots, V_n \rangle$ a **tail-circle path** from V_0 to V_n if for every i ($0 \leqslant i \leqslant n-1$), the edge between V_i and V_{i+1} is $V_i \mathrel{-\!\!\circ} V_{i+1}$.

Lemma A.3. *In $\mathcal{P}_{AFCI}$, the following hold*:

(i) *For any $A \mathrel{-\!\!\circ} B$, there is an uncovered tail-circle path from an endpoint of an undirected edge to B that ends with the edge $A \mathrel{-\!\!\circ} B$.*
(ii) *If p is an uncovered tail-circle path, then no two non-consecutive vertices on p are adjacent.*

Proof. Let **TC** be the set of $\mathrel{-\!\!\circ}$ edges in $\mathcal{P}_{AFCI}$. Order the members of **TC** by their order of occurrence in the orientation process. We show (i) by induction.

Base case: Let $X \mathrel{-\!\!\circ} Y$ be the "first" edge in **TC**—that is, it gets oriented as such before any other member of **TC** does. Of all the mark inference rules, only $\mathcal{R}6$ and $\mathcal{R}7$ could yield $\mathrel{-\!\!\circ}$ edges. If $X \mathrel{-\!\!\circ} Y$ is oriented by $\mathcal{R}6$, then obviously X is an endpoint of an undirected edge. Suppose $X \mathrel{-\!\!\circ} Y$ is oriented by $\mathcal{R}7$, which means there is a vertex Z such that Z, Y are not adjacent, and $Z \mathrel{-\!\!\circ} X \mathrel{\circ\!\!-\!\!\circ} Y$ is the configuration at the point of orienting $X \mathrel{\circ\!\!-\!\!\circ} Y$. If $Z \mathrel{-\!\!\circ} X$ remains in $\mathcal{P}_{AFCI}$, then it belongs to **TC**, and it occurs earlier than $X \mathrel{-\!\!\circ} Y$ does, which contradicts our choice of $X \mathrel{-\!\!\circ} Y$. So in $\mathcal{P}_{AFCI}$ it must be $Z - X$ (because no inference rule will orient $\mathrel{-\!\!\circ}$ into $\rightarrow$). Hence X is still an endpoint of an undirected edge. Then $X \mathrel{-\!\!\circ} Y$ is an uncovered tail-circle path from an endpoint of an undirected edge to Y.

Inductive step: Suppose the first n edges in **TC** satisfy (i); consider the $n+1^{st}$ edge, $U \mathrel{-\!\!\circ} W$, in **TC**. Again, it is oriented by $\mathcal{R}6$ or $\mathcal{R}7$. If it is oriented by $\mathcal{R}6$, then U is an endpoint of an undirected edge, and $U \mathrel{-\!\!\circ} W$ constitutes an uncovered tail-circle path from U to W. Suppose it is oriented by $\mathcal{R}7$, then there is a vertex V such that V, W are not adjacent, and $V \mathrel{-\!\!\circ} U \mathrel{\circ\!\!-\!\!\circ} W$ is the configuration at the point of orienting $X \mathrel{\circ\!\!-\!\!\circ} Y$. If $V \mathrel{-\!\!\circ} U$ remains in $\mathcal{P}_{AFCI}$, then it is one of the first n edges in **TC**. By the inductive hypothesis, there is an uncovered tail-circle path, p, from an endpoint of an undirected edge to U that includes the edge $V \mathrel{-\!\!\circ} U$. Since V, W are not adjacent, p appended to $U \mathrel{-\!\!\circ} W$ constitutes an uncovered tail-circle path from an endpoint of an undirected edge to W. If, on the other hand, $V \mathrel{-\!\!\circ} U$ is not in $\mathcal{P}_{AFCI}$, then it must be $V - U$, which makes U an endpoint of an undirected edge, and $U \mathrel{-\!\!\circ} W$ the desired path. Therefore, for every edge in **TC**, the property stated in (i) holds.

Next we prove (ii). If p has only one edge, the proposition trivially holds, because there is no pair of non-consecutive vertices; if p has two edges, the proposition also trivially holds, because p is uncovered, and the only pair of non-consecutive vertices on p are by definition non-adjacent.

Now suppose the proposition holds for those uncovered circle-tail paths that have fewer than n edges. Consider an uncovered circle-tail path with n edges: $V_0 \mathrel{-\!\!\circ} V_1 \cdots V_{n-1} \mathrel{-\!\!\circ} V_n$. By the inductive hypothesis, the only pair of non-consecutive vertices that could be adjacent is V_0 and V_n. By **P**2 (Lemma A.2), the edge between V_0 and V_n is not into V_0 or V_n. It is not an undirected edge either, for otherwise the circle at V_n on $V_{n-1} \mathrel{-\!\!\circ} V_n$ should have been oriented by $\mathcal{R}6$. However, $\langle V_0, V_1, \ldots, V_{n-1}, V_n, V_0 \rangle$ forms an uncovered cycle, so at least one of the $\mathrel{\circ\!\!-\!\!\circ}$ edges on the cycle should have been oriented as $-$ by $\mathcal{R}5$ before any$-$edge appears, which contradicts the fact that there is no$-$edge on the cycle. So V_0 and V_n are not adjacent. □

The main use of Lemma A.3 is to establish two more properties of $\mathcal{P}_{AFCI}$.

Lemma A.4. *In $\mathcal{P}_{AFCI}$, the following property holds*:

P3 *For any three vertices A, B, C, if $A \mathrel{-\!\!\circ} B \mathrel{\circ\!\!-\!\!*} C$, then A and C are adjacent. Furthermore, if $A \mathrel{-\!\!\circ} B \mathrel{\circ\!\!-\!\!\circ} C$, then $A \mathrel{-\!\!\circ} C$; if $A \mathrel{-\!\!\circ} B \mathrel{\circ\!\!\rightarrow} C$, then $A \rightarrow C$ or $A \mathrel{\circ\!\!\rightarrow} C$.*

Proof. The first claim is obvious. If $A \mathrel{-\!\!\circ} B \mathrel{\circ\!\!-\!\!*} C$, but A, C are not adjacent, then the circle at B on $B \mathrel{\circ\!\!-\!\!*} C$ should have been oriented by $\mathcal{R}7$.

Suppose, more specifically, that $A \mathrel{-\!\!\circ} B \mathrel{\circ\!\!-\!\!\circ} C$. Consider the edge between A and C. **P**1 (Lemma A.1) implies that it is not into C. **P**2 (Lemma A.2) implies that it is not into A. It is not undirected either, for otherwise the circle at C on $B \mathrel{\circ\!\!-\!\!\circ} C$ could be oriented by $\mathcal{R}6$. Hence it is either (1) $A \mathrel{\circ\!\!-} C$; or (2) $A \mathrel{\circ\!\!-\!\!\circ} C$; or (3) $A \mathrel{-\!\!\circ} C$. We now show that (1) and (2) are impossible.

Suppose for contradiction that (1) or (2) is the case. By (i) in Lemma A.3, there is an uncovered tail-circle path p from E, an endpoint of an undirected edge, to B that includes the edge $A \mathrel{-\!\!\circ} B$. We claim that for every vertex V on p, either $V \mathrel{\circ\!\!-\!\!\circ} C$ or $V \mathrel{\circ\!\!-} C$ is present. The argument goes by induction. Obviously B and A satisfy the claim. Suppose, starting from

B, the nth vertex on p, V_n, satisfies the claim. Consider the $n+1$st vertex on p, V_{n+1}. Since p is a tail-circle path, we have $V_{n+1} -\!\circ V_n$. By the inductive hypothesis, $V_n \circ\!\!-\!\!\circ C$ or $V_n \circ\!- C$. So, as already established, V_{n+1} and C must be adjacent. Again, $\mathcal{P}1$ implies that the edge between them is not into C. $\mathcal{P}2$ implies that the edge between them is not into V_{n+1}. The edge is not undirected either, for otherwise the circle at C on $B \circ\!\!-\!\!\circ C$ could be oriented by $\mathcal{R}6$. Furthermore, by (ii) in Lemma A.3, V_{n+1} and B are not adjacent. So the edge between V_{n+1} and C can't be $V_{n+1} -\!\circ C$, for otherwise the circle at C on $C \circ\!\!-\!\!\circ B$ could be oriented by $\mathcal{R}7$. It follows that either $V_{n+1} \circ\!\!-\!\!\circ C$ or $V_{n+1} \circ\!- C$. Therefore, every vertex on p, in particular the endpoint E, satisfies the claim. So either $E \circ\!\!-\!\!\circ C$ or $E \circ\!- C$ occurs. But E is an endpoint of an undirected edge, and hence the circle at E on $E \circ\!\!-\!\!\circ C$ or $E \circ\!- C$ could be oriented. Contradiction.

Hence neither (1) nor (2) is the case, which means $A -\!\circ C$ occurs in $\mathcal{P}_{AFCI}$.

On the other hand, if it is $A -\!\circ B \circ\!\!\rightarrow C$ that occurs in $\mathcal{P}_{AFCI}$, then **P**2 implies that the edge between A and C is not into A (due to the presence of $A -\!\circ B$). It follows that the edge mark at C is not a tail, for otherwise either $\mathcal{P}_{AFCI}$ would not be sound (with an arrowhead incident to an undirected edge) or **P**2 would be violated (with an arrowhead incident to a $-\!\circ$ edge). Note moreover that the edge mark at C cannot be a circle, for otherwise **P**1 would be violated. Hence the edge mark at C is an arrowhead, and the edge is either $A \rightarrow C$ or $A \circ\!\!\rightarrow C$. □

Lemma A.5. *In $\mathcal{P}_{AFCI}$, the following property holds*:

P4 *For any $A -\!\circ B$, there is no tail-circle path from B to A. That is, there is no such cycle as $A -\!\circ B -\!\circ C -\!\circ \cdots -\!\circ A$.*

Proof. We first argue that if there is any such cycle in $\mathcal{P}_{AFCI}$, then there is a cycle with only three edges, i.e., $A -\!\circ B -\!\circ C -\!\circ A$. To show this, note that for any such cycle $c = \langle V_0, V_1, V_2, \dots, V_n, V_0\rangle$ with more than three edges, c can't be uncovered, otherwise every edge on c would have been oriented as $-$ by $\mathcal{R}5$. That means there is a consecutive triple on c which is shielded. Without loss of generality, suppose $\langle V_0, V_1, V_2\rangle$ is shielded, i.e., V_0 and V_2 are adjacent. The edge between V_0 and V_2 can't contain an arrowhead, as Lemma A.2 shows; it can't be undirected, for otherwise some circle on c should been oriented by $\mathcal{R}6$; it can't be $\circ\!\!-\!\!\circ$, as implied by Lemma A.4 (because $V_0 -\!\circ V_1 -\!\circ V_2$ is present). So it is either $V_0 -\!\circ V_2$ or $V_2 -\!\circ V_0$. In either case, there is a shorter cycle than c that consists of $-\!\circ$ edges. Hence we have established that for any such cycle with more than three edges, there is a shorter one. It follows that if there is such a cycle at all, there must be one with only three edges.

So, to prove **P**4, it suffices to show that $A -\!\circ B -\!\circ C -\!\circ A$ is impossible. Suppose for contradiction that $A -\!\circ B -\!\circ C -\!\circ A$ appears in $\mathcal{P}_{AFCI}$. By (i) in Lemma A.3, there is an uncovered tail-circle path p from E, an endpoint of an undirected edge, to B that includes the edge $A -\!\circ B$. We claim that for every vertex V on p between A and E (including A and E), $C -\!\circ V$ is present in $\mathcal{P}_{AFCI}$. The argument is by induction. The vertex A, by supposition, satisfies the claim. Suppose, starting from A, the nth vertex on p, V_n, satisfies the claim. Consider the $n+1$st vertex on p, V_{n+1}. Since p is a tail-circle path, we have $V_{n+1} -\!\circ V_n$. By the inductive hypothesis, $C -\!\circ V_n$. So by Lemma A.4, V_{n+1} and C are adjacent. Lemma A.2 implies that the edge between them is not into either vertex. The edge is not undirected either, for otherwise the circle at C on $B -\!\circ C$ could be oriented by $\mathcal{R}6$. Furthermore, by (ii) in Lemma A.3, V_{n+1} and B are not adjacent. Since $B -\!\circ C$, the edge between V_{n+1} and C must be oriented as $C -\!\circ V_{n+1}$. Therefore, every vertex between A and E, in particular the endpoint E, satisfies the claim. But E is an endpoint of an undirected edge, and hence the circle at E on $C -\!\circ E$ could be oriented. This is a contradiction. □

With **P**1–**P**4, we are ready to prove Lemma 4.1 and Theorem 2.

Lemma 4.1. *For every edge $A \circ\!\!-\!\!\circ B$ in $\mathcal{P}^C_{AFCI}$, $\mathcal{P}^C_{AFCI}$ can be oriented into a DAG with no unshielded colliders in which $A \rightarrow B$ appears, and can be oriented into a DAG with no unshielded colliders in which $A \leftarrow B$ appears.*

Proof. Given Lemma 5 in [17]—which showed that all chordal undirected graphs have the desired property—it suffices to show that $\mathcal{P}^C_{AFCI}$ is chordal. Suppose for the sake of contradiction that there is a chordless cycle with four edges or more in $\mathcal{P}^C_{AFCI}$. Let $\langle V_0, V_1, V_2, V_3, \dots, V_0\rangle$ be a shortest such cycle, which implies that no two non-consecutive vertices on the cycle are adjacent in $\mathcal{P}^C_{AFCI}$. For every such pair of non-consecutive vertices V_i and V_j, they are not adjacent in $\mathcal{P}_{AFCI}$ either. The reason is that V_i and V_j are connected by a circle path in $\mathcal{P}_{AFCI}$, given which it is easy to derive from **P**1 and **P**3 that if V_i and V_j are adjacent in $\mathcal{P}_{AFCI}$, the edge between them must be $\circ\!\!-\!\!\circ$, and hence they would be adjacent in $\mathcal{P}^C_{AFCI}$. Therefore, the cycle remains a shortest chordless cycle consisting of $\circ\!\!-\!\!\circ$ edges in $\mathcal{P}_{AFCI}$, which should have been oriented by $\mathcal{R}5$. A contradiction. □

Theorem 2. *Let $\mathcal{H}$ be the graph resulting from the following procedure applied to $\mathcal{P}_{AFCI}$*:

(1) *orient the circles on $\circ\!\!\rightarrow$ edges in $\mathcal{P}_{AFCI}$ as tails, and orient the circles on $-\!\circ$ edges in $\mathcal{P}_{AFCI}$ as arrowheads* (*that is, turn all $\circ\!\!\rightarrow$ edges and all $-\!\circ$ edges into directed edges $\rightarrow$*); *and*
(2) *orient $\mathcal{P}^C_{AFCI}$ into a DAG with no unshielded colliders.*

Then $\mathcal{H}$ is a member of $[\mathcal{G}_T]$.

Proof. For interest of space, we will not give all the details, which are easy to construct given the sketch here. (Most details are also extremely similar to the proof of Theorem 4.2 in [2].) **P**2 and **P**4 together ensure that turning all circles on $-\!\!\circ$ edges into arrowheads will not create any directed cycle or almost directed cycle. **P**1 and **P**3 ensure that further turning all circles on $\circ\!\!\rightarrow$ edges into tails will not create any directed cycle or almost directed cycle. So after operation 1, no directed cycle or almost directed cycle is created.

For operation 2, **P**1 and **P**3 guarantee that no matter how we orient a $\circ\!\!-\!\!\circ$ edge, it will not yield a directed cycle or almost directed cycle that involves an edge outside $\mathcal{P}^C_{AFCI}$. So if $\mathcal{P}^C_{AFCI}$ is oriented into a DAG, no directed cycle or almost directed cycle will be created in $\mathcal{H}$.

Furthermore, no new undirected edges or bi-directed edges are created in constructing $\mathcal{H}$, and hence every undirected edge and bi-directed edge in $\mathcal{H}$ are already in $\mathcal{P}_{AFCI}$. It is then easy to show, given the soundness of $\mathcal{P}_{AFCI}$, that in $\mathcal{H}$ there is no edge into any vertex incident to an undirected edge, and that there is no inducing path between any two non-adjacent vertices. Therefore $\mathcal{H}$ is both ancestral and maximal.

To show Markov equivalence between $\mathcal{H}$ and $\mathcal{G}_T$, we just need to check that the conditions in Proposition 2 are satisfied. They have the same adjacencies given the correctness of the adjacency inference step in the FCI algorithm. **P**2 and **P**3 ensure that turning all circles on $-\!\!\circ$ edges in $\mathcal{P}_{AFCI}$ into arrowheads will not create any new unshielded collider. **P**1 implies that no matter how we orient a $\circ\!\!-\!\!\circ$ edge, it will not create a new unshielded collider that involves an edge outside $\mathcal{P}^C_{AFCI}$. So if $\mathcal{P}^C_{AFCI}$ is oriented into a DAG with no unshielded colliders, no more unshielded colliders than those already in $\mathcal{P}_{AFCI}$ are constructed in $\mathcal{H}$. So $\mathcal{H}$ and $\mathcal{G}_T$ have the same unshielded colliders. Finally, since no new bi-directed edges are created in constructing $\mathcal{H}$, it is not hard to verify condition (e3) in Proposition 2 concerning discriminating paths. It then follows that $\mathcal{H}$ is a member of $[\mathcal{G}_T]$. $\square$

Appendix B. Proof of Lemma 4.2 and Theorem 3

The proof of Lemma 4.2 is the most difficult part of our argument, and requires quite a few utility lemmas. Again, for interest of space, we will often note and skip easy or similar steps. We begin by noting some facts about (uncovered) p.d. paths (Definition 10) in $\mathcal{P}_{AFCI}$.

Lemma B.1. *If $p = \langle A, \ldots, B\rangle$ is a p.d. path from A to B in $\mathcal{P}_{AFCI}$, then some subsequence of p forms an uncovered p.d. path from A to B in $\mathcal{P}_{AFCI}$.*

Proof. The proof is by induction on the length of p. If there is only one edge on p, then it is trivially a (degenerate) uncovered p.d. path from A to B. If there are two edges on p, namely $p = \langle A, C, B\rangle$, either it is already uncovered, or it is covered so that A and B are adjacent. In the latter case, we show that the edge between A and B is not into A or out of B, and hence it constitutes a desired path between A and B.

We first argue that it is not into A. Suppose for contradiction that the mark at A on the edge between A and B is an arrowhead. Then the edge between A and C can't have a circle mark at A, for otherwise by **P**1 (Lemma A.1), the edge between C and B has an arrowhead at C, which contradicts the fact that p is potentially directed. It follows that the edge between A and C must have a tail at A in $\mathcal{P}_{AFCI}$. Since the edge between A and B is into A, it follows from **P**2 (Lemma A.2) that the edge between A and C is $A \to C$. Then the mark at C on the edge between C and B must be an arrowhead, as implied by $\mathcal{R}2$, a contradiction. So the edge between A and B is not into A.

Next we show that it is not out of B either. Suppose for contradiction that the mark at B on the edge between A and B is a tail. Then it is either $A - B$ or $A \circ\!\!- B$. The former implies that the edge between C and B has a tail at B by $\mathcal{R}6$, which contradicts the fact that p is potentially directed. So it can only be $A \circ\!\!- B$. Then **P**2 implies that there is no arrowhead into B. Since p is potentially directed, the edge between C and B is not out of B. Hence the mark at B on the edge between C and B is a circle. It is then easy to check that the only possible configurations consistent with **P**1, **P**2, and the fact that p is potentially directed are $A \circ\!\!-\!\!\circ C \circ\!\!-\!\!\circ B$, or $A \circ\!\!-\!\!\circ C -\!\!\circ B$, or $A -\!\!\circ C \circ\!\!-\!\!\circ B$ or $A -\!\!\circ C -\!\!\circ B$. The first three cases contradict **P**3 (Lemma A.4), and the last case contradicts **P**4 (Lemma A.5).

The inductive step is easy. Suppose the proposition holds when the length of p is $n-1$ ($n \geqslant 3$). Consider the case where p has n edges. Either p is already uncovered, or there is a triple $\langle X, Y, Z\rangle$ on the path which is shielded. In the latter case, by the foregoing argument, the edge between X and Z is not into X or out of Z. So if we replace $\langle X, Y, Z\rangle$ with the edge between X and Z on p, we get a subsequence of p which is a p.d. path from A to B with length $n-1$. By the inductive hypothesis, a subsequence of the new path, which is also a subsequence of p, forms an uncovered p.d. path from A to B. $\square$

Lemma B.2. *If p is an uncovered p.d. path from A to B in $\mathcal{P}_{AFCI}$, then*

(i) *if there is an $\circ\!\!\rightarrow$ or $-\!\!\circ$ edge on p, then any $\circ\!\!-\!\!\circ$ edge on p is before that edge, and any $\to$ edge on p is after that edge;*
(ii) *p does not include both a $\circ\!\!\rightarrow$ edge and a $-\!\!\circ$ edge; and*
(iii) *there is at most one $\circ\!\!\rightarrow$ edge on p.*

Proof. To see (i) is true, notice that since p is uncovered and potentially directed, any edge after a $\circ\!\!\rightarrow$ edge or a $\to$ edge on p must be oriented as $\to$ by $\mathcal{R}1$. So no $\circ\!\!-\!\!\circ$ can appear after a $\circ\!\!\rightarrow$ edge on p, and no $\to$ can appear before a $\circ\!\!\rightarrow$ edge on p. The same is true with a $-\!\!\circ$ edge. Since p is uncovered, any edge on p after $-\!\!\circ$ will be oriented as $-\!\!\circ$ or $\to$ by either $\mathcal{R}7$ or $\mathcal{R}1$.

(ii) and (iii) are evident given the argument for (i). For (iii), just note that any edge after a $\circ\!\!\to$ edge on p must be oriented as a $\to$ edge. For (ii), suppose for contradiction that p contains both a $\circ\!\!\to$ edge and a $-\!\!\circ$ edge. Then the $-\!\!\circ$ edge does not appear after the $\circ\!\!\to$ edge on p, because any edge after $\circ\!\!\to$ on p must be oriented as $\to$ by $\mathcal{R}1$. On the other hand, the $\circ\!\!\to$ does not appear after the $-\!\!\circ$ edge on p, because any edge after $-\!\!\circ$ on p is either $-\!\!\circ$ or $\to$. This is a contradiction. □

Lemma B.3. *In $\mathcal{P}_{AFCI}$, if there is a circle path—a path consisting of $\circ\!\!-\!\!\circ$ edges—between A and B, then for any other vertex C, $C{*\!\!\to}A$ if and only if $C{*\!\!\to}B$.*

Proof. This easily follows from **P**1. □

Lemma B.4. *In $\mathcal{P}_{AFCI}$, if there is a p.d. path from A to B, then the edge between A and B, if any, is not into A.*

Proof. By Lemma B.1, there is an uncovered p.d. path p from A to B. Suppose for contradiction that there is an edge between A and B which is into A, namely $A{\leftarrow\!\!*}B$. There can not be a $-\!\!\circ$ edge on p for the following reason: the first $-\!\!\circ$ edge, if any, is either incident to A or is connected to A by a circle path, according to Lemma B.2. In either case, by Lemma B.3, there is an edge into the tail endpoint of the $-\!\!\circ$ edge, which contradicts **P**2 (Lemma A.2).

So, by Lemma B.2, p is of the form: $A\circ\!\!-\!\!\circ\cdots\circ\!\!-\!\!\circ X\circ\!\!\to Y\to\cdots\to B$, where it could be that $A=X$ (there is no $\circ\!\!-\!\!\circ$ edge) and/or $X=Y$ (there is no $\circ\!\!\to$ edge) and/or $Y=B$ (there is no directed edge). If $Y=B$, it is easy to see that **P**1 is violated due to the supposed presence of $A{\leftarrow\!\!*}B$. If $Y\neq B$, then **P**1 and the supposed presence of $A{\leftarrow\!\!*}B$ entail that there is an edge between B and Y that is into Y. But Y is an ancestor of B. This contradicts the soundness of $\mathcal{P}_{AFCI}$. Hence the initial supposition of $A{\leftarrow\!\!*}B$ is false. □

Lemma B.5. *In $\mathcal{P}_{AFCI}$, if there is a p.d. path from A to B that is into B, then every uncovered p.d. path from A to B is into B.*

Proof. Suppose for contradiction that there is an uncovered p.d. path from A to B not into B. Then the last edge on the path must be $\circ\!\!-\!\!\circ$. (It is not $-\!\!\circ$ in light of **P**2, because there is a p.d. path into B.) It then follows from Lemma B.2 that the path is a circle path. Let C be the vertex adjacent to B on the p.d. path into B, so $C{*\!\!\to}B$. It follows from Lemma B.3 that $C{*\!\!\to}A$. But there is a p.d. path from A to C, which contradicts Lemma B.4. □

Corollary B.6. *In $\mathcal{P}_{AFCI}$, if A, B are adjacent, and there is a p.d. path from A to B that is into B, then the edge between A and B is either $A\circ\!\!\to B$ or $A\to B$.*

Proof. This easily follows from Lemmas B.4, B.5, and A.2. □

Lemma B.7. *If there is a circle path between two adjacent vertices in $\mathcal{P}_{AFCI}$, then the edge between the two vertices is $\circ\!\!-\!\!\circ$.*

Proof. This is very easy to see given **P**1 (or Lemma B.3) and **P**3. □

Lemma B.8. *Let u be an uncovered circle path in $\mathcal{P}_{AFCI}$. If A and B are two non-consecutive vertices on u, then A and B are not adjacent in $\mathcal{P}_{AFCI}$.*

Proof. It follows from Lemma B.7 and the fact that $\mathcal{P}^C_{AFCI}$ is chordal. □

The next two lemmas are useful facts about edges in **REL**($J\circ\!\!\to K$) (Definition 11).

Lemma B.9. *For every $A\circ\!\!\to B\in$ **REL**($J\circ\!\!\to K$), there is an uncovered p.d. path u from J to B in $\mathcal{P}_{AFCI}$ such that for every vertex V on u other than B, there is an edge $V\circ\!\!\to K$.*

Proof. The lemma holds trivially if $A=J$ or $B=K$. Suppose $A\neq J$ and $B\neq K$. By Definition 11, there is a p.d. path from J to A in $\mathcal{P}_{AFCI}$ such that no vertex on the path (including the endpoints) is a parent of K. Note that B is not on this p.d. path, for otherwise there would be a p.d. path from B to A, which, together with the presence of $A\circ\!\!\to B$, would contradict Lemma B.4. So we can concatenate the p.d. path with $A\circ\!\!\to B$ to form a p.d. path from J to B that is into B. In light of Lemma B.1, it follows that there is an uncovered p.d. path u from J to B such that every vertex on u other than B is not a parent of K. We can then prove by induction that for every vertex V on u other than B, there is an edge $V\circ\!\!\to K$ in $\mathcal{P}_{AFCI}$.

The base case $J\circ\!\!\to K$ is obvious. Suppose it holds of the nth vertex on u, V_n. Consider $V_{n+1}\neq B$. Since $B\neq K$, by Definition 11, B is a parent of K. This implies that there is a p.d. path from V_{n+1} to K. By Corollary B.6, if V_{n+1} and K are adjacent, then the edge is either $V_{n+1} \to K$ or $V_{n+1} \circ\!\!\rightarrow K$. But no vertex on u other than B is a parent of K, so it suffices to show that V_{n+1} is adjacent to K. Suppose otherwise. It is then easy to show that the circle at V_n on $V_n \circ\!\!\rightarrow K$ could have been oriented by $\mathcal{R}9$, which is a contradiction. Therefore V_{n+1} and K are adjacent, and the edge is $V_{n+1} \circ\!\!\rightarrow K$ in $\mathcal{P}_{AFCI}$. □

Lemma B.10. *If $A \circ\!\!\rightarrow B \in \mathbf{REL}(J \circ\!\!\rightarrow K)$, then $A \circ\!\!\rightarrow K$ appears in $\mathcal{P}_{AFCI}$.*

Proof. The lemma trivially holds if $A = J$ or $B = K$. Suppose $A \neq J$ and $B \neq K$. Since $A \circ\!\!\rightarrow B \in \mathbf{REL}(J \circ\!\!\rightarrow K)$, there is an uncovered p.d. path u from J to B satisfying the condition of Lemma B.9. By Lemma B.5, we know u is also into B. Let $X {*\!\!\rightarrow} B$ be the last edge on u. By Lemma B.9, we have $X \circ\!\!\rightarrow K$ in $\mathcal{P}_{AFCI}$. Also, because $B \neq K$, $B \to K$ is in $\mathcal{P}_{AFCI}$, so the edge between X and B can't be $X \to B$, for otherwise $X \circ\!\!\rightarrow K$ could be oriented by $\mathcal{R}8$. It follows that the edge is $X \circ\!\!\rightarrow B$ in $\mathcal{P}_{AFCI}$.

Note that if A and K are not adjacent, then the path $\langle A, B, X, K\rangle$ is a discriminating path for X (Definition 7). Hence the circle on $X \circ\!\!\rightarrow K$ could have been oriented by $\mathcal{R}4$, a contradiction. So A is adjacent to K. By Corollary B.6, the edge between A and K is either $A \to K$ or $A \circ\!\!\rightarrow K$. But by Definition 11, A is not a parent of K, so it must be $A \circ\!\!\rightarrow K$ in $\mathcal{P}_{AFCI}$. □

Our goal is to show that in the course of the *Orientation Algorithm*, no violation of $\mathbf{C_1}$–$\mathbf{C_3}$ (Definition 12) would occur. The next block of lemmas are important steps towards this goal. They amount to showing that if we choose a $\circ\!\!-\!\!\circ$ edge to orient away from violation of $\mathbf{C_1}$–$\mathbf{C_3}$ (as the *Orientation Algorithm* does), that orientation will not trigger any violation of $\mathbf{C_1}$–$\mathbf{C_3}$ by applications of $\mathbf{UR}_1$ alone.

Lemma B.11. *For any two vertices $B, C \in \mathbf{AR}(J \circ\!\!\rightarrow K)$, there is no uncovered circle path between B and C consisting of more than one edge in $\mathcal{P}_{AFCI}$.*

Proof. Given Lemma B.8, it suffices to show that B and C are adjacent. This is obviously true if one of B and C is K. Suppose $B \neq K$ and $C \neq K$, and hence both of them are parents of K by Definition 11. Let A be such a vertex that $A \circ\!\!\rightarrow B \in \mathbf{REL}(J \circ\!\!\rightarrow K)$. It follows from Lemma B.3 that either $A \circ\!\!\rightarrow C$ or $A \to C$ is in $\mathcal{P}_{AFCI}$. But it can't be $A \to C$ for otherwise $A \circ\!\!\rightarrow K$ (shown to be present in Lemma B.10) could be oriented by $\mathcal{R}8$. So it is $A \circ\!\!\rightarrow C$. Then B and C must be adjacent, for otherwise $A \circ\!\!\rightarrow K$ could be oriented by $\mathcal{R}10$. □

Lemma B.12. *Suppose $A \circ\!\!\rightarrow B \in \mathbf{REL}(J \circ\!\!\rightarrow K)$. If $A \circ\!\!-\!\!\circ C$ appears in $\mathcal{P}_{AFCI}$ and C is a parent of B in $\mathcal{P}_{AFCI}$ (i.e. the edge $A \circ\!\!-\!\!\circ C$ is required by condition $\mathbf{C_2}$ to be oriented as $A \leftarrow C$), then C is a parent of K in $\mathcal{P}_{AFCI}$.*

Proof. If $B = K$, it is trivial. Suppose $B \neq K$, and so B is a parent of K. By Lemma B.10, $A \circ\!\!\rightarrow K$ is present in $\mathcal{P}_{AFCI}$. It follows that C is adjacent to K, for otherwise $\langle C, B, A, K\rangle$ would constitute a discriminating path for A in $\mathcal{P}_{AFCI}$ to orient $A \circ\!\!\rightarrow K$ by $\mathcal{R}4$. Furthermore, the edge between C and K must be $C \to K$, as required by $\mathcal{R}2$ and $\mathcal{R}8$. Hence C is a parent of K. □

Lemma B.13. *Suppose $A \circ\!\!\rightarrow B \in \mathbf{REL}(J \circ\!\!\rightarrow K)$, $A \circ\!\!-\!\!\circ C$ and C is a parent of B in $\mathcal{P}_{AFCI}$ (i.e. the edge $A \circ\!\!-\!\!\circ C$ is required by condition $\mathbf{C_2}$ to be oriented as $A \leftarrow C$). Then*

(1) *if for some $D \in \mathbf{AR}(J \circ\!\!\rightarrow K)$, $C \circ\!\!-\!\!\circ D$ is in $\mathcal{P}_{AFCI}$, then $C \in \mathbf{AR}(J \circ\!\!\rightarrow K)$ (so that the edge $C \circ\!\!-\!\!\circ D$ is not subject to $\mathbf{C_1}$);*
(2) *If $u = \langle C, A, \ldots\rangle$ is an uncovered circle path, no vertex on u except possibly C is in $\mathbf{AR}(J \circ\!\!\rightarrow K)$.*

Proof. To show (1), note that if $D \in \mathbf{AR}(J \circ\!\!\rightarrow K)$, then there is some vertex X such that $X \circ\!\!\rightarrow D \in \mathbf{REL}(J \circ\!\!\rightarrow K)$. By **P**1 (Lemma A.1), $X \circ\!\!\rightarrow C$ or $X \to C$ is in $\mathcal{P}_{AFCI}$. By Lemma B.12, C is a parent of K. So it is not $X \to C$ in $\mathcal{P}_{AFCI}$, otherwise $X \circ\!\!\rightarrow K$, which is shown to be present by Lemma B.10, could be oriented as $X \to K$ by $\mathcal{R}8$. So it must be $X \circ\!\!\rightarrow C$ in $\mathcal{P}_{AFCI}$. Since $X \circ\!\!\rightarrow D \in \mathbf{REL}(J \circ\!\!\rightarrow K)$ and C is a parent of K, $X \circ\!\!\rightarrow C$ satisfies Definition 11, which means $C \in \mathbf{AR}(J \circ\!\!\rightarrow K)$.

To prove (2), suppose for contradiction that some vertex $E \neq C$ on u is in $\mathbf{AR}(J \circ\!\!\rightarrow K)$. Obviously $E \neq K$, otherwise $A \circ\!\!\rightarrow E$ would be present in $\mathcal{P}_{AFCI}$ by Lemma B.10, which contradicts Lemma B.3. So E is a parent of K. Now consider the edge $A \circ\!\!\rightarrow K$, shown to exist by Lemma B.10. $A \circ\!\!-\!\!\circ C$ is an uncovered p.d. path from A to C, a parent of K by Lemma B.12; $u(A, E)$ is an uncovered p.d. path from A to E, a parent of K. Since u is uncovered, $A \circ\!\!\rightarrow K$ could be oriented as $A \to K$ by $\mathcal{R}10$; a contradiction. □

Lemma B.14. *For every uncovered circle path $u = \langle A, \ldots, E\rangle$ in $\mathcal{P}_{AFCI}$, either the edge incident to A is not required by $\mathbf{C_2}$ to be oriented out of A, or the edge incident to E is not required by $\mathbf{C_2}$ to be oriented out of E.*

Proof. Suppose for contradiction that the contrary is true. By Lemma B.12, both A and E are parents of K. Let B be the vertex adjacent to A on u. By supposition and Definition 12, there is a vertex C such that $B \circ\!\!\rightarrow C \in \mathbf{REL}(J \circ\!\!\rightarrow K)$ (and A is a parent of C). Consider $B \circ\!\!\rightarrow K$ (cf. Lemma B.10). $B \circ\!\!-\!\!\circ A$ constitutes an uncovered p.d. path from B to A, a parent of K; $u(B, E)$ constitutes an uncovered p.d. path from B to E, a parent of K. A and E are not adjacent by Lemma B.8. Thus $B \circ\!\!\rightarrow K$ could be oriented as $B \to K$ by $\mathcal{R}10$; a contradiction. □

Lemma B.15. *If $A \circ\!\!\rightarrow B \in \mathbf{REL}(J \circ\!\!\rightarrow K)$, and $u = \langle A, C, \ldots \rangle$ is an uncovered circle path such that C is not adjacent to B in $\mathcal{P}_{AFCI}$ (so that the edge between A and C is required by $\mathbf{C_3}$ to be oriented as $A \to C$), then no vertex on u is a parent of K in $\mathcal{P}_{AFCI}$.*

Proof. Since $A \circ\!\!\rightarrow B \in \mathbf{REL}(J \circ\!\!\rightarrow K)$, by Lemma B.10, $A \circ\!\!\rightarrow K$ is present in $\mathcal{P}_{AFCI}$. Suppose for contradiction that a vertex D (which could be C) on u is a parent of K. We consider the two possible cases one by one.

Case 1: $B = K$, and hence K and C are not adjacent (which means D can't be C in this case). So $u(A, D) \oplus D \to K$ is a p.d. path from A to K such that the vertex adjacent to A on the path, namely C, is not adjacent to K. Let E be the first vertex after C on the path which is adjacent to K (there must be one, because D is adjacent to K). The edge between E and K, by Corollary B.6, is either $E \circ\!\!\rightarrow K$ or $E \to K$. It follows that $\langle A, C, \ldots, E, K \rangle$ forms an uncovered p.d. path from A to K such that C and K are not adjacent. Hence $A \circ\!\!\rightarrow K$ could be oriented as $A \to K$ by $\mathcal{R}9$; a contradiction.

Case 2: $B \to K$ is in $\mathcal{P}_{AFCI}$. Then $u(A, D)$ is an uncovered p.d. path from A to D, a parent of K, and $A \circ\!\!\rightarrow B$ is an uncovered p.d. path from A to B, a parent of K. Since C and B are not adjacent, the edge $A \circ\!\!\rightarrow K$ could be oriented as $A \to K$ by $\mathcal{R}10$; a contradiction. □

Lemma B.16. *Suppose $A \circ\!\!\rightarrow B, C \circ\!\!\rightarrow D \in \mathbf{REL}(J \circ\!\!\rightarrow K)$, $A \neq C$ and $u = \langle A, \ldots, C \rangle$ is an uncovered circle path in $\mathcal{P}_{AFCI}$. Either the vertex next to A on u is adjacent to B (so that $\mathbf{C_3}$ does* not *require orienting the edge out of A), or the vertex next to C on u is adjacent to D (so that $\mathbf{C_3}$ does* not *require orienting the edge out of C).*

Proof. Suppose for contradiction that the contrary is true. We consider three cases separately and derive a contradiction in each.

Case 1: $B = D$. In this case, since D is not adjacent to the vertex next to C on u, $u \oplus C \circ\!\!\rightarrow B$ is an uncovered p.d. path from A to B such that the vertex adjacent to A on the path is not adjacent to B. Hence $A \circ\!\!\rightarrow B$ could be oriented by $\mathcal{R}9$ as $A \to B$, a contradiction.

Case 2: $B \neq D$ and one of them is K. Without loss of generality, suppose $B = K$. Since $C \circ\!\!\rightarrow D \in \mathbf{REL}(J \circ\!\!\rightarrow K)$, and $D \neq K$, by Definition 11, D is a parent of K (B). Then $u \oplus C \circ\!\!\rightarrow D$ constitutes an uncovered p.d. path from A to D such that the vertex adjacent to A on the path is not adjacent to B. This is the same situation as *Case 1* in the proof of Lemma B.15, which leads to a contradiction.

Case 3: $B \neq D$ and neither of them is K. So both B and D are parents of K. Consider the edge $A \circ\!\!\rightarrow K$, which is shown to be present by Lemma B.10. Since $A \circ\!\!\rightarrow B$ is an uncovered p.d. path from A to B, a parent of K, $u \oplus C \circ\!\!\rightarrow D$ is an uncovered p.d. path from A to D, a parent of K, and that the vertex next to A on u is not adjacent to B, the edge $A \circ\!\!\rightarrow K$ could be oriented as $A \to K$ by $\mathcal{R}10$, a contradiction. □

Now it is time for our key lemma:

Lemma 4.2. *Let $\mathcal{D}_{J \circ\!\rightarrow K}$ be the DAG output of the* **Orientation Algorithm**. *$\mathcal{D}_{J \circ\!\rightarrow K}$ is a DAG orientation of $\mathcal{P}^C_{AFCI}$ free of unshielded colliders and agreeable to $J \circ\!\!\rightarrow K$.*

Proof. As noted in the main text, the correctness of Meek's algorithm [17] guarantees that $\mathcal{D}_{J \circ\!\rightarrow K}$ is a DAG free of unshielded colliders. We need to show that it is also agreeable (Definition 12). In other words, we need to show that no violation of $\mathbf{C_1}$–$\mathbf{C_3}$ occurs in $\mathcal{D}_{J \circ\!\rightarrow K}$. Below we give the details of our argument regarding $\mathbf{C_1}$. The argument regarding $\mathbf{C_2}$ and that regarding $\mathbf{C_3}$ are extremely parallel, of which we omit details.

Note that if any violation were to occur, it could only occur by the end of the third stage of the *Orientation Algorithm*, before all $\circ\!\!-\!\!\circ$ edges in $\mathbf{E_1} \cup \mathbf{E_2} \cup \mathbf{E_3}$ get oriented. So it suffices to show that by that stage, no violation of $\mathbf{C_1}$ occurs. In fact, we can prove something stronger. We show that for every vertex $W \in \mathbf{AR}(J \circ\!\!\rightarrow K)$, there is no $\circ\!\!-\!\!\circ$ edge that gets oriented as *into* W by the end of the third stage. Suppose for sake of contradiction that such an orientation occurs. Let the first occurrence be $A \circ\!\!-\!\!\circ B$ being oriented as $A \to B$, where $B \in \mathbf{AR}(J \circ\!\!\rightarrow K)$. We consider all the possible ways in which this orientation could occur and derive a contradiction in each. (We assume, without loss of generality, that $\mathbf{UR}_1$ has priority over $\mathbf{UR}_2$ and $\mathbf{UR}_3$.)

Case 1: $A \circ\!\!-\!\!\circ B$ is oriented as $A \to B$ to satisfy one of $\mathbf{C_1}$–$\mathbf{C_3}$. Since $B \in \mathbf{AR}(J \circ\!\!\rightarrow K)$, $\mathbf{C_1}$ does not dictate this orientation. Neither does $\mathbf{C_2}$, as entailed by (2) in Lemma B.13. So it is due to $\mathbf{C_3}$, which means there is a vertex E such that $A \circ\!\!\rightarrow E \in \mathbf{REL}(J \circ\!\!\rightarrow K)$ and E, B are not adjacent. Then Lemma B.15 implies that B is not a parent of K. Furthermore, by Lemma B.10, $A \circ\!\!\rightarrow K$ is present in $\mathcal{P}_{AFCI}$, which implies that $B \neq K$ (because of $A \circ\!\!-\!\!\circ B$). It follows that $B \notin \mathbf{AR}(J \circ\!\!\rightarrow K)$; a contradiction.

Case 2: $A \circ\!\!-\!\!\circ B$ is oriented as $A \to B$ by an application of $\mathbf{UR}_2$.[22] That is, there is a vertex C such that $A \circ\!\!-\!\!\circ C \circ\!\!-\!\!\circ B$ is in $\mathcal{P}^C_{AFCI}$, and is oriented as $A \to C \to B$ before $A \circ\!\!-\!\!\circ B$ is oriented. Then $C \circ\!\!-\!\!\circ B$ being oriented as $C \to B$ would be an earlier occurrence of orientation into B. This contradicts our choice of $A \circ\!\!-\!\!\circ B$.

Case 3: $A \circ\!\!-\!\!\circ B$ is oriented as $A \to B$ by an application of $\mathbf{UR}_3$. Again, it is easy to see that this contradicts the assumption that $A \to B$ is the first orientation into B.

[22] The case with $\mathbf{UR}_1$ is more complicated, and will be considered last.

Case 4: $A \circ\!\!-\!\!\circ B$ is oriented as $A \to B$ by an application of $\mathbf{UR}_1$. Generically this is the last (and possibly only) step in a chain of applications of $\mathbf{UR}_1$ to an uncovered circle path, initiated by a directed edge that is *not* oriented by $\mathbf{UR}_1$. Regarding this first initiating edge, there are three subcases to consider:

Case 4.1: the first edge is oriented to satisfy one of $\mathbf{C_1}$–$\mathbf{C_3}$. It can not be due to $\mathbf{C_1}$, for otherwise there would be an uncovered circle path in $\mathcal{P}^C_{AFCI}$ with more than one edge between two vertices in $\mathbf{AR}(J \circ\!\!\rightarrow K)$, which contradicts Lemma B.11. The rest goes exactly like the argument in *Case 1*.

Case 4.2: the first edge is oriented by $\mathbf{UR}_2$. That is, there are three vertices X, Y and Z (Z could be A) such that $X \circ\!\!-\!\!\circ Y \circ\!\!-\!\!\circ Z$ is in $\mathcal{P}^C_{AFCI}$, and is oriented as $X \to Y \to Z$, which in turn orients the edge $X \circ\!\!-\!\!\circ Z$ as $X \to Z$. And $X \to Z$ initiates a chain of $\mathbf{UR}_1$ applications on an uncovered circle path $u = \langle X, Z, \ldots, B\rangle$ that eventually leads to the orientation of $A \to B$. We claim that for every vertex V on u between Z and B (including B), there is an edge between Y and V already oriented as $Y \to V$ before $X \to Z$ is thus oriented. The argument is by induction. For the base case, let V_1 be the first vertex next to Z on u (V_1 is B if Z is A). Y and V_1 must be adjacent in $\mathcal{P}^C_{AFCI}$, for otherwise $Z \circ\!\!-\!\!\circ V_1$ would be oriented as $Z \to V_1$ by $\mathbf{UR}_1$ *before* $X \circ\!\!-\!\!\circ Z$ is oriented by $\mathbf{UR}_2$, according to our convention for the priority of $\mathbf{UR}_1$. Since X and V_1 are not adjacent (because u is uncovered), $Y \circ\!\!-\!\!\circ V_1$ should be oriented as $Y \to V_1$ by $\mathbf{UR}_1$ before $X \to Z$ is thus oriented. The inductive step is extremely similar. Therefore, the claim holds of every vertex V on u between Z and B, including B. In particular, $Y \to B$ is already present before $X \circ\!\!-\!\!\circ Z$ gets oriented, and hence before $A \circ\!\!-\!\!\circ B$ gets oriented. This contradicts our choice of $A \circ\!\!-\!\!\circ B$.

Case 4.3: the first edge is oriented by $\mathbf{UR}_3$. That is, there are four vertices X, Y, Z, W (Z could be A) such that $W \circ\!\!-\!\!\circ Y \circ\!\!-\!\!\circ Z$, $W \circ\!\!-\!\!\circ X \circ\!\!-\!\!\circ Z$, $X \circ\!\!-\!\!\circ Y$ are in $\mathcal{P}^C_{AFCI}$, and that W, Z are not adjacent. Furthermore, $W \circ\!\!-\!\!\circ Y \circ\!\!-\!\!\circ Z$ is oriented as $W \to Y \to Z$, which in turn orients the edge $X \circ\!\!-\!\!\circ Z$ as $X \to Z$. This then initiates a chain of $\mathbf{UR}_1$ applications on an uncovered circle path $u = \langle X, Z, \ldots, B\rangle$ that eventually leads to the orientation of $A \to B$. Notice that W, Z are not adjacent, so $\langle W, X, Z, \ldots, B\rangle$ is also an uncovered circle path in $\mathcal{P}^C_{AFCI}$, which implies that W is not adjacent to any vertex on u between Z and B. Then we can run the exact same argument as in *Case 4.2* to derive a contradiction with our choice of $A \circ\!\!-\!\!\circ B$.

Therefore, there is no occurrence of orienting a $\circ\!\!-\!\!\circ$ edge into W for any $W \in \mathbf{AR}(J \circ\!\!\rightarrow K)$ by the end of the third stage of the Orientation Algorithm. It follows that no violation of $\mathbf{C_1}$ occurs in $\mathcal{D}_{J \circ\!\rightarrow K}$.

The arguments regarding $\mathbf{C_2}$ and $\mathbf{C_3}$ are extremely similar, with different utility lemmas cited.[23] We omit the details to save space and tediousness. □

To prove Theorem 3, we need two more relatively simple facts about $\mathcal{P}_{AFCI}$.

Lemma B.17. *For any $A \circ\!\!\rightarrow B$ in $\mathcal{P}_{AFCI}$, if there is a p.d. path u other than $A \circ\!\!\rightarrow B$ from A to B, then some vertex on u is adjacent to both A and B.*

Proof. The argument is an easy induction on the length of u, with the upshot that if there is no such vertex, $A \circ\!\!\rightarrow B$ could have been oriented by $\mathcal{R}9$. □

Lemma B.18. *Suppose $C \leftarrow\!\!\circ A \circ\!\!\rightarrow B$ is in $\mathcal{P}_{AFCI}$. If C and B are not adjacent, then $A \circ\!\!\rightarrow B \notin \mathbf{REL}(J \circ\!\!\rightarrow K)$ or $A \circ\!\!\rightarrow C \notin \mathbf{REL}(J \circ\!\!\rightarrow K)$.*

Proof. Suppose for contradiction that $A \circ\!\!\rightarrow B \in \mathbf{REL}(J \circ\!\!\rightarrow K)$ and $A \circ\!\!\rightarrow C \in \mathbf{REL}(J \circ\!\!\rightarrow K)$. By Lemma B.10, $A \circ\!\!\rightarrow K$ is in $\mathcal{P}_{AFCI}$. It also follows that $B \neq K$ and $C \neq K$, for otherwise B and C would be adjacent. Then, by Definition 11, both B and C are parents of K, which implies that $A \circ\!\!\rightarrow K$ could be oriented by $\mathcal{R}10$ because C and B are not adjacent; a contradiction. □

Finally we can prove Theorem 3.

Theorem 3. *Let $J \circ\!\!\rightarrow K$ be a $\circ\!\!\rightarrow$ edge in $\mathcal{P}_{AFCI}$. Construct $\mathcal{H}$ from $\mathcal{P}_{AFCI}$ by the following procedure:*

(1) *orient $\circ\!\!\rightarrow$ edges in $\mathbf{REL}(J \circ\!\!\rightarrow K)$ as $\leftrightarrow$, and orient other $\circ\!\!\rightarrow$ edges as $\to$;*
(2) *orient $-\!\!\circ$ edges in $\mathcal{P}_{AFCI}$ as $\to$;*
(3) *orient $\mathcal{P}^C_{AFCI}$ into $\mathcal{D}_{J \circ\!\rightarrow K}$ with the Orientation Algorithm.*

Then $\mathcal{H}$ is a member of $[\mathcal{G}_T]$.

Proof. By Theorem 2, we can construct a member of $[\mathcal{G}_T]$ by turning all $\circ\!\!\rightarrow$ edges and $-\!\!\circ$ edges into directed edges, and orienting $\mathcal{P}^C_{AFCI}$ into $\mathcal{D}_{J \circ\!\rightarrow K}$. Denote this member by $\mathcal{H}_{J \circ\!\rightarrow K}$. It suffices to show that $\mathcal{H}$ is a MAG and Markov equivalent to $\mathcal{H}_{J \circ\!\rightarrow K}$.

[23] The argument for $\mathbf{C_2}$ is almost identical. The one regarding $\mathbf{C_3}$ is slightly more complicated in detail, but has the exact same structure.

Notice that the difference between the two is in regard to edges in **REL**($J\circ\!\!\rightarrow K$)—they correspond to directed edges in $\mathcal{H}_{J\circ\!\rightarrow K}$, but bi-directed edges in $\mathcal{H}$. In what follows, we show that **REL**($J\circ\!\!\rightarrow K$) can be transformed to $\mathcal{H}$ be a series of changes of directed edges into bi-directed edges, one edge at a time, such that each change will preserve MAG-ness and Markov equivalence. Our theorem then follows.

To show this, it suffices to establish the following. Let $\mathcal{M}$ be any MAG identical to $\mathcal{H}_{J\circ\!\rightarrow K}$ except possibly that some $\circ\!\!\rightarrow$ edges in **REL**($J\circ\!\!\rightarrow K$) are oriented as $\leftrightarrow$ (instead of $\rightarrow$) in $\mathcal{M}$. (Note that $\mathcal{H}_{J\circ\!\rightarrow K}$ is such a MAG.) Let

$$\mathbf{DIFF} = \left\{A \rightarrow B \text{ in } \mathcal{M} \mid A\circ\!\!\rightarrow B \text{ is in } \mathcal{P}_{AFCI} \text{ and } A\circ\!\!\rightarrow B \in \mathbf{REL}(J\circ\!\!\rightarrow K)\right\}.$$

We show that if **DIFF** is not empty, then some edge therein can be changed to $\leftrightarrow$ while preserving MAG-ness and Markov equivalence with $\mathcal{M}$. In other words, as long as $\mathcal{M}$ and $\mathcal{H}$ are still different, we can identify a directed edge in $\mathcal{M}$ that corresponds to an edge in **REL**($J\circ\!\!\rightarrow K$), and safely change it into a bi-directed edge so as to decrease the number of differences between $\mathcal{M}$ and $\mathcal{H}$. If it is true, obviously there is a desired transformation from $\mathcal{H}_{J\circ\!\rightarrow K}$ to $\mathcal{H}$.

We now prove it is true. Suppose **DIFF** is not empty. Let $\mathbf{W} = \{B \mid \exists A \ s.t.\ A \rightarrow B \in \mathbf{DIFF}\}$. **W** is also non-empty. Let Y be a member of **W** such that *no proper ancestor of* Y *in* $\mathcal{M}$ *belongs to* **W**. Let X be a vertex such that $X \rightarrow Y \in \mathbf{DIFF}$ and *no proper descendant of* X *in* $\mathcal{M}$ *has this property*. Let $\mathcal{M}^*$ be the graph resulting from changing $X \rightarrow Y$ in $\mathcal{M}$ into $X \leftrightarrow Y$. We show that $\mathcal{M}^*$ is a MAG, and is Markov equivalent to $\mathcal{M}$.

Obviously no directed cycle is created in this change. It does not create an almost directed cycle unless there is a directed path from X to Y in $\mathcal{M}$ other than the edge $X \rightarrow Y$. Suppose for sake of contradiction that there is a directed path from X to Y in $\mathcal{M}$ that does not contain $X \rightarrow Y$. The corresponding path in $\mathcal{P}_{AFCI}$ must be potentially directed. It follows from Lemma B.17 that some vertex Z on the path is adjacent to both X and Y. Since $\mathcal{M}$ is a MAG, we have $X \rightarrow Z \rightarrow Y$ in $\mathcal{M}$, and so the corresponding path $\langle X, Z, Y\rangle$ in $\mathcal{P}_{AFCI}$ is potentially directed. Notice that the edge between Z and Y can't be Z—$\circ Y$ in $\mathcal{P}_{AFCI}$ according to **P**2 (Lemma A.2), because $X\circ\!\!\rightarrow Y$ is present. So, by the definition of p.d. path, the edge between X and Z is either $X\circ\!\!-\!\!\circ Z$ or $X \rightarrow Z$ or $X\circ\!\!\rightarrow Z$ or X—$\circ Z$, and the edge between Z and Y is either $Z\circ\!\!-\!\!\circ Y$ or $Z \rightarrow Y$ or $Z\circ\!\!\rightarrow Y$. But none of the 12 combinations is possible. It would be tedious to go through them one by one. So we will just illustrate the kind of argument we would give by considering whether it is possible for $X\circ\!\!\rightarrow Z\circ\!\!-\!\!\circ Y$ to appear in $\mathcal{P}_{AFCI}$.

Suppose it is possible. Then $Z \notin \mathbf{AR}(J\circ\!\!\rightarrow K)$, for otherwise $X\circ\!\!\rightarrow Z \in \mathbf{REL}(J\circ\!\!\rightarrow K)$, and Z is a proper ancestor of Y in $\mathcal{M}$, which contradicts our choice of Y. However, $Z\circ\!\!-\!\!\circ Y$ is oriented as $Z \rightarrow Y$, which means that $\mathcal{D}_{J\circ\!\rightarrow K}$ is not agreeable to $J\circ\!\!\rightarrow K$ ($\mathbf{C}_1$ being violated). This contradicts Lemma 4.2. The other 11 cases can be similarly or more easily handled, in each of which one can derive a contradiction. So the initial supposition of a directed path from X to Y other than $X \rightarrow Y$ in $\mathcal{M}$ is false, and there is no almost directed cycle in $\mathcal{M}^*$ either.

Moreover, there is no configuration in $\mathcal{M}^*$ that violates (a3) in Definition 1. Suppose the contrary is true. Then the configuration can only be $Z - X \leftrightarrow Y$ for some Z in $\mathcal{M}^*$. But it is obvious that $Z - X$ must be also in $\mathcal{P}_{AFCI}$, which means $X\circ\!\!\rightarrow Y$ in $\mathcal{P}_{AFCI}$ could have been oriented by $\mathcal{R}6$; a contradiction. So $\mathcal{M}^*$ is ancestral.

What is left to show is that $\mathcal{M}^*$ is also maximal, and is Markov equivalent to $\mathcal{M}$. For this purpose, as established by Zhang and Spirtes [35] (their Lemma 1, see also [30]), it suffices to show the following hold of $\mathcal{M}$:

(T2) For every $Z \rightarrow X$ in $\mathcal{M}$, there is also an edge $Z \rightarrow Y$ in $\mathcal{M}$; for every $Z \leftrightarrow X$ in $\mathcal{M}$, there is also an edge $Z \rightarrow Y$ or $Z \leftrightarrow Y$ in $\mathcal{M}$.
(T3) In $\mathcal{M}$, there is no discriminating path for X on which Y is the endpoint adjacent to X.

We first establish (T2). For every $Z \rightarrow X$ in $\mathcal{M}$, it corresponds to either $Z \rightarrow X$ or $Z\circ\!\!\rightarrow X$ or $Z\circ\!\!-\!\!\circ X$ or Z—$\circ X$ in $\mathcal{P}_{AFCI}$. We claim Z and Y are adjacent in any case. In the former two cases, by **P**1, Z and Y are adjacent (since $X\circ\!\!\rightarrow Y$ is in $\mathcal{P}_{AFCI}$). In the case of $Z\circ\!\!-\!\!\circ X$, since it is oriented as $Z \rightarrow X$ in $\mathcal{M}$, Z is adjacent to Y, for otherwise $\mathcal{D}_{J\circ\!\rightarrow K}$ is not agreeable to $J\circ\!\!\rightarrow K$, which contradicts Lemma 4.2. In the case of Z—$\circ X$, by **P**3, Z and Y are adjacent. Moreover, the edge between Z and Y must be $Z \rightarrow Y$ in $\mathcal{M}$, because $Z \rightarrow X \rightarrow Y$ is in $\mathcal{M}$ and $\mathcal{M}$ is a MAG.

For every $Z \leftrightarrow X$ in $\mathcal{M}$, it corresponds to either $Z \leftrightarrow X$ or $Z\circ\!\!\rightarrow X$ or $Z\leftarrow\!\!\circ X$ in $\mathcal{P}_{AFCI}$. In the former two cases, Z and Y are adjacent by **P**1. In the latter case, $Z\leftarrow\!\!\circ X \in \mathbf{REL}(J\circ\!\!\rightarrow K)$ by our assumption about bi-directed edges in $\mathcal{M}$. It then follows from Lemma B.18 that Z and Y are adjacent. So in any case, Z and Y are adjacent in $\mathcal{M}$. Moreover, since $\mathcal{M}$ is a MAG, the edge between Z and Y is either $Z \rightarrow Y$ or $Z \leftrightarrow Y$ in $\mathcal{M}$. (T2) is true.

For (T3), suppose for sake of contradiction that in $\mathcal{M}$ there is a path $p = (V_0, V_1, \ldots, V_n = X, Y)$ which is discriminating for X. Without loss of generality, suppose p is a shortest such path. Below we derive a contradiction by (eventually) showing that p is already a discriminating path in $\mathcal{P}_{AFCI}$, and hence the circle at X on $X\circ\!\!\rightarrow Y$ could have been oriented by $\mathcal{R}4$.

Note first that the subpath $p(V_0, X)$ is into X in $\mathcal{M}$, for otherwise there would be a directed path from X to Y other than the edge $X \rightarrow Y$ (which follows from the definition of discriminating path). It follows that every edge on the subpath $p(V_1, X)$ is bi-directed in $\mathcal{M}$.

Next we claim that in $\mathcal{P}_{AFCI}$ the edge between V_0 and V_1 is $V_0 \ast\!\!\rightarrow V_1$, i.e., is into V_1. Suppose for contradiction that the contrary is true. Then the mark at V_1 must be a circle. Hence the edge is either V_0—$\circ V_1$ or $V_0\circ\!\!-\!\!\circ V_1$ or $V_0\leftarrow\!\!\circ V_1$ in $\mathcal{P}_{AFCI}$. In each of the three cases we can derive a contradiction. And two facts are useful for showing this: (i) $V_1 \leftrightarrow V_2$ (V_2 could be X) appears in $\mathcal{M}$ (as already noted); and (ii) In $\mathcal{P}_{AFCI}$ there isn't an edge between V_0 and V_2 that is into V_2.

For otherwise either $\langle V_0, V_2, \ldots, V_n = X, Y\rangle$ constitutes a shorter discriminating path in $\mathcal{M}$ (if $V_2 \neq X$), or $X \circ\!\!\rightarrow Y$ in $\mathcal{P}_{AFCI}$ could be oriented as $X \rightarrow Y$ by $\mathcal{R}1$ (if $V_2 = X$), either of which is a contradiction.

Again, we won't go through all three cases, and just use the most complicated case to illustrate our argument. Consider $V_0 \circ\!\!-\!\!\circ V_1$. Suppose this is true in $\mathcal{P}_{AFCI}$. Then $V_1 \leftrightarrow V_2$ is not already in $\mathcal{P}_{AFCI}$, for otherwise by Lemma B.3, there would also be an edge $V_0 \leftrightarrow V_2$ in $\mathcal{P}_{AFCI}$, which contradicts fact (ii). By our assumption about bi-directed edges in $\mathcal{M}$, either $V_1 \circ\!\!\rightarrow V_2$ or $V_1 \leftarrow\!\!\circ V_2$ appears in $\mathcal{P}_{AFCI}$ and belongs to $\mathbf{REL}(J \circ\!\!\rightarrow K)$. In the former case ($V_1 \circ\!\!\rightarrow V_2$), V_0 must be adjacent to V_2, for otherwise the orientation of $V_0 \circ\!\!-\!\!\circ V_1$ (into $V_0 \rightarrow V_1$) is not agreeable to $J \circ\!\!\rightarrow K$ ($\mathbf{C}_3$ being violated). By Corollary B.6, the edge between V_0 and V_2 is either $V_0 \rightarrow V_2$ or $V_0 \circ\!\!\rightarrow V_2$ in $\mathcal{P}_{AFCI}$, which contradicts fact (2). In the latter case ($V_1 \leftarrow\!\!\circ V_2$), by Lemma B.3, either $V_0 \leftarrow V_2$ or $V_0 \leftarrow\!\!\circ V_2$ is in $\mathcal{P}_{AFCI}$. Now if V_0 is not a parent of K, which means $V_0 \notin \mathbf{AR}(J \circ\!\!\rightarrow K)$ ($V_0 \neq K$ because Y belongs to $\mathbf{AR}(J \circ\!\!\rightarrow K)$ but is not adjacent to V_0 by the definition of discriminating path), then the orientation of $V_0 \circ\!\!-\!\!\circ V_1$ (into $V_0 \rightarrow V_1$) is not agreeable ($\mathbf{C}_1$ being violated). So V_0 is a parent of K—which also implies that $Y \neq K$. But then the edge $V_2 \circ\!\!\rightarrow K$—which is implied to be present in $\mathcal{P}_{AFCI}$ by Lemma B.10—could be oriented as $V_2 \rightarrow K$ by $\mathcal{R}10$ (because V_0 and Y are not adjacent by the definition of discriminating path, and the edge between V_2 and V_0 in $\mathcal{P}_{AFCI}$ constitutes an uncovered p.d. path from V_2 to V_0, and the edge between V_2 and Y constitutes an uncovered p.d. path in $\mathcal{P}_{AFCI}$ from V_2 to Y); a contradiction.

The other two cases can be handled more easily. It follows that the edge between V_0 and V_1 in $\mathcal{P}_{AFCI}$ is $V_0 *\!\!\rightarrow V_1$.

Finally we show that the supposed p would also be a discriminating path for X in $\mathcal{P}_{AFCI}$. We prove by induction that for every $1 \leqslant i \leqslant n-1$, V_i is a collider on p in $\mathcal{P}_{AFCI}$ and is a parent of Y in $\mathcal{P}_{AFCI}$. Consider V_1 as the base case. Since we have shown that $V_0 *\!\!\rightarrow V_1$ appears in $\mathcal{P}_{AFCI}$, and V_0 is not adjacent to Y, the edge between V_1 and Y is $V_1 \rightarrow Y$ in $\mathcal{P}_{AFCI}$ in virtue of $\mathcal{R}1$. So V_1 is a parent of Y in $\mathcal{P}_{AFCI}$. Suppose for contradiction that V_1 is not a collider on p in $\mathcal{P}_{AFCI}$. Since we have $V_0 *\!\!\rightarrow V_1$ in $\mathcal{P}_{AFCI}$, and we have $V_1 \leftrightarrow V_2$ in $\mathcal{M}$, the edge between V_1 and V_2 must be $V_1 \circ\!\!\rightarrow V_2$ in $\mathcal{P}_{AFCI}$. And by our assumption about bi-directed edges in $\mathcal{M}$, $V_1 \circ\!\!\rightarrow V_2 \in \mathbf{REL}(J \circ\!\!\rightarrow K)$. Then Lemma B.10 implies that there is an edge $V_1 \circ\!\!\rightarrow K$ in $\mathcal{P}_{AFCI}$. But either $Y = K$ or Y is a parent of K in $\mathcal{P}_{AFCI}$, which implies that V_1 is a parent of K or can be oriented as a parent of K by $\mathcal{R}8$ in $\mathcal{P}_{AFCI}$; a contradiction. So V_1 is a collider on p in $\mathcal{P}_{AFCI}$ and is a parent of Y in $\mathcal{P}_{AFCI}$.

The inductive step is very similar, except we will invoke $\mathcal{R}4$ where the base case invoked $\mathcal{R}1$. Therefore (T3) is also true. This concludes the proof. □

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