A Characterization of Markov Equivalance Classes for Ancestral Graphical Models

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Abstract

Ancestral graphical models form a superclass of directed acyclic graphical models, and unlike the latter, are closed under marginalization and conditioning. For this reason, ancestral graphs are particularly suitable to represent the conditional independence structures due to hidden common causes and/or hidden selection variables. Different ancestral graphs, however, can be Markov equivalent in the sense that they entail the same independence structure. In this paper, we give a set of orientation rules that can detect, given an arbitrary (maximal) ancestral graph, which features of the graph are specific to the graph, and which features of the graph are shared by all graphs Markov equivalent to it. By so doing, we solve the completeness problem for the FCI algorithm, an algorithm for causal discovery in the presence of latent confounders and selection bias. We regard this set of rules as a characterization of Markov equivalence classes for ancestral graphical models.

1 Introduction

Two virtues of graphical models have made them increasingly popular among researchers in statistics and artificial intelligence. On the one hand, graphical models use graphs to encode a set of conditional independence relations – an *independence model* – among random variables, which can usually facilitate multivariate statistical analysis by, for example, simplifying the likelihood function. On the other hand, the graphs employed in graphical modeling often bear interpretations related to data generating processes, which are meaningful for the purpose of selecting causal models. A good case in point is directed acyclic graph (DAG). The independence models associated with DAGs allows a neat and convenient factorization of the joint likelihood into several conditional likelihood functions. Meanwhile, the causal interpretation of DAGs elaborated in Pearl (2000) and Spirtes et al. (1993) enables principled search of causal models and inference of such novel quantities as intervention effects.

In this paper we consider the class of ancestral graphical models introduced by Richardson and Spirtes (2002), which properly includes the class of DAG models. The motivation behind ancestral graphs is likewise two-fold. On the statistical side, the class of DAG models is not closed under marginalization and conditioning, whereas the class of ancestral graph models is[1]. Hence, if an independence model $\mathcal{I}$ over variables $\mathbf{V} = \mathbf{O} \cup \mathbf{L} \cup \mathbf{S}$ is represented by a DAG, then the independence model over $\mathbf{O}$ obtained by marginalizing $\mathcal{I}$ over $\mathbf{L}$ and conditioning on $\mathbf{S}$ can always be represented by an ancestral graph over $\mathbf{O}$, even though it may not be representable by a DAG over $\mathbf{O}$. On the causal side, ancestral graphs can be used to meaningfully represent the causal relationships among a set of variables, even when the underlying data generating mechanism involves unobserved confounders and selection bias (Richardson and Spirtes

[1]In fact, the class of ancestral graphs is the smallest superclass of DAGs closed under marginalization and conditioning; see Richardson and Spirtes (2002).

2003). Thus, instead of searching among the infinite space of causal models represented by DAGs with latent variables and selection variables, one can search among the finite space of ancestral graphs for a suitable causal model.

Two different DAGs (over the same set of vertices) can be *Markov equivalent* in the sense that they entail the same independence model, i.e., the same set of conditional independence relations among the variables (represented by the vertices). This feature certainly holds for any superclass of DAG models, and in particular, for ancestral graphical models. Markov equivalent ancestral graphs cannot be distinguished by data, because they represent the same set of joint probability distributions (i.e., the set of distributions that satisfy the common independence model). So it is desirable to have a compact representation that characterizes the common features shared by all members of a Markov equivalence class of ancestral graphs. For one thing, it is important for the purpose of causal inference to distinguish graphical features that are shared by all members of a Markov equivalence class from ones that are not invariant across the class (see, e.g. Spirtes et al. 1993). For another, in model selection it is often recommendable to traverse the space of Markov equivalence classes (as contrasted to the space of graphs). This calls for a good representation of the Markov equivalence classes.

Two representation schemes have been proposed in the literature for Markov equivalence classes of ancestral graphs. One is Partial Ancestral Graphs (PAGs), used in Spirtes et al. (1999) to represent the output of their causal search algorithm, known as the FCI algorithm; the other is Joined Graphs (JGs), introduced by Ali (2002) as an analogue of essential graphs presented in Andersson et al. (1997). However, no full characterization of either representation is yet available. In this paper, we provide one for PAGs. Specifically, we give a set of rules that can detect all invariant orientations in a (maximal) ancestral graph. In other words, we can use these rules to construct a PAG that contains all and only those invariant features in a given (maximal) ancestral graph. We then give a characterization of PAGs based on these rules. Analogous works on Markov equivalence classes of DAGs include Meek (1995) and Andersson et al. (1997).

Section 2 introduces the background of ancestral graphs and a theorem on Markov equivalence we will rely on. The main result of this paper is presented in section 3. We conclude the paper with some discussion of related issues in section 4.

2 Ancestral Graphs and Markov Equivalence

As mentioned earlier, ancestral graphs are primarily motivated by the need to represent the presence of latent confounders and selection variables in the data generating process. For this task we need a richer formalism than typical directed graphs. Besides directed edges ($\rightarrow$), an ancestral graph can also contain bi-directed edges ($\leftrightarrow$, to represent the presence of latent confounders), and undirected edges (—, to represent the presence of selection variables). Before we introduce the definition of ancestral graphs, we need some basic terminology.[2]

A **mixed graph** is a graph consisting of vertices and edges that may contain any of the three kinds of edges (directed, bi-directed and undirected) and at most one edge between any two vertices. The two ends of an edge we call **marks** or **orientations**. Obviously two kinds of marks can appear in a mixed graph: **arrowhead** ($>$) or **tail** ($-$). Specifically, the marks of an undirected edge are both tails; the marks of a bi-directed edge are both arrowheads; and a directed edge has one arrowhead and one tail. We will be interested in characterizing marks that are invariant across a Markov equivalence class. Sometimes we say an edge is **into** (or **out of**) a vertex if the mark of the edge at the vertex is an

[2]The terminology and definitions introduced in this section follow Richardson and Spirtes (2002) closely.

arrowhead (or tail).

Two vertices are said to be **adjacent** in a 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 $\langle V_0, ..., V_n \rangle$ such that for $0 \leq i \leq n-1$, 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 $\langle V_0, ..., V_n \rangle$ such that for $0 \leq i \leq n-1$, 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. We use $\mathbf{Pa}, \mathbf{Ch}, \mathbf{Sp}, \mathbf{Ne}, \mathbf{An}, \mathbf{De}$ to denote the set of parents, children, spouses, neighbors, ancestors, and descendants of a vertex, respectively. 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) if there is an undirected edge between V_1 and V_2, i.e., $V_1 - V_2$, then V_1 and V_2 have no parents or spouses.

Obviously DAGs and undirected graphs (UGs) meet the definition, and hence 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 — that is, an arrowhead implies non-ancestorship — which induces a natural causal interpretation of ancestral graphs. The third condition requires that there is no edge into any vertex in the *undirected* component of an ancestral graph. This property simplifies parameterization and fitting of ancestral graphs (Richardson and Spirtes 2002, Drton and Richardson 2003).

Ancestral graphs encode conditional independence relations by a graphical criterion that generalizes the well-known *d-separation* for DAGs. Given a path u in a graph, a non-endpoint vertex V on u is called a **collider** if the two edges incident to V on u are both into V, otherwise V is called a **non-collider**.

Definition 2 (m-separation). *In an ancestral graph, a path u between vertices A and B is* **active** *(***m-connecting***) relative to a set of vertices $\mathbf{Z}$ ($A, B \notin \mathbf{Z}$) if*

i. every non-collider on u is not a member of $\mathbf{Z}$;

ii. every collider on u is an ancestor of some member of $\mathbf{Z}$.

A and B are said to be **m-separated** *by $\mathbf{Z}$ if there is no active path between A and B relative to $\mathbf{Z}$.*

Let $\mathbf{X}, \mathbf{Y}, \mathbf{Z}$ be three disjoint sets of vertices. $\mathbf{X}$ and $\mathbf{Y}$ are said to be m-separated by $\mathbf{Z}$ if $\mathbf{Z}$ m-separates every member of $\mathbf{X}$ from every member of $\mathbf{Y}$.

The following property is true of DAGs and UGs: if two vertices are not adjacent, then there is a set of some other vertices that m-separates the two. This, however, is not true of ancestral graphs in general. For example, the graph (a) in Figure 1 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:

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.*

As we already noted, DAGs and UGs are all maximal. In fact, maximality corresponds to the property known as pairwise Markov property, i.e., every

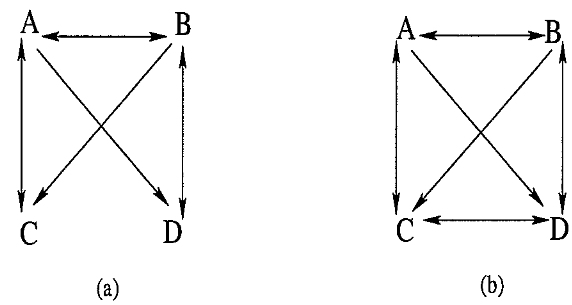

Figure 1: (a) an ancestral graph that is not maximal; (b) a maximal ancestral graph

missing edge corresponds to a conditional independence relation. It is shown in Richardson and Spirtes (2002) that every non-maximal ancestral graph has a unique supergraph that is ancestral and maximal, and furthermore, every non-maximal ancestral graph can be transformed into the maximal supergraph by a series of additions of bi-directed edges. For example, in Figure 1, (b) is the unique maximal supergraph of (a), which has an extra bi-directed edge between C and D. This justifies considering only those ancestral graphs that are maximal. From now on, we focus on maximal ancestral graphs (MAGs).

Maximality is closely related to the notion of inducing path, as defined below:

Definition 4 (inducing path). *In an ancestral graph, a path u between A and B is called an* **inducing path** *if every non-endpoint vertex on u is a collider and is an ancestor of either A or B.*

By this definition, if A and B are adjacent, then the edge between them is trivially an inducing path. In fact, the presence of an inducing path is necessary and sufficient for two vertices not to be m-separated by any set. We write it as a proposition here for later reference, the proof of which can be found in Richardson and Spirtes (2002).

Proposition 1. *An ancestral graph is maximal if and only if there is no in-*

ducing path between any two non-adjacent vertices.

A MAG represents the set of joint distributions (over its vertices) that satisfy its *global Markov property*, i.e., the set of distributions of which the conditional independence relations as implied by the m-separation relations in the MAG hold. Hence, if two MAGs share the same m-separation structures, then they represent the same set of distributions. In this case, we call them **Markov equivalent**.

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 $\mathcal{G}_2$.*

There are sufficient and necessary conditions for Markov equivalence of MAGs that can be checked in polynomial time (Spirtes and Richardson 1996, Ali et al. 2004). Before we present a version of the conditions, the following definitions are needed.

Definition 6 (unshielded collider). *In a MAG, a triple of vertices $\langle A, B, C\rangle$ forms an* **unshielded collider** *if A and C are not adjacent, and there is an edge between A and B and one between B and C such that both edges are into B.*

It is well known that two DAGs are Markov equivalent if and only if they have the same adjacencies and the same unshielded colliders (Verma and Pearl 1990). These conditions are still necessary for Markov equivalence between MAGs, but are not sufficient. For two MAGs to be Markov equivalent, some shielded colliders 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 D and C, $u = \langle D, \cdots, A, B, C\rangle$, is a* **discriminating path** *for B if* *i. u includes at least three edges;*

ii. B is a non-endpoint vertex on u, and is adjacent to C on u; and

iii. D is not adjacent to C, and every vertex between D and B is a collider on u and is a parent of C.

Note that we write a discriminating path in such a form $u = \langle D, \cdots, A, B, C \rangle$, that is, we specify the endpoints and the vertices adjacent to B, the vertex being *discriminated.* The ellipsis therein designates any number (possibly zero) of other vertices. More generally, we adopt it as a convention for depicting a path: the vertices specified in the sequence are understood as distinct ones, and the ellipsis could be any number (possibly zero) of vertices.

Discriminating paths behave similarly to unshielded triples in the following way: if a path between D can C is discriminating for B, then B is a collider on the path if and only if every set that m-separates D and C excludes B; and B is a non-collider on the path if and only if every set that m-separates D and C contains B. Thus we have the following proposition, proved in Spirtes and Richardson (1996):

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 u is a discriminating path for a vertex B in both graphs, then B 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 arbitrary MAG $\mathcal{G}$, we denote its Markov equivalence class, the set of MAGs Markov equivalent to $\mathcal{G}$, by $[\mathcal{G}]$. A mark in $\mathcal{G}$ is said to be **invariant** if the mark is the same in all members of $[\mathcal{G}]$. 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 variant across $[\mathcal{G}]$. In what follows, we aim to fully characterize the invariant marks in $\mathcal{G}$, or in other words, the common marks shared by every member of $[\mathcal{G}]$.

3 A Characterization of Markov Equivalence Classes

In this section we present the main results of the paper. In 3.1, we introduce the representation we are going to work with, called *complete partial ancestral graph (CPAG)*, which is complete with respect to the common marks shared by all members of a Markov equivalence class. In 3.2 we present a set of orientation rules that can, given an arbitrary MAG $\mathcal{G}$, yield the CPAG of $[\mathcal{G}]$. Then we give a syntactical characterization of CPAGs in 3.3 based on the orientation rules.

3.1 Complete Partial Ancestral Graphs (CPAGs)

Richardson (1996) introduced partial ancestral graphs (PAGs) to represent the output of his causal inference algorithm in linear feedback systems. Then PAGs are used by Spirtes et al. (1999) to represent the output of the FCI algorithm, an algorithm for causal inference in the presence of latent variables and selection bias. A PAG is a graph that can contain three kinds of marks: tail ($-$), arrowhead ($>$) and circle ($\circ$). (So, by simple combinatorics, there could be six sorts of edges: $-$, $\rightarrow$, $\leftrightarrow$, $\circ\!-$, $\circ\!-\!\circ$, $\circ\!\rightarrow$.) The circle is intended to be interpreted as an uninformative or ambiguous mark, which indicates that the corresponding mark is not invariant across the equivalence class. This intuition is captured in the definition below:

Definition 8 (CPAG). *Let $[\mathcal{G}]$ be the Markov equivalence class for an arbitrary MAG $\mathcal{G}$. The* **complete partial ancestral graph (CPAG)** *for $[\mathcal{G}]$, $\mathcal{P}_{\mathcal{G}}$, is* *a graph with (possibly) the three kinds of marks (and hence six kinds of edges:* $-$, $\rightarrow$, $\leftrightarrow$, $\circ\!-$, $\circ\!-\!\circ$, $\circ\!\!\rightarrow$*), such that*

i. $\mathcal{P}_{\mathcal{G}}$ *has the same adjacencies as* $\mathcal{G}$ *(and hence any member of* $[\mathcal{G}]$*) does;*

ii. A mark of arrowhead is in $\mathcal{P}_{\mathcal{G}}$ *if and only if it is invariant in* $[\mathcal{G}]$*; and*

iii. A mark of tail is in $\mathcal{P}_{\mathcal{G}}$ *if and only if it is invariant in* $[\mathcal{G}]$*.*

The difference between a CPAG and a PAG as previously employed in the literature[3] is of course that the latter is not alleged to contain all invariant arrowheads or tails. The difference between a CPAG and a joined graph introduced by Ali (2002) is that the latter only aims to represent all invariant arrowheads and hence do not distinguish invariant tails from variant marks. Clearly the most complete representation of a Markov equivalence class of MAGs is the CPAG.

Now we proceed to describe solutions to the following two problems:

- How to construct the CPAG for a Markov equivalence class given a single representative of that class; (section 3.2)
- How to characterize CPAGs without explicit reference to Markov equivalence classes. (section 3.3)

3.2 Construction of the CPAG

Suppose we are given a MAG $\mathcal{G}$. How can we construct the CPAG that represents $[\mathcal{G}]$? It is certainly infeasible to spell out all the members in $[\mathcal{G}]$ and build the CPAG according to Definition 8. For one thing, the size of $[\mathcal{G}]$ could be big; for another, it is not clear how one can list all the MAGs Markov equivalent to $\mathcal{G}$ without first figuring out the invariant edges or marks. The approach we

[3]It is worth noting that a graphical object named *partially oriented inducing path graph (POIPG)* is studied in Spirtes et al. (1993), which, however, can be shown to be just a PAG that is not complete in the sense of Definition 8.

take follows the spirit of Meek (1995), and more closely, the FCI algorithm in Spirtes et al. (1999). In particular, we start with a graph that has the same adjacencies as $\mathcal{G}$ does and every mark therein is a circle (i.e., every edge therein is of the form $\circ\!\!-\!\!\circ$)[4]. Then we apply a set of orientation rules that change some circles into informative marks: arrowheads or tails.

3.2.1 The Orientation Rules and Soundness

We need a few definitions of special paths to state some of the rules. Let us call any graph that may contain the three kinds of marks a **partial mixed graph (PMG)**.

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

Definition 10 (potentially directed path). *In a PMG, a path $u = \langle V_0, \cdots, V_n \rangle$ is said to be* **potentially directed** *(abbreviated as* **p.d.***) from V_0 to V_n if for every $0 \leq i \leq n-1$, the edge between V_i and V_{i+1} is not into V_i, nor is it 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 orienting circles into tails. A special case of a p.d. path is where every edge is of the form $\circ\!\!-\!\!\circ$. We will call such a path, a path that consists solely of $\circ\!\!-\!\!\circ$ edges, a **circle path**.

To state the orientation rules more efficiently, we need a meta-symbol $*$ that serves as a wildcard for marks. More specifically, if $*$ appears in an antecedent of a rule, that means it does not matter whether the mark at that place is an arrowhead, or a tail, or a circle. If $*$ appears in the consequence of a rule, that

[4]The adjacencies can be constructed even if we are not given a MAG, but instead given a set of independence facts (that can be revealed by data). See Spirtes et al. (1993), Spirtes et al. (1999).

means the mark at that place remains what it was (before the firing of the rule).

We break down the orientation process into four steps. Let $\mathcal{P}_0$ be the starting graph we just mentioned — the graph with the same adjacencies as $\mathcal{G}$ does and only $\circ\!\!-\!\!\circ$ edges. The first step is to introduce all unshielded colliders in $\mathcal{G}$, i.e., to apply the following rule to $\mathcal{P}_0$. (Greek letters are used in the orientation rules to denote generic vertices.)

$\mathcal{R}0$ For every triple $\alpha *\!\!-\!\!* \beta \circ\!\!-\!\!* \gamma$ s.t. α, γ are not adjacent, if it is an unshielded collider in $\mathcal{G}$[5], then orient the triple as $\alpha *\!\!\rightarrow \beta \leftarrow\!\!* \gamma$.

The soundness of $\mathcal{R}0$ readily follows from (e2) in Proposition 2, namely, Markov equivalent MAGs have the same unshielded colliders. Let $\mathcal{P}_1$ denote the resulting graph. The following lemma is thus evident.

Lemma 1. *$\mathcal{R}0$ is sound, i.e., every non-circle mark in $\mathcal{P}_1$ is invariant across $[\mathcal{G}]$.*

Proof. It follows from the fact that every graph in $[\mathcal{G}]$ contains the unshielded colliders in $\mathcal{G}$. □

The next step is to introduce more invariant arrowheads (as well as some invariant tails) by applying the following rules repeatedly until none can be fired.

$\mathcal{R}1$ 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 $\theta *\!\!\rightarrow \beta$.

[5] If we are not given a MAG directly, the antecedent of this rule can be formulated in terms of m-separation features, which, under suitable assumptions, are identifiable from data. See Spirtes et al. (1999) for details.

$\mathcal{R}4$ If $u = \langle\theta, ..., \alpha, \beta, \gamma\rangle$ is a discriminating path between θ and γ for β, and $\beta \circ\!\!-\!\!* \gamma$; then if $\beta \rightarrow \gamma$ appears in $\mathcal{G}$[6], orient $\beta \circ\!\!-\!\!* \gamma$ as $\beta \rightarrow \gamma$; otherwise orient the triple $\langle\alpha, \beta, \gamma\rangle$ as $\alpha \leftrightarrow \beta \leftrightarrow \gamma$.

The pictorial illustrations of these rules are given in Figure 2. These rules, together with $\mathcal{R}0$, will be referred to as *arrowhead orientation rules*, because the rest of the rules will not introduce more arrowheads. Let $\mathcal{P}_2$ be the graph resulting from repetitive (and exhaustive) applications of $\mathcal{R}1 - \mathcal{R}4$ to $\mathcal{P}_1$. We will show later that the arrowhead orientation rules are sufficient to identify all invariant arrowheads in $\mathcal{G}$. That is, all arrowheads that are common to members of $[\mathcal{G}]$ will be explicitly marked in $\mathcal{P}_2$. This means that these rules can be used to characterize, for example, the joined graph as defined in Ali (2002). In particular, if we change the remaining circles in $\mathcal{P}_2$ into tails, we get the joined graph for $[\mathcal{G}]$.

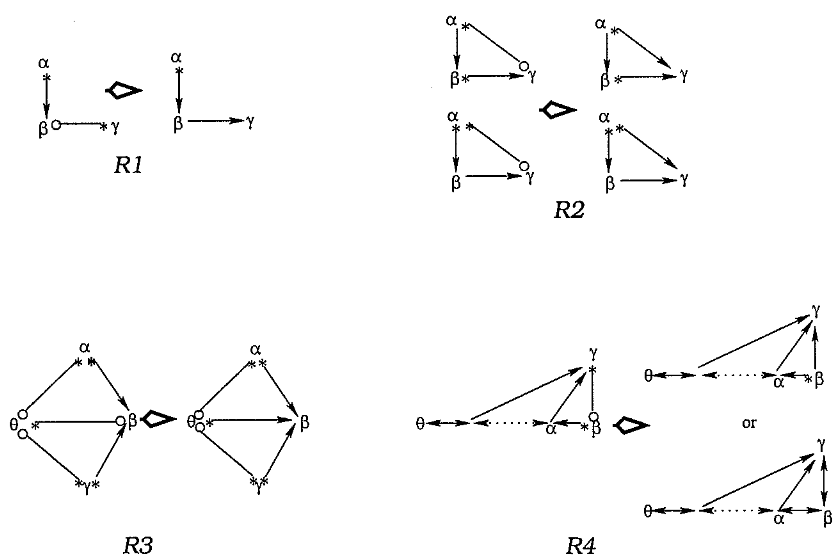

Figure 2: Graphical illustrations of $\mathcal{R}1 - \mathcal{R}4$

[6]Again, this rule shall be formulated in terms of m-separation features if $\mathcal{G}$ is not given directly.

For now we show that $\mathcal{R}1 - \mathcal{R}4$ are sound.

Lemma 2. *$\mathcal{R}1 - \mathcal{R}4$ are sound (and hence every non-circle mark in $\mathcal{P}_2$ is invariant across $[\mathcal{G}]$).*

Proof. It suffices to show that for each rule, if a mixed graph satisfies the antecedent of the rule but contains a mark different than what the rule requires, the graph is either not a MAG or not Markov equivalent to $\mathcal{G}$, and hence not a member of $[\mathcal{G}]$. In every case that follows, we assume the antecedent of the rule holds in the graph under consideration.

$\mathcal{R}1$: Suppose a mixed graph, contrary to what the rule requires, has an arrowhead at β. Then it contains an unshielded collider $\langle\alpha,\beta,\gamma\rangle$ which is not in $\mathcal{G}$, and so is not Markov equivalent to $\mathcal{G}$. Furthermore, if the mark at γ is a tail, then $\alpha *\!\!\rightarrow \beta - \gamma$ appears, which means the graph is not ancestral.

$\mathcal{R}2$: Suppose a mixed graph, contrary to what the rule requires, has a tail at γ. If it is $\alpha - \gamma$, the graph is not ancestral because the edge between β and γ is into γ. If it is $\alpha \leftarrow \gamma$, then either γ is an ancestor of β and $\beta *\!\!\rightarrow \gamma$, or β is an ancestor of α and $\alpha *\!\!\rightarrow \beta$. In either case the graph is not ancestral.

$\mathcal{R}3$: Suppose a mixed graph, contrary to what the rule requires, has a tail at β. If it is $\theta - \beta$, the graph is not ancestral because the edge between α and β is into β. Suppose it is $\theta \leftarrow \beta$ that appears in the graph. Notice that if the triple $\langle\alpha,\theta,\gamma\rangle$ is an unshielded collider in the graph, then the graph is not Markov equivalent to $\mathcal{G}$. On the other hand, if it is not a collider, then at least one of the two edges is out of θ. Note that neither the edge between α and θ, nor the edge between γ and θ can be undirected, for otherwise the graph is not ancestral due to the presence of $\theta \leftarrow \beta$. So either $\theta \rightarrow \alpha$, or $\theta \rightarrow \gamma$; that is, β is either an ancestor of α or an ancestor of γ. In either case, the graph is not ancestral because $\alpha *\!\!\rightarrow \beta \leftarrow\!\!* \gamma$ is present.

$\mathcal{R}4$: There are two cases to consider.

Case 1: $\beta \rightarrow \gamma$ appears in $\mathcal{G}$. So the triple $\langle\alpha,\beta,\gamma\rangle$ is not a collider. By (e3) in Proposition 2, in any MAG equivalent to $\mathcal{G}$, $\langle\alpha,\beta,\gamma\rangle$ is not a collider.

Suppose a mixed graph contains the triple as a non-collider, but contrary to what the rule requires, has an arrowhead at β on the edge between β and γ. Then the edge between β and α is out of β. If it is $\beta — \alpha$, then the graph is not ancestral because by our supposition there is an arrowhead at β; if it is $\beta \rightarrow \alpha$ that appears in the graph, remember that by the definition of discriminating path (Definition 7), α is a parent of γ. So β is an ancestor of γ, which, together with our supposition, makes the graph not ancestral. Furthermore, if the edge between β and γ is $\beta — \gamma$, then the graph is not ancestral because α is a parent of γ. Therefore, any MAG equivalent to $\mathcal{G}$ has to contain $\beta \rightarrow \gamma$, as the rule requires.

Case 2: $\beta \rightarrow \gamma$ does not appear in $\mathcal{G}$. By the definition of discriminating path, α is a parent of γ, that is, $\alpha \rightarrow \gamma$ appears in $\mathcal{G}$. This implies that the edge between β and γ is not undirected, and hence it is into β. It follows that $\langle \alpha, \beta, \gamma \rangle$ is a collider in $\mathcal{G}$, for otherwise the edge between α and β is either $\alpha \leftarrow \beta$ or $\alpha — \beta$, either of which would violate the definition of ancestral graphs. So, by Proposition 2, in any MAG equivalent to $\mathcal{G}$, the triple $\langle \alpha, \beta, \gamma \rangle$ is a collider. Also, by the definition of discriminating path, α is a collider on the path, which means $\alpha \leftrightarrow \beta \leftarrow\!\!* \gamma$ is in any MAG equivalent to $\mathcal{G}$. Furthermore, because $\alpha \rightarrow \gamma$ is present, $\alpha \leftrightarrow \beta \leftarrow \gamma$ will make the graph not ancestral. Therefore, $\alpha \leftrightarrow \beta \leftrightarrow \gamma$ is in any MAG equivalent to $\mathcal{G}$. $\square$

What comes next is a set of rules that can introduce more tails into $\mathcal{P}_2$. These rules can be further classified into two categories. We first list those that are primarily related to (invariant) undirected edges, the pictorial illustrations of which are given in Figure 3.

$\mathcal{R}5$ For every (remaining) $\alpha \circ\!\!—\!\!\circ \beta$, if there is a path $u = \langle \alpha, \gamma, \cdots, \theta, \beta \rangle$ that is an uncovered circle path 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 u as undirected (—).

$\mathcal{R}6$ If $\alpha - \beta \circ\!\!-\!\!* \gamma$, 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 $\beta -\!\!* \gamma$.

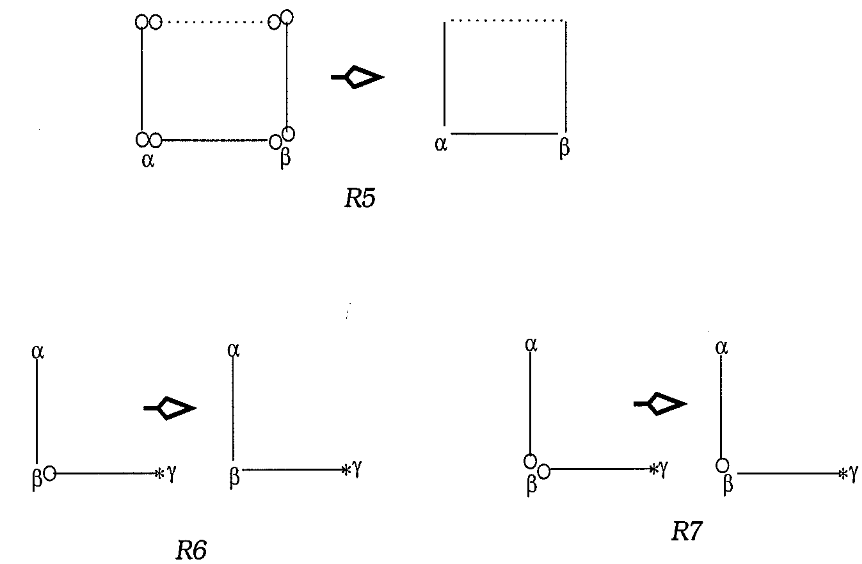

Figure 3: Graphical illustrations of $\mathcal{R}5 - \mathcal{R}7$

We add a quantifier in $\mathcal{R}5$ to indicate that it will be executed once and for all (before $\mathcal{R}6$ and $\mathcal{R}7$), as is the case with $\mathcal{R}0$. It should be clear from the ensuing proof of soundness that $\mathcal{R}5 - \mathcal{R}7$ are primarily motivated by the third condition in the definition of ancestral graphs ((a3) in Definition 1), namely, the restriction on the endpoints of undirected edges.

Lemma 3. *$\mathcal{R}5 - \mathcal{R}7$ are sound.*

Proof. Again, we show that any mixed graph that violates the rule does not belong to $[\mathcal{G}]$.

$\mathcal{R}5$: Note that the antecedent of this rule implies that $\langle \alpha, \gamma, \cdots, \theta, \beta, \alpha \rangle$ 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. By our argument for the soundness of $\mathcal{R}1$, it should be clear that the cycle must be oriented as a directed cycle to avoid unshielded colliders that are not in $\mathcal{G}$. But then the graph is not ancestral.

$\mathcal{R}6$: It is clear that 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 $\alpha \rightarrow \beta \leftarrow\!\!* \gamma$ is present, in which case the graph contains an unshielded collider that is not in $\mathcal{G}$. $\square$

Let $\mathcal{P}_3$ be the graph resulting from repetitive (and exhaustive) applications of $\mathcal{R}5 - \mathcal{R}7$ to $\mathcal{P}_2$. By the above lemma, every non-circle mark in $\mathcal{P}_3$ is invariant across $[\mathcal{G}]$. Furthermore, as our proof of completeness will show, in $\mathcal{P}_3$ every circle on either $\circ\!\!—\!\!\circ$ or $\circ\!\!—$ corresponds to a variant mark in $\mathcal{G}$. That is, only circles on $\circ\!\!\rightarrow$ possibly hide invariant marks. So the last bunch of our rules aims exclusively at orienting $\circ\!\!\rightarrow$ into $\rightarrow$.

$\mathcal{R}8$ If $\alpha \rightarrow \beta \rightarrow \gamma$ or $\alpha —\!\!\circ\, \beta \rightarrow \gamma$, and $\alpha \circ\!\!\rightarrow \gamma$, orient $\alpha \circ\!\!\rightarrow \gamma$ as $\alpha \rightarrow \gamma$.

$\mathcal{R}9$ If $\theta \rightarrow \beta \rightarrow \gamma$, $\alpha \circ\!\!\rightarrow \gamma$, and $u = \langle \alpha, \cdots, \theta \rangle$ is an uncovered p.d. path from α to θ such that the vertex adjacent to α on u is not adjacent to γ, then orient $\alpha \circ\!\!\rightarrow \gamma$ as $\alpha \rightarrow \gamma$.

$\mathcal{R}10$ If $\alpha \circ\!\!\rightarrow \gamma$, and $u = \langle \alpha, \beta, \theta, \cdots, \gamma \rangle$ is an uncovered p.d. path from α to γ such that γ and β are not adjacent, then orient $\alpha \circ\!\!\rightarrow \gamma$ as $\alpha \rightarrow \gamma$.

$\mathcal{R}11$ Suppose $\alpha \circ\!\!\rightarrow \gamma$, $\beta \rightarrow \gamma \leftarrow \theta$, u_1 is an uncovered p.d. path from α to β, and u_2 is an uncovered p.d. path from α to θ. Let μ be the vertex adjacent to α on u_1 (μ could be β), and ω be the vertex adjacent to α on u_2 (ω could be θ). If μ and ω are not adjacent, then orient $\alpha \circ\!\!\rightarrow \gamma$ as $\alpha \rightarrow \gamma$.

Figure 4 contains pictorial illustrations of these rules. Again, the soundness of these rules is not hard to verify.

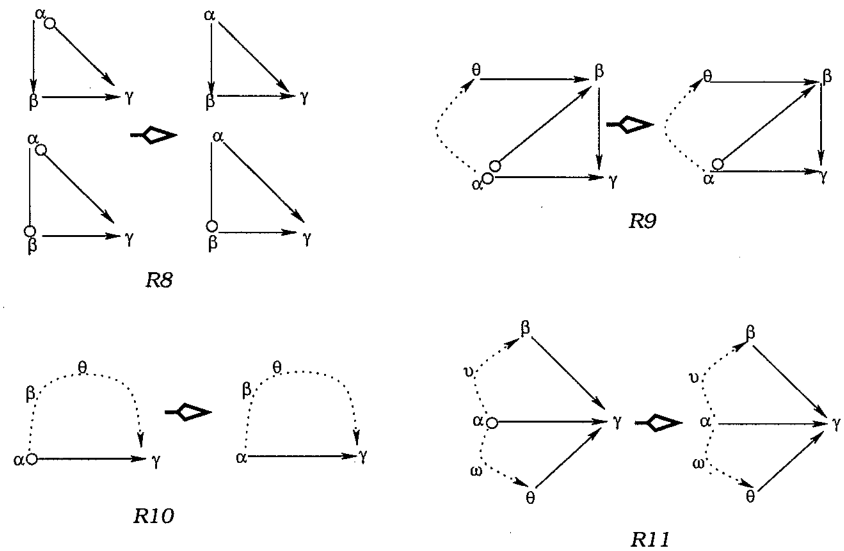

Figure 4: Graphical illustrations of $\mathcal{R}8 - \mathcal{R}11$

Lemma 4. *$\mathcal{R}8 - \mathcal{R}11$ are sound.*

Proof. We show that, for each of the four rules, if a mixed graph has an arrowhead in the place where the rule requires a tail, the graph is not a member of $[\mathcal{G}]$.

$\mathcal{R}8$: 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.

$\mathcal{R}9$: If a mixed graph, contrary to what the rule requires, contains $\alpha \leftrightarrow \gamma$, the uncovered path u must be a directed path (from α to θ) in the graph, to avoid unshielded colliders which are not present in $\mathcal{G}$. But then α is an ancestor of γ, which, together with $\alpha \leftrightarrow \gamma$, makes the graph not ancestral.

$\mathcal{R}10$: The same argument for the soundness of $\mathcal{R}5$ applies here. If a mixed graph, contrary to what the rule requires, contains $\alpha \leftrightarrow \gamma$, then the uncovered path u must be a directed path (from α to γ) in a graph, to avoid unshielded colliders which are not present in $\mathcal{G}$. But then the graph is not ancestral.

$\mathcal{R}11$: This rule is analogous to $\mathcal{R}3$. The antecedent of the rule implies that the triple $\langle \mu, \alpha, \omega \rangle$ is not a collider in $\mathcal{G}$, which means at least one of the two edges involved in the triple is out of α in any MAG equivalent to $\mathcal{G}$. Now, suppose a mixed graph, 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 u_1 or u_2 is a directed path in the graph to avoid unshielded colliders which are not in $\mathcal{G}$. In either case, α is an ancestor of γ, and hence the graph is not ancestral. $\square$

So, every non-circle mark in $\mathcal{P}_4$, the resulting graph from repetitive applications of $\mathcal{R}8 - \mathcal{R}11$ to $\mathcal{P}_3$, is also invariant across $[\mathcal{G}]$. We write it down as a theorem here.

Theorem 1 (Soundness). *Every non-circle mark in $\mathcal{P}_4$ is invariant.*

The main aim of this paper, however, is to show that $\mathcal{P}_4 = \mathcal{P}_{\mathcal{G}}$, i.e., $\mathcal{P}_4$ is the CPAG for the Markov equivalence class of $\mathcal{G}$. For this purpose we need to demonstrate that each remaining circle in $\mathcal{P}_4$ represents a variant mark, that is, there is a member of $[\mathcal{G}]$ in which the circle is marked as an arrowhead and there is a member of $[\mathcal{G}]$ in which the circle is marked as a tail. Before we turn to the rather involved demonstration of this fact, we make some further remarks about the orientation rules, which are summarized in Figures 5 and 6 for easy reference.

We broke down our presentation of $\mathcal{R}0 - \mathcal{R}11$ into several steps to highlight the modularity in the process. Application of $\mathcal{R}0$ gives us $\mathcal{P}_1$, which, in the case of DAGs, would be an (incomplete) pattern or a PDAG, in the terminology of Chickering (2002). Then $\mathcal{R}1 - \mathcal{R}4$ constitutes the first block of rules to be applied to $\mathcal{P}_1$. The resulting graph $\mathcal{P}_2$, reveals all invariant arrowheads

Arrowhead Orientation Rules:

$\mathcal{R}0$ For every triple $\alpha *\!\!-\!\!* \beta \circ\!\!-\!\!* \gamma$ s.t. α, γ are not adjacent, if it is an unshielded collider in $\mathcal{G}$, then orient the triple as $\alpha *\!\!\rightarrow \beta \leftarrow\!\!* \gamma$.

$\mathcal{R}1$ 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 $\theta *\!\!\rightarrow \beta$.

$\mathcal{R}4$ If $u = \langle \theta, ..., \alpha, \beta, \gamma \rangle$ is a discriminating path between θ and γ for β, and $\beta \circ\!\!-\!\!* \gamma$ then if $\beta \rightarrow \gamma$ appears in $\mathcal{G}$, orient $\beta \circ\!\!-\!\!* \gamma$ as $\beta \rightarrow \gamma$; otherwise orient the triple

Figure 5: Summary of the arrowhead orientation rules

and some special invariant tails[7]. The rest two blocks of rules, $\mathcal{R}5 - \mathcal{R}7$ and $\mathcal{R}8 - \mathcal{R}11$, are independent of each other in the sense that any firing of a rule in one block will not trigger any extra firing of a rule in the other. (And for that matter, of course, $\mathcal{R}1 - \mathcal{R}4$ is also independent of these two blocks). We listed $\mathcal{R}5 - \mathcal{R}7$ first, because, as will become clear later, they are the necessary steps in transforming a PAG into a MAG in which all bi-directed edges and undirected edges are invariant. That is, suppose we construct $\mathcal{P}_2$ out of data rather than a given MAG, and would like to turn it into a representative MAG with a minimum number of bi-directed and undirected edges (perhaps for the purpose of fitting and scoring, as in Spirtes et al. (1997)), then we need to apply $\mathcal{R}5 - \mathcal{R}7$ but do not need to apply $\mathcal{R}8 - \mathcal{R}11$. On the other hand, since $\mathcal{R}5 - \mathcal{R}7$ are relevant only when undirected edges may be present, they

[7]The reason why the tails contained in $\mathcal{P}_2$ are special is related to the identification of intervention effects, the discussion of which shall be left to another paper.

Tail Orientation Rules:

$\mathcal{R}5$ For every $\alpha \circ\!\!-\!\!\circ \beta$, if there is a path $u = \langle \alpha, \gamma, \cdots, \theta, \beta \rangle$ that is an uncovered circle path 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 u as undirected ($-$).

$\mathcal{R}6$ If $\alpha - \beta \circ\!\!-\!\!* \gamma$, 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 $\beta -\!\!* \gamma$.

$\mathcal{R}8$ 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 $\theta \to \beta \to \gamma$, $\alpha \circ\!\!\to \gamma$, and $u = \langle \alpha, \cdots, \theta \rangle$ is an uncovered p.d. path from α to θ such that the vertex adjacent to α on u is not adjacent to γ, then orient $\alpha \circ\!\!\to \gamma$ as $\alpha \to \gamma$.

$\mathcal{R}10$ If $\alpha \circ\!\!\to \gamma$, and $u = \langle \alpha, \beta, \theta, \cdots, \gamma \rangle$ 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 $\alpha \to \gamma$.

$\mathcal{R}11$ Suppose $\alpha \circ\!\!\to \gamma$, $\beta \to \gamma \leftarrow \theta$, u_1 is an uncovered p.d. path from α to β, and u_2 is an uncovered p.d. path from α to θ. Let μ be the vertex adjacent to α on u_1 (μ could be β), and ω be the vertex adjacent to α on u_2 (ω could be θ). If μ and ω are not adjacent, then orient $\alpha \circ\!\!\to \gamma$ as $\alpha \to \gamma$.

Figure 6: Summary of the tail orientation rules

will not be invoked in such tasks as causal discovery in the presence of latent confounders but no selection bias.

It is also worth noting the resemblance between $\mathcal{R}10$ and $\mathcal{R}5$. (In fact, the latter essentially amounts to a double application of the former plus $\mathcal{R}7$.) So $\mathcal{R}10$, just as $\mathcal{R}5$, need only be checked once for each relevant edge. The implementation details shall not concern us in this paper, so we simply note that the antecedent of each rule that involves (uncovered) paths, in the worst case, can be checked in $O(mn)$, with m being the number of edges and n being the number of vertices in the graph. More efficient implementation is possible given a further elaboration of the property of uncovered p.d. paths.

3.2.2 Completeness w.r.t Arrowheads

In what follows, we prove the completeness of $\mathcal{R}0-\mathcal{R}11$, or simply put, $\mathcal{P}_4 = \mathcal{P}_{\mathcal{G}}$, where $\mathcal{P}_4$ is the output from the process described in section 3.2.1, and $\mathcal{P}_{\mathcal{G}}$ is the CPAG for $[\mathcal{G}]$. We first show that $\mathcal{P}_4$ is complete with respect to arrowhead[8], namely all invariant arrowheads have been included in $\mathcal{P}_4$. In other words, for every circle in $\mathcal{P}_4$, there is a MAG in $[\mathcal{G}]$ in which the circle is oriented as a tail. To demonstrate this fact, we need to establish some properties of $\mathcal{P}_4$. Certain properties are already evident given Theorem 1. For example, the defining properties of ancestral graphs, i.e., (a1)-(a3) in Definition 1 all hold of $\mathcal{P}_4$, and there is no inducing path between two non-adjacent vertices. Other properties are not so obvious. The following lemma establishes a property of $\mathcal{P}_4$ which is analogous to the one proved by Meek (1995) in the context of DAGs. We will call this property **CP**1, as this property together with some others will be used to characterize **CP**AGs later.

Lemma 5. *In $\mathcal{P}_4$, the following property holds:*

CP1 *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 $A \leftrightarrow C$).*

Proof. We prove that **CP**1 holds of $\mathcal{P}_2$, the graph resulting from exhaustive applications of the arrowhead orientation rules $\mathcal{R}0 - \mathcal{R}4$. The fact that it also holds of $\mathcal{P}_4$ obviously follows, because no extra arrowheads are introduced in $\mathcal{P}_4$.

[8]This part is joint work with Ali and Richardson, which is also reported, in a slightly different framework, in Ali et al. 2005.

Let $\mathbf{M} = \{Y | \exists X, Z$ such that $X {*\!\!\rightarrow} Y \circ\!\!- * Z$ but not $X {*\!\!\rightarrow} Z$ is in $\mathcal{P}_2\}$. We need to show that $\mathbf{M}$ is empty. Suppose for the sake of contradiction that $\mathbf{M}$ is not empty. Let Y_0 be a vertex in $\mathbf{M}$ such that no *proper ancestor*[9] of Y_0 in $\mathcal{P}_2$ is in $\mathbf{M}$. (This specification is legitimate because there is no directed cycle in $\mathcal{P}_2$.) Let $\mathbf{F}_{Y_0} = \{X | \exists Z$ such that $X {*\!\!\rightarrow} Y_0 \circ\!\!- * Z$ but not $X {*\!\!\rightarrow} Z$ is in $\mathcal{P}_2\}$. Since $Y_0 \in \mathbf{M}$, $\mathbf{F}_{Y_0}$ is not empty. Choose X_0 in $\mathbf{F}_{Y_0}$ such that no proper *descendant* of X_0 in $\mathcal{P}_2$ is in $\mathbf{F}_{Y_0}$. Finally, choose any Z_0 such that $X_0 {*\!\!\rightarrow} Y_0 \circ\!\!- * Z_0$ but not $X_0 {*\!\!\rightarrow} Z_0$ is in $\mathcal{P}_2$. We will manage to derive a contradiction out of this.

Note that X_0 and Z_0 must be adjacent, otherwise the circle at Y_0 on $Y_0 \circ\!\!- * Z_0$ would have been oriented by $\mathcal{R}0$ or $\mathcal{R}1$. Furthermore, the edge between X_0 and Z_0 is not out of Z_0, i.e., the mark at Z_0 on the edge is not a tail. The reason is this: it is evident that no $-$ or $\circ\!\!-$ could result from applications of $\mathcal{R}0 - \mathcal{R}4$, and hence none is present in $\mathcal{P}_2$. So if the edge between X_0 and Z_0 is out of Z_0, then it must be $X_0 \leftarrow Z_0$. But then $Y_0 \circ\!\!- * Z_0$ would have been oriented as $Y_0 \leftarrow\!\! * Z_0$ by $\mathcal{R}2$. This is a contradiction. Hence the edge between X_0 and Z_0 is not out of Z_0. Since by our supposition, the edge is not into Z_0 either, the mark at Z_0 on the edge between X_0 and Z_0 has to be a circle, namely $X_0 * \!\!-\!\!\circ Z_0$.

Below we enumerate the ways in which the arrowhead at Y_0 on $X_0 {*\!\!\rightarrow} Y_0$ could have been oriented, and derive a contradiction in each case.

Case 1: $X_0 {*\!\!\rightarrow} Y_0$ is oriented by $\mathcal{R}0$. That means there is a vertex W such that W is not adjacent to X_0, and $X_0 {*\!\!\rightarrow} Y_0 \leftarrow\!\! * W$ appears in $\mathcal{P}_2$. This implies that Z_0 and W are adjacent, for otherwise the circle at Y_0 on $Y_0 \circ\!\!- * Z_0$ would have been oriented by either $\mathcal{R}0$ or $\mathcal{R}1$. Furthermore, because $X_0 * \!\!-\!\!\circ Z_0$, it is not the case that $Z_0 \leftarrow\!\! * W$, otherwise the circle at Z_0 would have been oriented by $\mathcal{R}0$ or $\mathcal{R}1$. It follows that either $Z_0 \circ\!\!- * W$ or $Z_0 \rightarrow W$ (again, because no $-$ or $-\!\!\circ$ is present). In the former case, $X_0 * \!\!-\!\!\circ Z_0 \circ\!\!- * W$ and $X_0 {*\!\!\rightarrow} Y_0 \leftarrow\!\! * W$, and hence $Y_0 \circ\!\!- * Z_0$ should have been oriented as $Y_0 \leftarrow\!\! * Z_0$ by $\mathcal{R}3$; in the latter case, $Z_0 \rightarrow W {*\!\!\rightarrow} Y_0$, and hence $Y_0 \circ\!\!- * Z_0$ should have been oriented as $Y_0 \leftarrow\!\! * Z_0$ by

[9]A **proper ancestor** of a vertex is an ancestor distinct from the vertex itself.

$\mathcal{R}2$. So in either case it is a contradiction.

Case 2: $X_0 {*\!\!\rightarrow} Y_0$ is oriented by $\mathcal{R}1$, which means that there is a vertex W not adjacent to Y_0 such that $W {*\!\!\rightarrow} X_0 \rightarrow Y_0$ is in $\mathcal{P}_2$. It is not the case that $X_0 \leftarrow\!\circ Z_0$, otherwise $Y_0 \circ\!\!-\!* Z_0$ would be oriented by $\mathcal{R}2$ to be $Y_0 \leftarrow\!* Z_0$. So $X_0 \circ\!\!-\!\!\circ Z_0$ is in $\mathcal{P}_2$. It follows that W and Z_0 are adjacent, otherwise the circle at X_0 on $X_0 \circ\!\!-\!\!\circ Z_0$ would be oriented by $\mathcal{R}0$ or $\mathcal{R}1$. Now the unshielded triple $Y_0 \circ\!\!-\!* Z_0 *\!\!-\!* W$ cannot be a collider, for otherwise $X_0 \rightarrow Y_0 \circ\!\!\rightarrow Z_0$, and $X_0 \circ\!\!-\!\!\circ Z_0$ would be oriented as $X_0 \circ\!\!\rightarrow Z_0$ by $\mathcal{R}2$. Since it is a non-collider, it cannot be that $W {*\!\!\rightarrow} Z_0$, otherwise $Y_0 \circ\!\!-\!* Z_0$ would be oriented as $Y_0 \leftarrow Z_0$. Now we have $W {*\!\!\rightarrow} X_0 \circ\!\!-\!\!\circ Z_0$ but not $W {*\!\!\rightarrow} Z_0$ in $\mathcal{P}_2$. So X_0 is in $\mathbf{M}$ and is a parent of Y_0, which contradicts our choice of Y_0.

Case 3: $X_0 {*\!\!\rightarrow} Y_0$ is oriented by $\mathcal{R}2$. There are two sub-cases to consider.

Case 3.1: There is a vertex W such that $X_0 \rightarrow W {*\!\!\rightarrow} Y_0$ appears in $\mathcal{P}_2$. Then W and Z_0 must be adjacent, for otherwise the circle at Y_0 on $Y_0 \circ\!\!-\!* Z_0$ would be oriented by either $\mathcal{R}0$ or $\mathcal{R}1$. Furthermore, it is not the case that $W {*\!\!\rightarrow} Z_0$, otherwise by $\mathcal{R}2$, $X_0 {*\!\!\rightarrow} Z_0$, a contradiction. Now we have $W {*\!\!\rightarrow} Y_0 \circ\!\!-\!* Z_0$ but not $W {*\!\!\rightarrow} Z_0$. So W is in $\mathbf{F}_{Y_0}$ and is a child of X_0, which contradicts our choice of X_0.

Case 3.2: There is a vertex W such that $X_0 {*\!\!\rightarrow} W \rightarrow Y_0$ appears in $\mathcal{P}_2$. Again, W and Z_0 must be adjacent, for the same reason as in *3.1*. Furthermore, it must be the case that $W \circ\!\!-\!* Z_0$. If not, either $W \rightarrow Z_0$ or $W \leftarrow\!* Z_0$. In the former case, $\mathcal{R}2$ would dictate that $X_0 {*\!\!\rightarrow} Z_0$, which contradicts our assumption; In the latter case, $\mathcal{R}2$ would dictate that $Y_0 \leftarrow\!* Z_0$, which also contradicts our assumption. Now we have $X_0 {*\!\!\rightarrow} W \circ\!\!-\!* Z_0$ but not $X_0 {*\!\!\rightarrow} Z_0$. So W is in $\mathbf{M}$ and is a parent of Y_0, which contradicts our choice of Y_0.

Case 4: $X_0 {*\!\!\rightarrow} Y_0$ is oriented by $\mathcal{R}3$. That means there are two non-adjacent vertices U and V such that $U *\!\!-\!* X_0 *\!\!-\!* V$ is a non-collider (which, at the time $X_0 {*\!\!\rightarrow} Y_0$ gets oriented, is $U *\!\!-\!\!\circ X_0 \circ\!\!-\!* V$), and $U {*\!\!\rightarrow} Y_0 \leftarrow\!* V$ is a collider in $\mathcal{P}_2$. U and V must be adjacent to Z_0, otherwise the circle at Y_0 on $Y_0 \circ\!\!-\!* Z_0$

would be oriented by either $\mathcal{R}0$ or $\mathcal{R}1$. Furthermore, since $U *\!\!-\!\!* X_0 *\!\!-\!\!* V$ is a non-collider, either $U *\!\!-\!\!\circ X_0 \circ\!\!-\!\!* V$, or $U \leftarrow X_0$, or $X_0 \rightarrow U$ appears in $\mathcal{P}_2$. It follows that the triple $\langle U, Z_0, V\rangle$ is not a collider, otherwise $X_0 *\!\!-\!\!\circ Z_0$ should be oriented as $X_0 *\!\!\rightarrow Z_0$ by $\mathcal{R}3$ or $\mathcal{R}2$, contrary to our assumption. Also, neither $Z_0 \rightarrow U$ nor $Z_0 \rightarrow V$ is the case, otherwise $Y_0 \circ\!\!-\!\!* Z_0$ should be oriented as $Y_0 \leftarrow\!\!* Z_0$ by $\mathcal{R}2$, contrary to our assumption. Then it must be the case that $U *\!\!-\!\!\circ Z_0 \circ\!\!-\!\!* V$. Again, by $\mathcal{R}3$, $Y_0 \circ\!\!-\!\!* Z_0$ should be oriented as $Y_0 \leftarrow\!\!* Z_0$, a contradiction.

Case 5: $X_0 *\!\!\rightarrow Y_0$ is oriented by $\mathcal{R}4$. There are three sub-cases to consider.

Case 5.1: There is a discriminating path $u = \langle U, ..., W, X_0, Y_0\rangle$ for X_0 in $\mathcal{P}_2$ (and $X_0 \rightarrow Y_0$ is in $\mathcal{G}$), which orients the edge as $X_0 \rightarrow Y_0$. By the definition of discriminating path, $W \leftarrow\!\!* X_0$ and $W \rightarrow Y_0$. So W is adjacent to Z_0, otherwise the circle at Y_0 on $Y_0 \circ\!\!-\!\!* Z_0$ would be oriented by either $\mathcal{R}0$ or $\mathcal{R}1$. It is not the case that $W \rightarrow Z_0$, for otherwise $X_0 *\!\!-\!\!\circ Z_0$ would be oriented as $X_0 *\!\!\rightarrow Z_0$ by $\mathcal{R}2$. It is not the case that $W \leftarrow\!\!* Z_0$, for otherwise $Y_0 \circ\!\!-\!\!* Z_0$ would be oriented as $Y_0 \leftarrow\!\!* Z_0$ by $\mathcal{R}2$, contrary to our assumption. So it has to be that $W \circ\!\!-\!\!* Z_0$. Now we have $X_0 *\!\!\rightarrow W \circ\!\!-\!\!* Z_0$ but not $X_0 *\!\!\rightarrow Z_0$. So W is in $\mathbf{M}$ and is a parent of Y_0, which contradicts our choice of Y_0.

Case 5.2: There is a discriminating path $u = \langle U, ..., X_0, Y_0, W\rangle$ for Y_0 in $\mathcal{P}_2$ (and $X_0 \rightarrow Y_0$ is not in $\mathcal{G}$), which orients the triple as $X_0 \leftrightarrow Y_0 \leftrightarrow W$. Then W is adjacent to Z_0; if not, the circle at Y_0 on $Y_0 \circ\!\!-\!\!* Z_0$ would be oriented by either $\mathcal{R}0$ or $\mathcal{R}1$. By the definition of discriminating path, X_0 is a parent of W, i.e., $X_0 \rightarrow W$. Hence it is not the case that $W *\!\!\rightarrow Z_0$, otherwise $X_0 *\!\!\rightarrow Z_0$ by $\mathcal{R}2$, contrary to what we established at the beginning. So we have $W \leftrightarrow Y_0 \circ\!\!-\!\!* Z_0$ but not $W *\!\!\rightarrow Z_0$, which means W is in $\mathbf{F}_{Y_0}$. But W is a child of X_0, which contradicts our choice of X_0.

Case 5.3: There is a discriminating path $u = \langle U, ..., W, Y_0, X_0\rangle$ for Y_0 in $\mathcal{P}_2$ (and $X_0 \rightarrow Y_0$ is not in $\mathcal{G}$), which orients the triple as $W \leftrightarrow Y_0 \leftrightarrow X_0$. The contradiction in this case is the least obvious, and needs several non-trivial steps to be revealed.

Note that Z_0 is not on u because it is not the case that $Z_0 \to X_0$ as we showed at the beginning. As a first step, we show that for every vertex Q on u between U and W (including W), it is not the case that $Q \leftarrow\!\!* Z_0$. Otherwise, for any such Q, $u(U,Q) \oplus Q \leftarrow\!\!* Z_0 \oplus Z_0 \circ\!\!-\!\!* X_0$ is a discriminating path for Z_0. (We use $\oplus$ to denote the concatenation operation of paths). So the circle at Z_0 on $Z_0 \circ\!\!-\!\!* X_0$ would be oriented by $\mathcal{R}4$, a contradiction.

Next, we establish that every vertex on u between U and W (including U and W) is adjacent to Z_0. Suppose not, let V be the closest vertex to Y_0 on $u(U,W)$ that is not adjacent to Z_0. If $V = W$, the circle at Y_0 on $Y_0 \circ\!\!-\!\!* Z_0$ would be oriented by either $\mathcal{R}0$ or $\mathcal{R}1$. If $V \neq W$, let T be the first vertex after V on $u(V,W)$, which is adjacent to Z_0 (because of our choice of V). Because u is a discriminating path, the edge between V and T is $V *\!\!\rightarrow T$. Since $\langle V, T, Z_0 \rangle$ is an unshielded triple, the edge between T and Z_0 is either $T \to Z_0$ or $T \leftarrow\!\!* Z_0$. Hence it is $T \to Z_0$, as the latter case has been ruled out in the previous step. Then we can show that every vertex on $u(T,W)$ (including W) is a parent of Z_0. Otherwise, let R be the closest vertex to T on $u(T,W)$ that is not a parent of Z_0. Then $u(V,R) \oplus R *\!\!-\!\!* Z_0$ is a discriminating path for R (because every vertex between T and R is a parent of Z_0, by our choice of R). Since it is not the case that $R \to Z_0$, the edge between R and Z_0 must be oriented as $R \leftrightarrow Z_0$, which, however, has been shown impossible. Hence every vertex on $u(T,W)$ (including W) is a parent of Z_0. Then $u(V,Y_0) \oplus Y_0 \circ\!\!-\!\!* Z_0$ is a discriminating path for Y_0, which means the circle at Y_0 on $Y_0 \circ\!\!-\!\!* Z_0$ would be oriented by $\mathcal{R}4$, a contradiction. So every vertex on $u(U,W)$ (including U and W) is adjacent to Z_0.

The contradiction we are about to carry out is on the adjacency between U and Y_0. We first argue that U is not adjacent to Y_0. Suppose for contradiction that they are adjacent. By the definition of discriminating path, U is not adjacent to X_0, so $U *\!\!-\!\!* Y_0 \leftrightarrow X_0$ is an unshielded triple. It follows that either

$\mathcal{R}0$ or $\mathcal{R}1$ could apply here, and it is either $U \leftarrow Y_0 \leftrightarrow X_0$ or $U {*\!\!\rightarrow} Y_0 \leftarrow X_0$. The former case is impossible, because that would make u an inducing path between U and X_0, two non-adjacent vertices, which contradicts the maximality of $\mathcal{G}$. In the latter case, we claim that $U {*\!\!-\!\!\circ}\, Z_0$ is present. Otherwise, either $U {*\!\!\rightarrow} Z_0$ or $U \leftarrow Z_0$. In the former case the circle at Z_0 on $Z_0 \circ\!\!-\!\!* X_0$ would be oriented by either $\mathcal{R}0$ or $\mathcal{R}1$; in the latter case, let S be the vertex next to U on u. Then by $\mathcal{R}2$, the edge between S and Z_0 would be oriented as $S \leftarrow\!\!* Z_0$, which we have shown to be impossible. So $U {*\!\!-\!\!\circ}\, Z_0 \circ\!\!-\!\!* X_0$ is present. Now, by $\mathcal{R}3$, the edge between Y_0 and Z_0 would be oriented as $Y_0 \leftarrow\!\!* Z_0$, a contradiction. Hence U and Y_0 are not adjacent.

An immediate corollary of the above argument is that it is not the case that $Y_0 {\circ\!\!\rightarrow} Z_0$. Otherwise, the edge between U and Z_0 would be oriented either as $U {*\!\!\rightarrow} Z_0$ or as $U \leftarrow Z_0$ (because U and Y_0 are not adjacent). But neither of the two cases can be true, as shown in the above argument. It follows that $Y_0 \circ\!\!-\!\!\circ Z_0$ is present.

Now we are ready to complete the argument. We show (by induction) that every vertex on u between W and U, and in particular U, is adjacent to Y_0, which yields a contradiction. Obviously W is adjacent to Y_0. In the inductive step, we show that if a vertex S_1 between W and U is adjacent to Y_0, then the next vertex S_2 (the one further from W) is also adjacent to Y_0. Suppose otherwise, that S_1 is adjacent to Y_0 but S_2 is not. Because $S_2 *\!\!-\!\!* Z_0 \circ\!\!-\!\!\circ Y_0$ is an unshielded triple, it is not the case that $S_2 {*\!\!\rightarrow} Z_0$. Note that this further rules out $S_1 \rightarrow Z_0$, as the latter implies the former by $\mathcal{R}2$. $S_2 \leftarrow Z_0$ is also impossible, for in that case we have $S_1 \leftarrow\!\!* Z_0$ by $\mathcal{R}2$, which we have ruled out. Hence the only possible case is $S_2 {*\!\!-\!\!\circ}\, Z_0 \circ\!\!-\!\!\circ Y_0$. Now let us focus on the triple $S_2 {*\!\!\rightarrow} S_1 *\!\!-\!\!* Y_0$. It is an unshielded triple, which implies either $S_1 \leftarrow\!\!* Y_0$ or $S_1 \rightarrow Y_0$. In the former case, we can apply $\mathcal{R}3$ to orient the edge between S_1 and Z_0 as $S_1 \leftarrow\!\!* Z_0$, which we have shown to be impossible; in the latter case, since neither $S_1 \rightarrow Z_0$ and $S_1 \leftarrow\!\!* Z_0$ can be true, it must be $S_1 \circ\!-\!* Z_0$. Thus we have $S_2 {*\!\!\rightarrow} S_1 \circ\!-\!* Z_0$ but not $S_2 {*\!\!\rightarrow} Z_0$. Hence S_1 is in $\mathbf{M}$ and is a parent of Y_0. This contradicts our choice of Y_0. So S_2 is also adjacent to Y_0, and by induction U is also adjacent to Y_0. Hence a contradiction, which concludes *Case 5.3.*

Hence, the initial supposition that $\mathbf{M}$ is non-empty leads to contradiction. Furthermore, for any $A \rightarrow B \circ\!\!-\!* C$ in $\mathcal{P}_2$, it is not the case that $A \leftrightarrow C$, for otherwise the circle at B on $B \circ\!\!-\!* C$ could be oriented as an arrowhead by $\mathcal{R}2$. Since we have shown that $A {*\!\!\rightarrow} C$ appears, it is either $A \rightarrow C$ or $A \circ\!\!\rightarrow C$. So **CP**1 holds of $\mathcal{P}_2$, and hence also holds of $\mathcal{P}_4$. □

The following lemma concerning the endpoints of circle paths immediately follows from **CP**1.

Lemma 6. *In $\mathcal{P}_4$, for any two vertices A and B, if there is a circle path, i.e., a path consisting of $\circ\!\!-\!\!\circ$ edges, between A and B, then:*

(i) if there is an edge between A and B, the edge is not into A or B.

(ii) for any other vertex C, $C {*\!\!\rightarrow} A$ if and only if $C {*\!\!\rightarrow} B$. Furthermore, $C \leftrightarrow A$ if and only if $C \leftrightarrow B$.

Proof. We do induction on the length of the circle path. For (i), the base case is trivial. In the inductive step, suppose the proposition holds when there is a circle path consisting of n $\circ\!\!-\!\!\circ$ edges between any two vertices. Consider the case in which the circle path between A and B has $n+1$ edges. Let D be the vertex adjacent to B on the circle path. By the inductive hypothesis, the edge between A and D, if any, is not into D. This implies that the edge between A and B, if any, is not into B, otherwise **CP**1 does not hold of the triple $A {*\!\!\rightarrow} B \circ\!\!-\!\!\circ D$. By symmetry, the edge between A and B, if any, is not into A either. Hence (i) is true.

For (ii), notice that it is a direct consequence of **CP**1 that if $A \circ\!\!-\!\!\circ B$, then for any other vertex C, $C {*\!\!\rightarrow} A$ iff. $C {*\!\!\rightarrow} B$. Furthermore, if $C \leftrightarrow A$, then the edge between C and B can't be $C \circ\!\!\rightarrow B$, for then the triple $A \leftrightarrow C \circ\!\!\rightarrow B$ would violate **CP**1. Neither can it be $C \rightarrow B$, for then $C \rightarrow B \circ\!\!-\!\!\circ A$ would violate **CP**1 (because $C \leftrightarrow A$ is present). So it has to be $C \leftrightarrow B$. By symmetry, $C \leftrightarrow B$ also implies $C \leftrightarrow A$. Thus the base case holds. The inductive step is similar to that in (i). $\square$

Next, we establish a property concerning $-\!\!\circ$ edges, which we will call **CP**2.

Lemma 7. *In $\mathcal{P}_4$, the following property holds:*

CP2 *For any two vertices A, B, if $A -\!\!\circ B$, then there is no edge into A or B.*

Proof. Note that by **CP**1, for any $A -\!\!\circ B$, if $C {*\!\!\rightarrow} B$, then $C {*\!\!\rightarrow} A$. So it suffices to prove that for any $A -\!\!\circ B$, there is no edge into A. Let $\mathbf{E} = \{X -\!\!\circ Y | \exists Z$ s.t. $Z {*\!\!\rightarrow} X\}$. We need to show that $\mathbf{E}$ is empty. Suppose for contradiction that it is not empty. Let $X_0 -\!\!\circ Y_0 \in \mathbf{E}$ be the member of $\mathbf{E}$ that gets oriented first in the orientation process, that is, the tail marks on the other edges in $\mathbf{E}$ 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 $\mathcal{P}_4$. 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 $\mathcal{P}_4$. But then $Z_0 {*\!\!\rightarrow} X_0 - W$ violates (a3) in the definition of ancestral graphs, which contradicts the soundness of $\mathcal{P}_4$.

Case 2: It is oriented by $\mathcal{R}7$. That means there is a vertex W such that W, Y_0 are not adjacent, and $W -\!\!\circ X_0$ or $W - X_0$ appears in $\mathcal{P}_4$. The latter case has been ruled out in the above case. In the former case, since $Z_0 {*\!\!\rightarrow} X_0$ is in $\mathcal{P}_4$, by **CP**1, $Z_0 {*\!\!\rightarrow} W$ is in $\mathcal{P}_4$, too. But then $W -\!\!\circ X_0$ is in $\mathbf{E}$ and gets oriented before $X_0 -\!\!\circ Y_0$ does, which contradicts our choice of $X_0 -\!\!\circ Y_0$.

Hence the supposition that $\mathbf{E}$ is not empty is false. **CP**2 holds of $\mathcal{P}_4$. $\square$

Since $\mathcal{P}_4$ is sound, i.e., every non-circle mark therein is invariant in $[\mathcal{G}]$, any MAG equivalent to $\mathcal{G}$ should contain the non-circle marks in $\mathcal{P}_4$. In other words, every MAG equivalent to $\mathcal{G}$ is a further orientation of $\mathcal{P}_4$ in the sense of changing circles into arrowheads or tails. To prove arrowhead completeness, we need to show that every circle can be oriented into a tail in some MAG orientation of $\mathcal{P}_4$. The following operation takes care of all circles on $\circ\!\!\rightarrow$ and $\circ\!\!-$ edges (and some circles on $\circ\!\!-\!\!\circ$ edges).

Definition 11 (Tail Augmentation). *Let $\mathcal{H}$ be any partial mixed graph.* **Tail augmentation** *of $\mathcal{H}$ is defined as the following set of operations on $\mathcal{H}$:*

- *change all $\circ\!\!\rightarrow$ edges into directed edges $\rightarrow$;*
- *change all $\circ\!\!-$ edges into undirected edges $-$;*
- *for any $A \circ\!\!-\!\!\circ B$, if there is no arrowhead into A or B, then change the edge into an undirected edge $A - B$.*

The resulting graph is called the **tail augmented graph (TAG)** *of $\mathcal{H}$, denoted by $\mathcal{H}_{tag}$.*

It is clear that the tail augmentation changes some circles in a PMG to tails, but does not affect any non-circle mark already in the PMG. Furthermore, after tail augmentation, all the remaining circles, if any, belong to $\circ\!\!-\!\!\circ$ edges. Now consider the TAG of $\mathcal{P}_4$, $\mathcal{P}_{4tag}$. It is obvious that **CP**1 still holds of $\mathcal{P}_{4tag}$ as well as (a1)-(a3) in Definition 1. Furthermore, Lemma 6 and Lemma 7 ensure that no endpoint of a (remaining) $\circ\!\!-\!\!\circ$ edge is an endpoint of an undirected edge in $\mathcal{P}_{4tag}$.

Lemma 8. *Let $\mathcal{P}_{4tag}$ be the TAG of $\mathcal{P}_4$. In $\mathcal{P}_{4tag}$,*

(i) (a1)-(a3) (in Definition 1) and **CP**1 *hold;*

(ii) there is no inducing path between two non-adjacent vertices; and

(iii) there is no such triple as $A - B \circ\!\!-\!\!\circ C$.

Proof. First we prove (i). For (a1), suppose for contradiction that there is a directed cycle. Let $c = \langle V_0, \cdots, V_n, V_0\rangle$ be a shortest directed cycle in $\mathcal{P}_{4tag}$, that is, no other directed cycle has fewer edges than c does. Since no directed cycle is present in $\mathcal{P}_4$, the corresponding cycle in $\mathcal{P}_4$ must contain a $\circ\!\!\rightarrow$ edge. That is, there exists i such that $V_{i-1}{*\!\!\rightarrow}\, V_i{\circ\!\!\rightarrow}\, V_{i+1}$ is in $\mathcal{P}_4$. Because **CP**1 holds of $\mathcal{P}_4$, there is an edge $V_{i-1}{*\!\!\rightarrow}\, V_{i+1}$ in $\mathcal{P}_4$. The edge can't be $V_{i-1} \leftrightarrow V_{i+1}$ for the following reason: the edge between V_{i-1} and V_i is either $V_{i-1}{\circ\!\!\rightarrow}\, V_i$ or $V_{i-1} \rightarrow V_i$. In the former case, the triple $V_{i+1} \leftrightarrow V_{i-1}{\circ\!\!\rightarrow}\, V_i$ would violate **CP**1; in the latter case, the circle at V_i on $V_i \circ -* V_{i+1}$ should have been oriented by $\mathcal{R}2$. So either $V_{i-1}{\circ\!\!\rightarrow}\, V_{i+1}$ or $V_{i-1} \rightarrow V_{i+1}$ is in $\mathcal{P}_4$, which means $V_{i-1} \rightarrow V_{i+1}$ is in $\mathcal{P}_{4tag}$. But then $\langle V_0, \cdots, V_{i-1}, V_{i+1}, \cdots, V_n, V_0\rangle$ is a shorter cycle than c is, hence a contradiction. So there is no directed cycle in $\mathcal{P}_{4tag}$.

For (a2), suppose for contradiction that there is an almost directed cycle in $\mathcal{P}_{4tag}$. Let $c = \langle V_0, \cdots, V_n, V_0\rangle$ be a shortest one. Without loss of generality, suppose the bi-directed edge in the cycle is $V_0 \leftrightarrow V_n$, and $\langle V_0, V_1, \cdots, V_n\rangle$ is a directed path from V_0 to V_n. It is obvious that $V_0 \leftrightarrow V_n$ is also in $\mathcal{P}_4$, because no extra arrowheads are introduced in $\mathcal{P}_{4tag}$. Since no almost directed cycle is present in $\mathcal{P}_4$, the corresponding path between V_0 and V_n in $\mathcal{P}_4$ contains a $\circ\!\!\rightarrow$ edge. If the edge between V_0 and V_1 is not $\circ\!\!\rightarrow$, then there must exist $1 \leq i \leq n-1$ such that $V_{i-1}{*\!\!\rightarrow}\, V_i{\circ\!\!\rightarrow}\, V_{i+1}$ is in $\mathcal{P}_4$. By the same argument we went through in proving (a1), there is a shorter directed path from V_0 to V_n and hence a shorter almost directed cycle. So it is $V_0{\circ\!\!\rightarrow}\, V_1$ that appears in $\mathcal{P}_4$, then by **CP**1, $V_n{*\!\!\rightarrow}\, V_1$ is in $\mathcal{P}_4$, which means either $V_n \rightarrow V_1$ or $V_n \leftrightarrow V_1$ is in $\mathcal{P}_{4tag}$. In the former case, there is a directed cycle in $\mathcal{P}_{4tag}$, which we have shown to be impossible; in the latter case, there is a shorter almost directed cycle, a contradiction.

For (a3), note that any $X - Y$ in $\mathcal{P}_{4tag}$ corresponds to either $X - Y$ or $X -\!\!\circ Y$ or $X \circ\!\!-\!\!\circ Y$ in $\mathcal{P}$. In the first case, there is no edge into X or Y due to the soundness of $\mathcal{P}_4$; in the second case, **CP**2 (Lemma 7) guarantees that there is no edge into X or Y; in the third case, the definition of tail augmentation guarantees that there is no edge into X or Y.

For **CP1**, note that no extra arrowheads are introduced in $\mathcal{P}_{4tag}$ and hence any pattern of $*\!\!\rightarrow \circ\!\!-\!\!*$ in $\mathcal{P}_{4tag}$ is also in $\mathcal{P}_4$. Since **CP1** holds of $\mathcal{P}_4$, it also holds of $\mathcal{P}_{4tag}$.

Next, we prove (ii). It is convenient to define the *rank* of an inducing path. By definition (Definition 4), an inducing path is one on which every vertex (except the endpoints) is a collider and is an ancestor of one of the endpoints. In other words, from each interior vertex on the path there is a directed path to one of the endpoints. Let the *rank* of each interior vertex on the path be the length of a shortest directed path from that vertex to one of the endpoints. We define the *rank* of an inducing path as the length of the path plus the sum of the ranks of the interior vertices.

Suppose for contradiction that in $\mathcal{P}_{4tag}$ there is an inducing path between two non-adjacent vertices X and Y. Let $p = \langle X = V_0, V_1, \cdots, V_{n-1}, Y = V_n \rangle$ be the one of the lowest rank. By definition, V_i's $(1 \leq i \leq n-1)$ are colliders on the path and are ancestors of either X or Y. This implies that V_1 is an ancestor of Y and V_{n-1} is an ancestor of X, otherwise there would be a directed or almost directed cycle in $\mathcal{P}_{4tag}$, which we have shown to be absent. For the same reason, the edge between X and V_1 is $X \leftrightarrow V_1$, and the edge between V_{n-1} and Y is $V_{n-1} \leftrightarrow Y$. So every edge on p is bi-directed. Since no extra arrowheads are introduced in $\mathcal{P}_{4tag}$, these bi-directed edges on p are also in $\mathcal{P}_4$.

Furthermore, note that $\mathcal{P}_4$ is sound and hence should not contain any inducing path between X and Y. It follows that not every interior vertex on p is an ancestor of X or Y in $\mathcal{P}_4$. Let V_j $(1 \leq j \leq n-1)$ be such a vertex, that is, V_j is not an ancestor of X or Y in $\mathcal{P}_4$. Without loss of generality, suppose in $\mathcal{P}_{4tag}$, V_j is an ancestor of Y. Let d be a shortest directed path from V_j to Y in $\mathcal{P}_{4tag}$. Since d is not a directed path in $\mathcal{P}_4$, d must contain a $\circ\!\!\rightarrow$ edge in $\mathcal{P}_4$. Since d is a shortest one, **CP1** implies that $\circ\!\!\rightarrow$ can only appear as the first edge on the directed path (by the argument we have used several times above).

That is, let V_{j1} be the vertex adjacent to V_j on d, then $V_j \circ\!\!\rightarrow V_{j1}$ is in $\mathcal{P}_4$.

Now we argue that there is a V_k $(j+1 \leq k \leq n-1)$ such that $V_k \leftrightarrow V_{j1}$ is in $\mathcal{P}_4$. Suppose not; we prove by induction that for every $j+1 \leq i \leq n$, either $V_i \circ\!\!\rightarrow V_{j1}$ or $V_i \rightarrow V_{j1}$ is present in $\mathcal{P}_4$. The base case is easy. Since $V_{j+1} \leftrightarrow V_j \circ\!\!\rightarrow V_{j1}$ is in $\mathcal{P}_4$, by $\mathbf{P}_4$, we have $V_{j+1} *\!\!\rightarrow V_{j1}$. Since it is not bi-directed by the supposition, it is either $V_{j+1} \circ\!\!\rightarrow V_{j1}$ or $V_{j+1} \rightarrow V_{j1}$. In the inductive step, suppose $V_{j+1}, ..., V_m$ all satisfy the claim, we argue that V_{m+1} also satisfies the claim. V_{m+1} must be adjacent to V_{j1}, otherwise either a $V_k \circ\!\!\rightarrow V_{j1}$ will be oriented as $V_k \leftrightarrow V_{j1}$ $(j+1 \leq k \leq m)$ by $\mathcal{R}4$, or all $V_k \circ\!\!\rightarrow V_{j1}$ will be oriented into $V_k \rightarrow V_{j1}$, and hence $V_j \circ\!\!\rightarrow V_{j1}$ will be oriented by $\mathcal{R}4$. Furthermore, the edge between V_{m+1} and V_{j1} is $V_{m+1} *\!\!\rightarrow V_{j1}$. This is because either $V_m \circ\!\!\rightarrow V_{j1}$ or $V_m \rightarrow V_{j1}$ appears. In the former case, $V_{m+1} *\!\!\rightarrow V_{j1}$ by **CP**1; in the latter case, $V_{m+1} *\!\!\rightarrow V_{j1}$ by $\mathcal{R}2$. Lastly, since the edge between V_{m+1} and V_{j1} is not bi-directed (in the case of $V_{m+1} = Y$, it is not $Y \leftrightarrow V_{j1}$ because V_{j1} is an ancestor of Y in $\mathcal{P}_{4tag}$), it is either $V_{m+1} \circ\!\!\rightarrow V_{j1}$ or $V_{m+1} \rightarrow V_{j1}$. This completes the induction. But then either $Y \circ\!\!\rightarrow V_{j1}$ or $Y \rightarrow V_{j1}$, which contradicts the fact that V_{j1} is an ancestor of Y in $\mathcal{P}_{4tag}$. So there is a V_k $(j+1 \leq k \leq n-1)$ such that $V_k \leftrightarrow V_{j1}$ is in $\mathcal{P}_4$.

By essentially the same argument, we can show that there is a V_h $(0 \leq h \leq j-1)$ such that $V_h \leftrightarrow V_{j1}$ is in $\mathcal{P}_4$. (The only difference is that we rule out the case $X \circ\!\!\rightarrow V_{j1}$ and the case $X \rightarrow V_{j1}$ not because V_{j1} is an ancestor of X, but because X cannot be an ancestor of Y in $\mathcal{P}_{4tag}$, for otherwise an almost directed cycle would be present.) This implies that the path $\langle V_0 = X, \cdots, V_h, V_{j1}, V_k, \cdots, V_n = Y \rangle$ (V_h could be V_0) is an inducing path between X and Y but is of a lower rank than p, a contradiction. Hence there is no inducing path between two non-adjacent vertices in $\mathcal{P}_{4tag}$.

Lastly, we demonstrate (iii). Suppose for contradiction that there is such a triple $X - Y \circ\!\!-\!\!\circ Z$ in $\mathcal{P}_{4tag}$. By the definition of tail augmentation, in $\mathcal{P}_4$ the edge between X and Y is either $X \,—Y$ or $X \circ\!— Y$ or $X \circ\!\!—\!\!\circ Y$. In the first case, obviously the circle at Y on $Y \circ\!\!—\!\!\circ Z$ should have been oriented by $\mathcal{R}_6$; in the second case, by $\mathbf{CP_2}$, there is no edge into Y, and then by Lemma 6, there is no edge into Z either, so $Y \circ\!\!—\!\!\circ Z$ should be changed to $Y \,—Z$ in the tail augmentation; in the third case, since $X \circ\!\!—\!\!\circ Y$ is changed to $X \,—Y$ in the tail augmentation, there is no edge into Y in $\mathcal{P}_4$, which implies, by Lemma 6, that there is no edge into Z either, and hence $Y \circ\!\!—\!\!\circ Z$ should be changed to $Y \,—Z$ in the tail augmentation. Therefore, each case leads to a contradiction. □

Let the **circle component** of any PMG be the induced subgraph that consists of all $\circ\!\!—\!\!\circ$ edges in the PMG. We denote the circle component of $\mathcal{P}_{4tag}$ by $\mathcal{P}^c_{4tag}$. Since **CP1** holds of $\mathcal{P}_{4tag}$, no matter how we orient the remaining $\circ\!\!—\!\!\circ$ edges (i.e., $\mathcal{P}^c_{4tag}$), no new unshielded colliders or directed cycles or almost directed cycles would be created that involve the arrowheads already present in $\mathcal{P}_{4tag}$. In particular, as shown in the next lemma, if we orient $\mathcal{P}^c_{4tag}$ into a directed acyclic graph with no unshielded colliders, then the resulting graph is a maximal ancestral graph and is Markov equivalent to $\mathcal{G}$.

Lemma 9. *Let $\mathcal{P}_{4tag}$ be the TAG of $\mathcal{P}_4$. If we further orient $\mathcal{P}^c_{4tag}$, the circle component of $\mathcal{P}_{4tag}$, into a DAG with no unshielded colliders, the resulting graph is a MAG and is Markov equivalent to $\mathcal{G}$.*

Proof. Let $\mathcal{H}$ denote the resulting graph. We first show that $\mathcal{H}$ is a MAG. Since $\mathcal{H}$ is obviously a mixed graph, we only need to check that $(a1) - (a3)$ in Definition 1 hold, and that there is no inducing path between two non-adjacent vertices. The argument is very similar to the one we saw in the previous lemma, so we will only highlight the strategy.

There is no directed cycle in $\mathcal{H}$. Otherwise let c be a shortest one. The corresponding cycle in $\mathcal{P}_{4tag}$ must contain $\rightarrow \circ\!\!—\!\!\circ$, because there is no directed cycle in $\mathcal{P}_{4tag}$ and by assumption $\mathcal{P}^c_{4tag}$ is oriented into a DAG. Then **CP1** implies that there is a shorter directed cycle in $\mathcal{H}$, a contradiction.

For almost the same reason, there is no almost directed cycle in $\mathcal{H}$. Otherwise a shortest such cycle must be present in $\mathcal{P}_{4tag}$.

For any X — Y in $\mathcal{H}$, it is also in $\mathcal{P}_{4tag}$, because no new undirected edge is created in $\mathcal{H}$. We have shown that there is no edge into X or Y in $\mathcal{P}_{4tag}$, and that there is no $\circ\!\!-\!\!\circ$ edge incident to X or Y in $\mathcal{P}_{4tag}$. It obviously follows that there is no edge into X or Y in $\mathcal{H}$.

To show that $\mathcal{H}$ is maximal, we will again use the rank of an inducing path as defined in the proof of the previous lemma. Suppose for contradiction that there is an inducing path between two non-adjacent vertices X and Y in $\mathcal{H}$. Consider one that is of the lowest rank, $p = \langle V_0 = X, V_1, \cdots, V_{n-1}, V_n = Y \rangle$. As we have shown in the proof of the previous lemma, every edge on p is bi-directed, which is also in $\mathcal{P}_{4tag}$, because no new bi-directed edge is created in $\mathcal{H}$. Then we shall argue that in $\mathcal{P}_{4tag}$ it is also the case that every V_i $(1 \leq i \leq n-1)$ is an ancestor of either X or Y, and hence p is also an inducing path in $\mathcal{P}_{4tag}$, which contradicts the last lemma. Here is the argument. For an arbitrary V_i $(1 \leq i \leq n-1)$, by supposition, it is an ancestor of X or Y in $\mathcal{H}$. Without loss of generality, suppose it is an ancestor of Y. Let d be a shortest directed path from V_i to Y. Then d must also be a directed path in $\mathcal{P}_{4tag}$. Suppose not, then it contains a $\circ\!\!-\!\!\circ$ in $\mathcal{P}_{4tag}$. Furthermore, the first edge must be $V_i \circ\!\!-\!\!\circ V_{i1}$, for otherwise $\rightarrow \circ\!\!-\!\!\circ$ would appear on the path and **CP1** implies there is a shorter directed path in $\mathcal{H}$. Now by Lemma 6, we have $V_{i-1} \leftrightarrow V_{i1}$ and $V_{i+1} \leftrightarrow V_{i1}$, which means we can replace V_i with V_{i1} and create an inducing path with a lower rank (because the directed path from V_{i1} to Y is shorter than the one from V_i to Y). Contradiction. So d is also a directed path in $\mathcal{P}_{4tag}$, which means V_i is also an ancestor of Y in $\mathcal{P}_{4tag}$. That is, p is also an inducing path between X and Y in $\mathcal{P}_{4tag}$, which contradicts the previous lemma.

Therefore $\mathcal{H}$ is a maximal ancestral graph.

Now that we have shown $\mathcal{H}$ to be a MAG, we only need to check the conditions in Proposition 2 to demonstrate its Markov equivalence with $\mathcal{G}$. Obviously they have the same adjacencies, i.e., $(e1)$ holds. For $(e2)$, notice that every unshielded collider in $\mathcal{G}$ is also in $\mathcal{P}_4$ – which is guaranteed by $\mathcal{R}0$ – and hence is also in $\mathcal{H}$. Conversely, for any unshielded collider in $\mathcal{H}$, in $\mathcal{P}_{4tag}$, the triple is either $*\!\!\rightarrow\leftarrow\!\!*$, or $*\!\!\rightarrow$ o—o, or o—o o—o. The latter two cases are impossible, because by **CP1** $*\!\!\rightarrow$ o—o implies that the triple is shielded; and by assumption, the circle component is oriented into a DAG with no unshielded colliders. So it must be the first case. Then the unshielded collider is also in $\mathcal{P}_4$ (because no arrowhead is introduced in tail augmentation), and hence also in $\mathcal{G}$.

Thus if $\mathcal{H}$ and $\mathcal{G}$ are not Markov equivalent, it is due to a violation of $(e3)$. That is, there is a path $u = \langle W, ..., X, Y, Z\rangle$ that is discriminating for Y in both graphs, but the triple $\langle X, Y, Z\rangle$ is a collider in one of the graphs but a non-collider in the other. Note that if the triple is a collider in $\mathcal{H}$, then it is easy to deduce from the definition of discriminating path that $X \leftrightarrow Y \leftrightarrow Z$ is in $\mathcal{H}$. But every bi-directed edge in $\mathcal{H}$ is also in $\mathcal{P}_4$ (because neither tail augmentation nor the further orientation of $\mathcal{P}_{4tag}$ creates any new bi-directed edge), so $A \leftrightarrow B \leftrightarrow C$ is also in $\mathcal{G}$. Therefore, it can only be the case that $\langle A, B, C\rangle$ is a collider in $\mathcal{G}$ and a non-collider in $\mathcal{H}$. We will derive a contradiction from this.

First of all, we argue that if every collider on $u(W, Y) = \langle W, \cdots, X, Y\rangle$ is present in $\mathcal{P}_4$, then every vertex between W and X (including A) is a parent of Z in $\mathcal{P}_4$. The argument goes by induction. Let U be the vertex next to W on u. $\langle W, U, Z\rangle$ is an unshielded triple (because by the definition of discriminating path, W and Z are not adjacent). Since by assumption U is a collider on the path, $W{*\!\!\rightarrow}\, U$ is in $\mathcal{P}_4$; so the edge between U and Z is either oriented as $U \leftarrow\!\!* Z$ by $\mathcal{R}0$ or $U \rightarrow Z$ by $\mathcal{R}1$. It cannot be the former case, because in $\mathcal{G}$ (and in $\mathcal{H}$) we have $U \rightarrow Z$. Hence $U \rightarrow Z$ is in $\mathcal{P}_4$. Now suppose the first n vertices after W on u are all parents of Z in $\mathcal{P}_4$. Then the edge between the $n+1^{st}$ vertex and Z can be oriented by $\mathcal{R}4$. Because it is a parent of Z in $\mathcal{G}$, the edge should be oriented as a directed edge into Z. End of induction. Therefore, if every collider on $u(W, Y)$ is present in $\mathcal{P}_4$, u is also a discriminating path in $\mathcal{P}_4$, which means the triple $\langle X, Y, Z\rangle$ would be oriented as a collider, as is the case in $\mathcal{G}$. Then it would be a collider in $\mathcal{H}$, too, a contradiction.

Thus some collider on $u(W, Y)$ is not present in $\mathcal{P}_4$. In other words, some arrowheads on the path correspond to circles in $\mathcal{P}_4$. Note also that only the first and/or the last collider on the path can be absent from $\mathcal{P}_4$, because bi-directed edges in $\mathcal{H}$, if any, are all in $\mathcal{P}_4$ as well. Below we consider three cases separately.

Case 1: $u(W, Y)$ only has three vertices, $\langle W, X, Y\rangle$. So in $\mathcal{P}_4$, it is either (a) $W \circ\!\!-\!\!\circ X \leftarrow\!\!* Y$, or (b) $W *\!\!\rightarrow X \circ\!\!-\!\!\circ Y$, or (c) $W \circ\!\!-\!\!\circ X \circ\!\!-\!\!\circ Y$ (because extra arrowheads are only introduced in the orientation of the circle component of $\mathcal{P}_{4tag}$). In (a) and (b), by **CP1**, W and Y are adjacent. In (c), because $\langle W, X, Y\rangle$ is oriented as a collider in $\mathcal{H}$, and by assumption no unshielded collider is introduced in the orientation of $\mathcal{P}^c_{4tag}$, W and Y must also be adjacent ($W \circ\!\!-\!\!\circ Y$). So $\langle W, Y, Z\rangle$ is an unshielded triple, in any case. Since $\langle X, Y, Z\rangle$ is a non-collider in $\mathcal{H}$, it must be that $Y \rightarrow Z$, which can be easily deduced from the definition of discriminating path. Thus $\langle W, Y, Z\rangle$ is an unshielded non-collider in $\mathcal{H}$. We already showed that $\mathcal{G}$ and $\mathcal{H}$ have the same unshielded colliders, so $\langle W, Y, Z\rangle$ is also an unshielded non-collider in $\mathcal{G}$. Furthermore, since $\langle X, Y, Z\rangle$ is a collider in $\mathcal{G}$, we have $X \leftrightarrow Y \leftrightarrow Z$ in $\mathcal{G}$, and hence the edge between W and Y must be $W \leftarrow Y$ (to avoid collider). But then the path u is an inducing path between W and Z in $\mathcal{G}$, which contradicts the fact that $\mathcal{G}$ is maximal.

Case 2: $u(W, Y)$ has four vertices, $\langle W, U, X, Y\rangle$. So in $\mathcal{P}_4$, it is either (a) $W \circ\!\!-\!\!\circ U \leftrightarrow X \leftarrow\!\!* Y$, or (b) $W *\!\!\rightarrow U \leftrightarrow X \circ\!\!-\!\!\circ Y$, or (c) $W \circ\!\!-\!\!\circ U \leftrightarrow X \circ\!\!-\!\!\circ Y$. In (c), it is easy to deduce from Lemma 6 that $W \leftrightarrow Y$ is in $\mathcal{P}_4$, and hence is in both $\mathcal{G}$ and $\mathcal{H}$. But then the triple $\langle W, Y, Z\rangle$ is an unshielded collider in $\mathcal{G}$ but not in $\mathcal{H}$, contrary to what we already showed. In (a), Lemma 6 implies that $W \leftrightarrow X$. Hence $X \rightarrow Z$ is also present in $\mathcal{P}_4$. So the path $\langle W, X, Y, Z\rangle$ is a discriminating path for Y in $\mathcal{P}_4$, which means the edge between Y and Z

should be the same in $\mathcal{G}$ and $\mathcal{H}$, contrary to the assumption. In (b), Lemma 6 implies that $U \leftrightarrow Y$. For the same reason as in (a), the path $\langle W, U, Y, Z\rangle$ is a discriminating path for Y in $\mathcal{P}_4$, hence the edge between Y and Z should be the same in $\mathcal{G}$ and $\mathcal{H}$, contrary to the assumption.

Case 3: $u(W, Y)$ has more than four vertices, $\langle W, U, V_1, ..., V_2, X, Y\rangle$ (V_1 and V_2 could be the same vertex). Again there are three cases: (a) $W \circ\!\!-\!\!\circ U \leftrightarrow V_1 \cdots V_2 \leftrightarrow X \leftarrow\!\!* Y$, or (b) $W *\!\!\rightarrow U \leftrightarrow V_1 \cdots V_2 \leftrightarrow X \circ\!\!-\!\!\circ Y$, or (c) $W \circ\!\!-\!\!\circ U \leftrightarrow V_1 \cdots V_2 \leftrightarrow X \circ\!\!-\!\!\circ Y$. In any of the three cases, by essentially the same argument as we saw in *Case 2*, there would be a discriminating path in $\mathcal{P}_4$ for Y that ends at Z, so the edge between Y and Z should be the same in $\mathcal{G}$ and $\mathcal{H}$, contrary to the assumption.

Therefore, the initial supposition of non-equivalence is false. $\mathcal{H}$ and $\mathcal{G}$ are Markov equivalent. $\square$

To orient $\mathcal{P}^c_{4tag}$ into a DAG is trivial – an arbitrary ordering over the vertices in $\mathcal{P}^c_{4tag}$ would do. But that does not in general yield a DAG with no unshielded colliders. In fact, as is well known, an undirected graph can be oriented into a DAG with no unshielded colliders if and only if it is chordal (see, e.g., Meek (1995). A graph is **chordal** (a.k.a **triangular**) if there is no cycle of length 4 or more without an edge (chord) linking two non-consecutive vertices on the cycle. The chordality of $\mathcal{P}^c_{4tag}$ is not hard to see.

Lemma 10. *The circle component of $\mathcal{P}_{4tag}$, $\mathcal{P}^c_{4tag}$, is chordal.*

Proof. Suppose for contradiction that there is a cycle $\langle V_0, V_1, \cdots, V_{n-1}, V_n, V_0\rangle$ in $\mathcal{P}^c_{4tag}$ such that no non-consecutive vertices on the cycle are adjacent. We argue that the cycle is also chordless in $\mathcal{P}_{4tag}$, and hence chordless in $\mathcal{P}_4$ (because $\mathcal{P}_{4tag}$ and $\mathcal{P}_4$ have the same adjacencies). Suppose on the contrary that in $\mathcal{P}_{4tag}$ there is an edge linking two nonadjacent vertices on the cycle, say, V_i and V_j. The edge is either $V_i - V_j$ or is into at least one of them. By Lemma 8, there is no such pattern as $- \circ\!\!-\!\!\circ$ in $\mathcal{P}_{4tag}$, so the former case is impossible. By

Lemma 6, since there is a circle path between V_i and V_j, the edge between V_i and V_j, if any, is not into V_i or V_j in $\mathcal{P}_4$, and hence is not into V_i or V_j in $\mathcal{P}_{4tag}$. So the latter case is also impossible. Hence the cycle is also chordless in $\mathcal{P}_4$. But then the edge $V_0 \circ\!\!-\!\!\circ V_1$ (as well as other edges on the cycle) should have been oriented by $\mathcal{R}5$. Contradiction. Therefore, there is no such cycle in $\mathcal{P}^c_{4tag}$ in the first place, which means $\mathcal{P}^c_{4tag}$ is chordal. □

Therefore, $\mathcal{P}^c_{4tag}$ can be oriented into a DAG with no unshielded colliders. By Lemma 9, there is a MAG in $[\mathcal{G}]$ — the Markov equivalence class to which $\mathcal{G}$ belongs — in which all circles except possibly ones in $\mathcal{P}^c_{4tag}$ are marked as tails. In other words, these circles do not hide invariant arrowheads. The next lemma due to Meek (1995) entails that the circles in $\mathcal{P}^c_{4tag}$ do not hide invariant arrowheads either.

Lemma 11 (Meek). *Let X and Y be any two vertices adjacent in a chordal graph. That graph can be oriented into a directed acyclic graph with no unshielded colliders in which the edge between X and Y is oriented as $X \to Y$.*

The completeness of $\mathcal{P}_4$ with respect to arrowheads is now evident.

Theorem 2. *$\mathcal{P}_4$ is complete with respect to arrowheads. That is, for every circle in $\mathcal{P}_4$, there is a member of $[\mathcal{G}]$ in which the circle is oriented as a tail.*

Proof. It follows readily from Lemma 9, Lemma 10 and Lemma 11. □

3.2.3 Completeness w.r.t Tails

Now we turn to the even more involved task of showing that $\mathcal{P}_4$ is also complete with respect to tails, that is, for every circle in $\mathcal{P}_4$, there is a MAG equivalent to $\mathcal{G}$ in which the circle is oriented as an arrowhead. The following operation introduces arrowheads to the circles on the $-\!\!\circ$ edges.

Definition 12 (Arrowhead Augmentation). *Let $\mathcal{H}$ be any partial mixed graph.* **Arrowhead augmentation** *of $\mathcal{H}$ is defined as the following set of operations on $\mathcal{H}$:*

- *change all $\circ\!\!\rightarrow$ edges into directed edges $\rightarrow$;*
- *change all $-\!\!\circ$ edges into directed edges $\rightarrow$.*

The resulting graph is called the **arrowhead augmented graph (AAG)** *of $\mathcal{H}$, denoted by $\mathcal{H}_{aag}$.*

Thus the arrowhead augmentation and the tail augmentation are common in their treatments of $\circ\!\!\rightarrow$ edges. They are distinguished by their treatments of $-\!\!\circ$ edges: the tail augmentation turns the circles into tails, whereas the arrowhead augmentation turns the circles into arrowheads. Furthermore, unlike the tail augmentation, the arrowhead augmentation does not affect any $\circ\!\!-\!\!\circ$ edge.

Let $\mathcal{P}_{4aag}$ be the AAG of $\mathcal{P}_4$. We will prove a lemma about $\mathcal{P}_{4aag}$ analogous to Lemma 8. For that purpose, we need to establish some properties of $\mathcal{P}_4$ concerning $-\!\!\circ$ edges. A path $\langle V_0, \cdots, V_n \rangle$ is called a **tail-circle path** from V_0 to V_n if for every i $(0 \leq i \leq n-1)$, $V_i -\!\!\circ V_{i+1}$.

Lemma 12. *In $\mathcal{P}_4$, the following hold:*

(i) For any $A -\!\!\circ B$, there is an uncovered tail-circle path from an endpoint of an undirected edge to B that includes the edge $A -\!\!\circ B$.

(ii) If u is an uncovered tail-circle path, then any two non-consecutive vertices on u are not adjacent.

Proof. Let **TC** be the set of $-\!\!\circ$ edges in $\mathcal{P}_4$. We can order the members of **TC** by their order of occurrence in the orientation process. (i) can be proved by induction. Let $X -\!\!\circ Y$ be the "first" edge in **TC** – that is, it gets oriented as such before any other member of **TC** does (i.e., the others were still $\circ\!\!-\!\!\circ$ edges). Among all the orientation rules, only $\mathcal{R}6$ and $\mathcal{R}7$ could yield $-\!\!\circ$ edges. If $X -\!\!\circ Y$ is oriented by $\mathcal{R}6$, then obviously X is an endpoint of an undirected edge; if $X \multimap Y$ is oriented by $\mathcal{R}7$, which means there is a vertex Z such that Z, Y are not adjacent, and $Z \multimap X \circ\!\!-\!\!\circ Y$ is the configuration at the point of orienting $X \circ\!\!-\!\!\circ Y$. If $Z \multimap X$ remains in $\mathcal{P}_4$, then it belongs to **TC**, and it occurs earlier than $X \multimap Y$ does, which contradicts our assumption about $X \multimap Y$. So in $\mathcal{P}_4$ it must be $Z - X$ (because no orientation rule will orient $\multimap$ into $\rightarrow$). Hence in either case X is an endpoint of an undirected edge. Then $X \multimap Y$ is an uncovered tail-circle path from an endpoint of an undirected edge to Y.

Now we show the inductive step. Suppose the first n edges in **TC** satisfy (i); consider the $n+1^{st}$ edge, $U \multimap W$, 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 $U \multimap W$ constitutes an uncovered tail-circle path from U to W; if it is oriented by $\mathcal{R}7$, then there is a vertex V such that V, W are not adjacent, and $V \multimap U \circ\!\!-\!\!\circ W$ is the configuration at the point of orienting $X \circ\!\!-\!\!\circ Y$. If $V \multimap U$ remains in $\mathcal{P}_4$, then it is one of the first n edges in **TC**. By the inductive hypothesis, there is an uncovered tail-circle path, T, from an endpoint of an undirected edge to U that includes the edge $V \multimap U$. Since V, W are not adjacent, T appended to $U \multimap W$ constitutes an uncovered tail-circle path from an endpoint of an undirected edge to W. If, on the other hand, $V \multimap U$ is not in $\mathcal{P}_4$, then it must be $V - U$, which makes U an endpoint of an undirected edge, and $U \multimap W$ the desired path. Therefore, for every edge in **TC**, the property stated in (i) holds.

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

Now suppose u consists of more than two edges. We prove (ii) by induction on the length of u. The base case is that u has three edges: $X \multimap Y \multimap$

$Z \multimap W$. Suppose for contradiction that a pair of non-consecutive vertices on u is adjacent. Because u is uncovered, this pair must be X and W. By **CP**2 (Lemma 7), the edge between X and W is not into X or W. It is not an undirected edge either, for otherwise the circle at W on $Z \multimap W$ should have been oriented by $\mathcal{R}6$. However, $\langle X, Y, Z, W, X \rangle$ forms an uncovered cycle, so at least one of the $\circ\!\!-\!\!\circ$ edges on the cycle should have been oriented as $-$ by $\mathcal{R}5$ before any $\multimap$ edge appears. Contradiction. So X and W are not adjacent.

In the inductive step, suppose the proposition holds for those uncovered circle-tail paths that have fewer than n edges. Consider an uncovered circle-tail path with $n+1$ edges: $V_0 \multimap V_1 \cdots V_n \multimap V_{n+1}$. By the inductive hypothesis, the only pair of non-consecutive vertices that could be adjacent is V_0 and V_{n+1}. But then the same argument applies. That is, the edge between V_0 and V_{n+1} is not into X or W, nor is it an undirected edge. But we have an uncovered cycle $\langle V_0, V_1, \cdots, V_n, V_{n+1}, V_0 \rangle$, which means at least one of the $\circ\!\!-\!\!\circ$ edges on the cycle should have been oriented as $-$ by $\mathcal{R}5$ before any $\multimap$ edge appears. This yields a contradiction. So V_0 and V_{n+1} are not adjacent. $\square$

The main utility of Lemma 12 is to prove the next two lemmas.

Lemma 13. *In $\mathcal{P}_4$, the following property holds:*

CP3 *For any three vertices A, B, C, if $A \multimap B \circ\!\!-\!\!* C$, then A and C are adjacent. Furthermore, if $A \multimap B \circ\!\!-\!\!\circ C$, then $A \multimap C$; if $A \multimap B \circ\!\!\rightarrow C$, then $A \rightarrow C$ or $A \circ\!\!\rightarrow C$.*

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

Suppose, more specifically, that $A \multimap B \circ\!\!-\!\!\circ C$. Consider the edge between A and C. Lemma 5 implies that it is not into C. Lemma 7 implies that it is not into A. It is not undirected either, for otherwise the circle at C on $B \circ\!\!-\!\!\circ C$ could be oriented by $\mathcal{R}6$. Hence it is either (1) $A \circ\!\!- C$; or (2) $A \circ\!\!-\!\!\circ C$; or (3) $A \multimap C$. We now show that (1) and (2) are impossible.

Suppose for contradiction that (1) or (2) is the case. By (i) in Lemma 12, there is an uncovered tail-circle path u from an endpoint of an undirected edge E to B that includes the edge $A \multimap B$. We claim that for every vertex V on u, either $V \circ\!\!-\!\!\circ C$ or $V \circ\!\!- C$ is present. The argument goes by induction. Obviously B and A satisfy the claim. Suppose, starting from B, the n'th vertex on u, V_n, satisfies the claim. Consider the $n+1$'st vertex on u, V_{n+1}. Since u is a tail-circle path, we have $V_{n+1} \multimap V_n$. By the inductive hypothesis, $V_n \circ\!\!-\!\!\circ C$ or $V_n \circ\!\!- C$. So, as we have established, V_{n+1} and C must be adjacent. Again, Lemma 5 implies that the edge between them is not into C. Lemma 7 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 12, V_{n+1} and B are not adjacent. So the edge between V_{n+1} and C can't be $V_{n+1} \multimap C$, 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 u, in particular the endpoint E satisfies the claim. 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.

So neither (1) nor (2) could be the case, which means $A \multimap C$ is the case.

Lastly, if it is $A \multimap B \circ\!\!\rightarrow C$, then Lemma 7 implies that the edge between A and C has an arrowhead (due to the arrowhead on $B \circ\!\!\rightarrow C$), and that there is no arrowhead at A (due to the presence of $A \multimap B$). So it is either $A \rightarrow C$ or $A \circ\!\!\rightarrow C$. □

Lemma 14. *In $\mathcal{P}_4$, the following property holds:*

CP4 *For any $A \multimap B$, there is no tail-circle path from B to A. That is, there is no such cycle as $A \multimap B \multimap C \multimap \cdots \multimap A$.*

Proof. We first argue that if there is any such cycle in $\mathcal{P}_4$, then there is a cycle with only three edges, i.e., $A \multimap B \multimap C \multimap A$. To show this, note that for any such cycle $c = \langle V_0, V_1, V_2, \cdots, V_n, V_0 \rangle$ 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 7 shows; it can't be undirected, for otherwise some circle on c should been oriented by $\mathcal{R}6$; it can't be ∘—∘, as implied by Lemma 13 (because V_0 —∘ V_1 —∘ V_2 is present). So it is either V_0 —∘ V_2 or V_2 —∘ V_0. In either case, there is a shorter cycle than c that consists of —∘ 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 **CP**4, it suffices to show that A —∘ B —∘ C —∘ A is impossible. Suppose for contradiction that A —∘ B —∘ C —∘ A appears in $\mathcal{P}_4$. By (i) in Lemma 12, there is an uncovered tail-circle path u from an endpoint of an undirected edge E to B that includes the edge A —∘ B. We claim that for every vertex V on u between A and E (including A and E), C —∘ V is present in $\mathcal{P}_4$. The argument is by induction. The vertex A, by supposition, satisfies the claim. Suppose, starting from A, the n'th vertex on u, V_n, satisfies the claim. Consider the $n+1^{st}$ vertex on u, V_{n+1}. Since u is a tail-circle path, we have V_{n+1} —∘ V_n. By the inductive hypothesis, C —∘ V_n. So by Lemma 13, V_{n+1} and C are adjacent. Lemma 7 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 —∘ C could be oriented by $\mathcal{R}6$. Furthermore, by (ii) in Lemma 12, V_{n+1} and B are not adjacent. Since B —∘ C, the edge between V_{n+1} and C must be oriented as C —∘ 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 —∘ E could be oriented. This is a contradiction. □

We now prove a lemma about $\mathcal{P}_{4aag}$ analogous to Lemma 8.

Lemma 15. *Let $\mathcal{P}_{4aag}$ be the AAG of $\mathcal{P}_4$. In $\mathcal{P}_{4aag}$,*

(i) (a1)-(a3) (in Definition 1) and **CP1** *hold;*

(ii) there is no inducing path between two non-adjacent vertices;

(iii) there is no such triple as $A - B \circ\!\!-\!\!\circ C$; and

(iv) every unshielded collider in $\mathcal{P}_{4aag}$ is also in $\mathcal{P}_4$, i.e., arrowhead augmentation does not create any new unshielded colliders.

Proof. We first demonstrate (i). For (a1), suppose for contradiction that there is a directed cycle in $\mathcal{P}_{4aag}$. Since there is no directed cycle in $\mathcal{P}_{4tag}$, as proved in Lemma 8, at least one edge in the cycle must correspond to a $-\!\!\circ$ edge in $\mathcal{P}_4$ (because the treatment of $\circ\!\!\rightarrow$ edges is the same in both tail augmentation and arrowhead augmentation). On the other hand, not all edges in the cycle correspond to $-\!\!\circ$ edges in $\mathcal{P}_4$, as implied by **CP**4 (Lemma 14). This means at least one arrowhead in the cycle is already present in $\mathcal{P}_4$. It follows that there will be an arrowhead meeting a $-\!\!\circ$ edge in $\mathcal{P}_4$, which contradicts **CP**2 (Lemma 7). So there is no directed cycle in $\mathcal{P}_{4aag}$.

For (a2), suppose for contradiction that there is an almost directed cycle in $\mathcal{P}_{4aag}$. Again, one edge therein must correspond to a $-\!\!\circ$ edge in $\mathcal{P}_4$, since we already showed that there is no almost directed cycle in $\mathcal{P}_{4tag}$ (Lemma 8). Also, because no new bi-directed edge is introduced by the arrowhead augmentation, the bi-directed edge in the cycle is also in $\mathcal{P}_4$. Then it is easy to see that there must be an arrowhead meeting a $-\!\!\circ$ edge in $\mathcal{P}_4$, which contradicts **CP2**. So there is no almost directed cycle in $\mathcal{P}_{4aag}$.

For (a3), note that no new undirected edge is introduced in the arrowhead augmentation, and new arrowheads are introduced only by way of changing $-\!\!\circ$ into $\rightarrow$. Since $\mathcal{P}_4$ satisfies (a3), and no such pattern as $-\!\!\circ -$ appears in $\mathcal{P}_4$ (for otherwise the circle could be oriented by $\mathcal{R}6$), it obviously follows that (a3) holds of $\mathcal{P}_{4aag}$.

The fact that **CP1** also holds of $\mathcal{P}_{4aag}$ follows directly from **CP3** of $\mathcal{P}_4$

(Lemma 13).

To see (ii) is true, it suffices to note the following: if there is an inducing path in $\mathcal{P}_{4aag}$ between two non-adjacent vertices, the path must consist of bi-directed edges (which follows from (a1) and (a2), as we have seen). Every bi-directed edge in $\mathcal{P}_{4aag}$ is also in $\mathcal{P}_4$, so every vertex on the inducing path would have an arrowhead into it in $\mathcal{P}_4$. It follows that no edge on any directed path from a vertex on the path to one of the endpoints corresponds to a $-\!\!\circ$ edge in $\mathcal{P}_4$, for otherwise **CP**2 would be violated. So if there is any inducing path in $\mathcal{P}_{4aag}$ between two non-adjacent vertices, it would also be present in $\mathcal{P}_{4tag}$, which we have shown to be impossible. Therefore (ii) is true in $\mathcal{P}_{4aag}$.

(iii) is obvious because no new undirected edge is introduced in the arrowhead augmentation.

(iv) follows from **CP**2 and **CP**3 of $\mathcal{P}_4$. Specifically, **CP**2 implies that the extra colliders produced by the arrowhead augmentation can only come from such patterns as $-\!\!\circ\ \circ\!\!-$ in $\mathcal{P}_4$, but **CP**3 implies that they are shielded. □

This immediately leads to the following result, analogous to Lemma 9.

Lemma 16. *Let $\mathcal{P}_{4aag}$ be the AAG of $\mathcal{P}_4$. If we further orient $\mathcal{P}^c_{4aag}$, the circle component of $\mathcal{P}_{4aag}$, into a DAG with no unshielded colliders, the resulting graph is a MAG and is Markov equivalent to $\mathcal{G}$.*

Proof. Let $\mathcal{H}$ be the resulting MAG. Given Lemma 15, the exact same argument as in Lemma 15 can be used to to argue that $\mathcal{H}$ is a MAG.

The argument for the Markov equivalence between $\mathcal{H}$ and $\mathcal{G}$ is also similar. (iv) in Lemma 15 (plus the argument in Lemma 9) ensure that they have the same unshielded colliders. So if they are not Markov equivalent, it must be that there is a path $u = \langle W, ..., X, Y, Z\rangle$ that is discriminating for Y in both graphs, but the triple $\langle X, Y, Z\rangle$ is a collider in one of the graphs but a non-collider in the other. By the same argument as in Lemma 9, we can show that it must be a collider in $\mathcal{G}$ and a non-collider in $\mathcal{H}$. If none of the edges in u corresponds to a $-\!\!\circ$ edge in $\mathcal{P}_4$, obviously the same argument as in 9 can be applied to derive a contradiction. So some edge on u must corresponds to a $-\!\!\circ$ edge in $\mathcal{P}_4$. But by **CP**2 (Lemma 7), this is only possible if no arrowhead on u is already in $\mathcal{P}_4$, which means there is no vertex between W and X on u (for otherwise there will be bi-directed edges), and either $W -\!\!\circ\, X \circ\!\!-\, Y$, or $W \circ\!\!-\!\!\circ X \circ\!\!-\, Y$, or $W -\!\!\circ\, X \circ\!\!-\!\!\circ Y$ appears in $\mathcal{P}_4$. In the first two cases, $\langle X, Y, Z\rangle$ are non-colliders in both graphs. In the last case, by **CP**3 (Lemma 13), we have $W -\!\!\circ\, Y$ in $\mathcal{P}_4$. It must be oriented as $W \rightarrow Y$ in $\mathcal{G}$, because $\langle X, Y, Z\rangle$ is a collider in $\mathcal{G}$ (and hence it can't be $W - Y$). We also know that $Y \rightarrow Z$ is in $\mathcal{H}$, since $\langle X, Y, Z\rangle$ is a (discriminated) non-collider in $\mathcal{H}$. But then $\langle W, Y, Z\rangle$ is an unshielded collider in $\mathcal{G}$ but not in $\mathcal{H}$, contrary to what we already established.

Therefore, $\mathcal{H}$ and $\mathcal{G}$ are Markov equivalent. □

Lemma 17. *The circle component of $\mathcal{P}_{4aag}$, $\mathcal{P}^c_{4aag}$, is chordal.*

Proof. The proof is the same as the one for Lemma 10. □

Lemma 11, Lemma 16, Lemma 17 together confirm a remark we made earlier: after $\mathcal{R}5 - \mathcal{R}7$ are done, the circles on the $\circ\!\!-\!\!\circ$ and $-\!\!\circ$ edges do not hide any invariant tails. In other words, for any circle on $\circ\!\!-\!\!\circ$ or $-\!\!\circ$, there is a MAG belonging to $[\mathcal{G}]$ in which the circle is marked as an arrowhead. So what is left to show is that $\mathcal{R}8 - \mathcal{R}11$ are sufficient to identify all the invariant tails hidden in the $\circ\!\!\rightarrow$ edges.

Before we delve into the complicated demonstration of this last fact, we note a corollary that follows from the foregoing arguments. It is the fact that every Markov equivalence class of MAGs has a representative with the minimum number of bi-directed edges and undirected edges, or put it differently, a representative whose bi-directed edges and undirected edges are all invariant (and hence appear in every member of the class).

Corollary 18. *For every MAG $\mathcal{G}$, there is a MAG $\mathcal{H}$ Markov equivalent to $\mathcal{G}$ such that all bi-directed and undirected edges in $\mathcal{H}$ are invariant, and every directed edge in $\mathcal{G}$ is also in $\mathcal{H}$.*

Proof. If follows from Lemma 16 that as long as we orient $\mathcal{P}^c_{4aag}$, the circle component of $\mathcal{P}_{4aag}$, into a DAG with no unshielded colliders, we get a MAG Markov equivalent to $\mathcal{G}$ such that all bi-directed and undirected edges therein are invariant, because no additional bi-directed edges or undirected edges are created in the arrowhead augmentation of $\mathcal{P}_4$.

Let $\mathcal{G}^*$ be the subgraph of $\mathcal{G}$ that corresponds to $\mathcal{P}^c_{4aag}$. It is easy to see that all directed edges that belong to $\mathcal{G}$ but not $\mathcal{G}^*$ are already in $\mathcal{P}_{4aag}$. Hence, to prove $\mathcal{H}$ as requested exists, it suffices to show that $\mathcal{P}^c_{4aag}$ can be oriented into a DAG with no unshielded colliders that retains all the directed edges of $\mathcal{G}^*$.

This is not hard to show. Let $\mathcal{G}^*_u$ be the undirected component of $\mathcal{G}^*$. It is chordal, otherwise it would have been oriented in $\mathcal{P}_4$ as undirected. So the part of $\mathcal{P}^c_{4aag}$ that corresponds to $\mathcal{G}^*_u$ can be oriented into a DAG with no unshielded colliders. Orient it into any such DAG, $\mathcal{D}_1$.

The rest of $\mathcal{P}^c_{4aag}$ will be oriented as follows. The ancestor relationship in $\mathcal{G}^*$ naturally induces a partial order over the vertices therein. Since $\mathcal{G}^*$ is ancestral (as it is a subgraph of an ancestral graph), no edge is into the vertices of $\mathcal{G}^*_u$, which implies that no vertex precedes any vertex of $\mathcal{G}^*_u$ in the partial order. Thus we can extend this partial order to a total order such that every vertex of $\mathcal{G}^*_u$ precedes every vertex not in $\mathcal{G}^*_u$. Orient the rest of $\mathcal{P}^c_{4aag}$ according to this total order, and we get a DAG $\mathcal{D}_2$. $\mathcal{D}_2$ obviously retains all the directed edges of $\mathcal{G}^*$, as it respects the partial order induced by $\mathcal{G}^*$. So every arrowhead in $\mathcal{D}_2$ is also in $\mathcal{G}^*$, which implies that $\mathcal{D}_2$ does not contain any unshielded collider (for otherwise $\mathcal{G}^*$ would contain unshielded colliders too, which contradicts the fact that it is a counterpart of $\mathcal{P}^c_{4aag}$).

Let $\mathcal{D}$ denote the resulting DAG orientation of $\mathcal{P}^c_{4aag}$, i.e., the union of $\mathcal{D}_1$ and $\mathcal{D}_2$. This union will not create any unshielded collider, because every edge between a vertex in $\mathcal{D}_1$ and a vertex not in $\mathcal{D}_1$ is out of the former, by our construction of $\mathcal{D}_2$. So $\mathcal{D}$ is the desirable DAG orientation of $\mathcal{P}^c_{4aag}$ that has no unshielded colliders and retains all the directed edges of $\mathcal{G}^*$. □

A special case of this Corollary will be useful in proving a transformational property of directed MAGs, analogous to the one for DAGs established by Chickering (1995). We shall present that result in another paper. The following related lemma, however, is useful for the purpose of the current paper. It gives sufficient and necessary conditions under which changing a directed edge ($\rightarrow$) into a bi-directed edge ($\leftrightarrow$) preserves equivalence.

Lemma 19. *Let $\mathcal{G}$ be an arbitrary MAG, and $A \rightarrow B$ an arbitrary directed edge in $\mathcal{G}$. Let $\mathcal{G}'$ be the graph identical to $\mathcal{G}$ except that the edge between A and B is $A \leftrightarrow B$. (In other words, $\mathcal{G}'$ is the result of simply changing the mark at A on $A \rightarrow B$ from an tail into an arrowhead.) $\mathcal{G}'$ is a MAG and Markov equivalent to $\mathcal{G}$ if and only if*

(t1) A is not an endpoint of an undirected edge;

(t2) there is no directed path from A to B other than $A \rightarrow B$;

(t3) For any $C \rightarrow A$ in $\mathcal{G}$, $C \rightarrow B$ is also in $\mathcal{G}$; and for any $D \leftrightarrow A$ in $\mathcal{G}$, either $D \rightarrow B$ or $D \leftrightarrow B$ is in $\mathcal{G}$;

(t4) There is no discriminating path for A on which B is the endpoint adjacent to A.

Proof. We first show that each of the conditions is necessary (**only if**). Obviously if (t1) or (t2) fails, $\mathcal{G}'$ will not be ancestral. The failure of (t3) could be due to one of the following two cases:

Case 1: there is a vertex C which is a parent of A but not a parent of B. If B and C are not adjacent, then there is an unshielded collider in $\mathcal{G}'$ but not in $\mathcal{G}$, and hence the two graphs are not Markov equivalent. If B and C are adjacent, then $\mathcal{G}$ can't be ancestral (unless we have $C \rightarrow B$).

Case 2: there is a vertex C which is a spouse of A but not a parent or spouse of B. Again, if B and C are not adjacent, the two graphs can't be Markov equivalent because there is an unshielded collider in $\mathcal{G}$ but not in $\mathcal{G}'$. If B and C are adjacent, the edge between them must be $B \rightarrow C$ by the supposition. But then there is an almost directed cycle in $\mathcal{G}$.

If (t4) fails, that is, there is a discriminating path $u = \langle U, \cdots, V, A, B\rangle$ for A. If the edge between V and A is into A, then $\mathcal{G}$ and $\mathcal{G}'$ are not Markov equivalent, because (e3) in Proposition 2 is violated. If, on the other hand, the edge between V and A is not into A, then it must be $A \rightarrow V$. By the definition of discriminating path (Definition 7), V is a parent of B. So we have $A \rightarrow V \rightarrow B \leftrightarrow A$ in $\mathcal{G}'$, an almost directed cycle.

Next, we demonstrate the sufficiency of the conditions (**if**). Suppose (t1)-(t4) are met. We first verify that $\mathcal{G}'$ is a MAG, i.e., it is both ancestral and maximal. Suppose for contradiction that $\mathcal{G}'$ is not ancestral. Since $\mathcal{G}$ is ancestral, and $\mathcal{G}'$ differs from $\mathcal{G}$ only regarding the edge between A and B, in $\mathcal{G}'$ the violation of the definition of ancestral graphs (Definition 1) must involve the edge between A and B. So it can't be a violation of (a1), because a directed cycle would not involve $A \leftrightarrow B$. If it is a violation of (a2), i.e., there is an almost directed cycle in $\mathcal{G}'$. That cycle includes $A \leftrightarrow B$, which means either A is an ancestor of B or B is an ancestor of A in $\mathcal{G}'$. The former case contradicts (t2), and the latter case yields a directed cycle in $\mathcal{G}$. So there can't be any violation of (a2) in $\mathcal{G}'$. Lastly, if there is a violation of (a3) in $\mathcal{G}'$, it must be that there is an undirected edge incident to A, which contradicts (t1). Hence $\mathcal{G}'$ must be ancestral.

To show that $\mathcal{G}'$ is maximal, suppose for the sake of contradiction that there is an inducing path u in $\mathcal{G}'$ between two non-adjacent vertices, D and E. Then

u must include $A \leftrightarrow B$, otherwise u is also an inducing path in $\mathcal{G}$. Furthermore, A is not an endpoint of u, otherwise u is still an inducing path in $\mathcal{G}$ (in fact, there will be an almost directed path in $\mathcal{G}$ in that case). Suppose, without loss of generality, that D is the endpoint closer to A on u than it is to B. We show that some vertex on $u(D, A)$ other than A is B's spouse. Suppose not; we argue by induction that every vertex on $u(A, D)$, and in particular D, is a parent of B. By (t3), the vertex adjacent to A on $u(D, A)$ is either a parent or a spouse of B, but it is not a spouse by supposition, so it is a parent. In the inductive step, suppose the first n vertices next to A on $u(D, A)$ are B's parents, then the $n + 1^{st}$ vertex V must be adjacent to B, otherwise the sub-path of u between this vertex and B forms a discriminating path for A which contradicts (t4). The edge between V and B obviously can't be undirected. Furthermore, by supposition, V is not a spouse of B, i.e., it is not $V \leftrightarrow B$. It can't be $V \leftarrow B$ either, because in that case there would be an almost directed cycle in $\mathcal{G}'$ (as the vertex before V, by the inductive hypothesis, is a parent of B), which we have shown to be impossible. So V must be a parent of B. Thus we have shown that every vertex on $u(A, D)$, and in particular D, is a parent of B. Then B must be an ancestor of E, because by the definition of inducing path (Definition 4), B is an ancestor of either D or E. So D is an ancestor of E, and it is obvious that the vertex adjacent to E on u must be an ancestor of D, which implies that there is an almost directed cycle in $\mathcal{G}'$. which we have shown to be absent. Hence a contradiction. So some vertex on $u(D, A)$ other than A is a spouse of B. Let C be such a vertex on $u(D, A)$. Replacing $u(C, B)$ on u with $C \leftrightarrow B$ yields an inducing path between D and E in $\mathcal{G}$, which contradicts the fact that $\mathcal{G}$ is maximal.

Having shown that $\mathcal{G}'$ is a MAG, we now verify that $\mathcal{G}$ and $\mathcal{G}'$ satisfy the conditions for Markov equivalence in Proposition 2. Obviously they have the same adjacencies, and share the same colliders except possibly A. But A will not be a collider in an unshielded triple, for condition (t3) requires that any vertex that is incident to an edge into A is also adjacent to B. So the only worry is that a triple $\langle C, A, B\rangle$ might be discriminated by a path, but (t4) guarantees that there is no such path. Therefore, $\mathcal{G}'$ is Markov equivalent to $\mathcal{G}$. $\square$

Let us turn to the final task of showing that for every $\circ\!\!\rightarrow$ edge in $\mathcal{P}_4$, there is a MAG equivalent to $\mathcal{G}$ in which the edge is oriented as $\leftrightarrow$. The argument is going to be a little roundabout, with two major steps. Let $J\circ\!\!\rightarrow K$ be an arbitrary $\circ\!\!\rightarrow$ edge in $\mathcal{P}_4$. In the first step, we show that we can orient $\mathcal{P}_4^c$ — the circle component of $\mathcal{P}_4$, which is the same as $\mathcal{P}_{4aag}^c$, the circle component of the AAG of $\mathcal{P}_4$ — into a DAG with no unshielded colliders that satisfies certain conditions relative to $J\circ\!\!\rightarrow K$. By Lemma 16, the arrowhead augmentation together with this DAG orientation of $\mathcal{P}_4^c$ yield a MAG equivalent to $\mathcal{G}$. In the second step, we argue that this particular MAG can be transformed into a MAG containing $J \leftrightarrow K$ through a sequence of equivalence-preserving changes of $\rightarrow$ to $\leftrightarrow$. It then follows that the resulting MAG with $J \leftrightarrow K$ is also equivalent to $\mathcal{G}$.

The following definitions specify the conditions we want a DAG orientation of $\mathcal{P}_4^c$ ($\mathcal{P}_{4aag}^c$) to satisfy.

Definition 13. *Let $J\circ\!\!\rightarrow K$ be an arbitrary $\circ\!\!\rightarrow$ edge in $\mathcal{P}_4$. For any $A\circ\!\!\rightarrow B$ in $\mathcal{P}_4$, it is said to be* **relevant** *to $J\circ\!\!\rightarrow K$ if*

(i) $A = J$ or there is a p.d. path from J to A in $\mathcal{P}_4$ 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 $B \rightarrow K$) in $\mathcal{P}_4$.

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

Informally, relevant edges are those that may have to be changed to bi-directed edges ($\leftrightarrow$) before the edge between J and K can be so oriented. The rationale behind the formal definition above will be revealed by the proof of Lemma 42. We use $\mathbf{REL}(J\circ\!\!\rightarrow K)$ to denote the set of $\circ\!\!\rightarrow$ edges relevant to $J\circ\!\!\rightarrow K$ in $\mathcal{P}_4$. Notice that $J\circ\!\!\rightarrow K$ itself belongs to this set. It will also be convenient to 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 14. *A DAG orientation of $\mathcal{P}_4^c$ – the circle component of $\mathcal{P}_4$ – is said to be* **agreeable** *to $J\circ\!\!\rightarrow K$ if the following three conditions hold:*

$\mathbf{C_1}$ *For any $A\circ\!\!\rightarrow B \in \mathbf{REL}(J\circ\!\!\rightarrow K)$ and $B\circ\!\!-\!\!\circ C$ in $\mathcal{P}_4$, if $C \notin \mathbf{AR}(J\circ\!\!\rightarrow K)$, then $B \circ\!\!-\!\!\circ C$ is oriented as $B \rightarrow C$ in the DAG;*

$\mathbf{C_2}$ *For any $A\circ\!\!\rightarrow B \in \mathbf{REL}(J\circ\!\!\rightarrow K)$ and $A \circ\!\!-\!\!\circ C$ in $\mathcal{P}_4$, if C is a parent of B (namely $C \rightarrow B$) in $\mathcal{P}_4$, then $A \circ\!\!-\!\!\circ C$ is oriented as $A \leftarrow C$ in the DAG;*

$\mathbf{C_3}$ *For any $A\circ\!\!\rightarrow B \in \mathbf{REL}(J\circ\!\!\rightarrow K)$ and $A \circ\!\!-\!\!\circ C$ in $\mathcal{P}_4$, if C is not adjacent to B in $\mathcal{P}_4$, then $A \circ\!\!-\!\!\circ C$ is oriented as $A \rightarrow C$ in the DAG.*

Since we will henceforth refer to $\mathbf{C_1} - \mathbf{C_3}$ very frequently, some further explanation of them is in order. Roughly they are all motivated as necessary for a $\circ\!\!\rightarrow$ edge (relevant to $J\circ\!\!\rightarrow K$) to meet the conditions in Lemma 19. This is especially clear in $\mathbf{C_2}$ and $\mathbf{C_3}$. Regarding the relevant edge $A\circ\!\!\rightarrow B$ (which will be $A \rightarrow B$ after arrowhead augmentation), violation of $\mathbf{C_2}$ will fail condition (t2) in Lemma 19, and violation of $\mathbf{C_3}$ will fail condition (t3) in Lemma 19. For $\mathbf{C_1}$, notice that if the antecedent holds, we have either $A \rightarrow C$ or $A\circ\!\!\rightarrow C$ in $\mathcal{P}_4$, by the property **CP1** (Lemma 5). In either case, $A \rightarrow C$ will appear in $\mathcal{P}_{4aag}$. So if $\mathbf{C_1}$ is violated, i.e., if $B\circ\!\!-\!\!\circ C$ is oriented as $B \leftarrow C$, then (t2) in Lemma 19 fails. (It will not matter, however, if $C \in \mathbf{AR}(J\circ\!\!\rightarrow K)$; because in that case, as will become clear later, $A\circ\!\!\rightarrow C$ is in $\mathcal{P}_4$. Then $A\circ\!\!\rightarrow C \in \mathbf{REL}(J\circ\!\!\rightarrow K)$, which can be dealt with before $A\circ\!\!\rightarrow B$.)

It is far less obvious, however, that $\mathbf{C_1} - \mathbf{C_3}$ suffice to ensure the existence of a sequence of equivalence-preserving changes that can eventually turn $J \rightarrow K$

into $J \leftrightarrow K$. The demonstration of this fact will be postponed until Lemma 42. Before that, we need to establish the even less obvious fact that $\mathcal{P}_4^c$ can be oriented into a DAG with no unshielded colliders that satisfies $\mathbf{C_1} - \mathbf{C_3}$ relative to $J \circ\!\!\rightarrow K$.

One way to orient a chordal graph into a DAG free of unshielded colliders is given in Meek (1995):

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 $A \rightarrow B$ and close orientations under the following rules:[10]

UR$_1$ If $A \rightarrow B \circ\!\!-\!\!\circ C$, A and C are not adjacent, orient as $B \rightarrow C$.

UR$_2$ If $A \rightarrow B \rightarrow C$ and $A \circ\!\!-\!\!\circ C$, orient as $A \rightarrow C$.

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 $\mathcal{H}$.

We now adopt the algorithm to fit our purpose. Given an arbitrary edge $J \circ\!\!\rightarrow K$ in $\mathcal{P}_4$, let $\mathbf{E_n}, n = 1, 2, 3$ denote the set of $\circ\!\!-\!\!\circ$ edges whose orientations are required by condition $\mathbf{C_n}$ in Definition 14. (Note that they are not necessarily disjoint.)

Orientation Algorithm

Input: $\mathcal{P}_4^c$, $\mathcal{P}_4$, and an edge $J \circ\!\!\rightarrow K$ therein

[10]There is another rule in Meek (1995) which will not be used in orienting a chordal graph into a DAG *with no unshielded colliders*.

Output: a DAG orientation of $\mathcal{P}_4^c$ with no unshielded colliders

Let $\mathcal{D} = \mathcal{P}_4^c$

Repeat

If some edge in $\mathbf{E_1}$ is yet unoriented 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 yet unoriented 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 yet unoriented 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 $A \to B$ and close orientations under $\mathbf{UR}_1, \mathbf{UR}_2, \mathbf{UR}_3$.

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

Return $\mathcal{D}$

Given the correctness of Meek's algorithm, the output from the above *Orientation Algorithm* is obviously a DAG orientation of $\mathcal{P}_4^c$ with no unshielded colliders. The question is whether it is also agreeable to $J \circ\!\!\rightarrow K$. We answer this question affirmatively in Corollary 39, to which we now proceed.

We begin by noting some facts about (uncovered) p.d. paths (see Definition 10) in $\mathcal{P}_4$.

Lemma 20. *If $u = \langle A, \cdots, B \rangle$ is a p.d. path from A to B in $\mathcal{P}_4$, then a subsequence of u forms an uncovered p.d. path from A to B.*

Proof. We prove it by induction on the length of u. If there is only one edge on u, then it is trivially an uncovered p.d. path from A to B. If there are two edges on u, namely $u = \langle A, C, B \rangle$, 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 constitutes an uncovered p.d. path from A to B, or in other words, the edge between A and B is not into A or out of 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 **CP**1 (Lemma 5), the edge between C and B has an arrowhead at C, which contradicts the fact that u is potentially directed. It follows that the edge between A and C must have a tail at A in $\mathcal{P}_4$. Since the edge between A and B is into A, it follows from **CP**2 (Lemma 7) that the edge between A and C is $A \rightarrow C$. 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 argue 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 u is potentially directed. So it must be $A \circ\!\!- B$. It obviously follows, by **CP**2, that there can't be any arrowhead on u, so it is either $A \circ\!\!-\!\!\circ C \circ\!\!-\!\!\circ B$, 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 **CP**3 (Lemma 13), and the last case contradicts **CP**4 (Lemma 14).

Now the inductive step is very easy. Suppose the proposition holds when the length of u is $n-1$ ($n \geq 3$). Consider the case where u has n edges.

Either u 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 u, we get a subsequence of u 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 u, forms an uncovered p.d. path from A to B. This concludes our argument. $\square$

Lemma 21. *If u is an uncovered p.d. path from A to B in $\mathcal{P}_4$, then*

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

Proof. To see (i) is true, notice that since u is uncovered and potentially directed, any edge after a $\circ\!\!\rightarrow$ edge or a $\rightarrow$ edge on u must be oriented as $\rightarrow$ by $\mathcal{R}1$. So no $\circ\!\!-\!\!\circ$ can appear after a $\circ\!\!\rightarrow$ edge on u, and no $\rightarrow$ can appear before a $\circ\!\!\rightarrow$ edge on u. The same is true with a $-\!\!\circ$ edge. Since u is uncovered, any edge on u after $-\!\!\circ$ will be oriented as $-\!\!\circ$ or $\rightarrow$ 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 $\circ\!\!\rightarrow$ edge on u must be oriented as a $\rightarrow$ edge. For (ii), Suppose for contradiction that u contains both a $\circ\!\!\rightarrow$ edge and a $-\!\!\circ$ edge. Then the $-\!\!\circ$ edge does not appear after the $\circ\!\!\rightarrow$ edge on u, because any edge after $\circ\!\!\rightarrow$ on u must be oriented as $\rightarrow$ by $\mathcal{R}1$. On the other hand, the $\circ\!\!\rightarrow$ does not appear after the $-\!\!\circ$ edge on u, because any edge after $-\!\!\circ$ on u is either $-\!\!\circ$ or $\rightarrow$. This is a contradiction. $\square$

Lemma 22. *In $\mathcal{P}_4$, 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 20, there is an uncovered p.d. path u from A to B. Suppose for contradiction that there is an edge between A and B which is into A, namely $A \leftarrow\!\!* B$ is in $\mathcal{P}_4$. There can't be a $-\!\!\circ$ edge on u 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 21. In either case, by Lemma 6, there is an edge into the tail endpoint of the $-\!\!\circ$ edge, which contradicts **CP2** (Lemma 7).

So, by Lemma 21, u is of the form: $\circ\!-\!\circ \cdots \circ\!\!\rightarrow\rightarrow \cdots \rightarrow$. It takes little effort to see that Lemma 6 entails that there is an edge between B and an ancestor of B which is into that ancestor. This contradicts the soundness of $\mathcal{P}_4$. □

Lemma 23. *In $\mathcal{P}_4$, 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 an uncovered p.d. path from A to B is not into B. That is, the last edge on the path is not $\circ\!\!\rightarrow$ or $\rightarrow$. The last edge can't be $-\!\!\circ$ either, because there is a p.d. path into B. So the last edge must be $\circ\!-\!\circ$, and hence by Lemma 21, the path must be a circle path. Let C be the vertex adjacent to B on the p.d. path into B, which means $C *\!\!\rightarrow B$. Since there is a circle path between A and B, it follows from Lemma 6 that $C *\!\!\rightarrow A$. But there is a p.d. path from A to C, which contradicts Lemma 22. □

Corollary 24. *In $\mathcal{P}_4$, 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 $A \circ\!\!\rightarrow B$ or $A \rightarrow B$.*

Proof. By Lemma 22, the edge between A and B is not into A. It follows that it is not out of B, because there is a path into B, which rules out the possibility of $A - B$ or $A \circ\!- B$ by Lemma 7. Hence the edge between A and B is an uncovered p.d. path from A to B. By Lemma 23, it is into B, which means it is either $A \circ\!\!\rightarrow B$ or $A \rightarrow B$. □

Lemma 25. *If there is a circle path between two adjacent vertices in $\mathcal{P}_4$, then the edge between the two vertices is $\circ\!-\!\circ$.*

Proof. By Lemma 6, there is no arrowhead on the edge between the two vertices. The edge obviously can't be —. If it is —o, then it is easy to derive a contradiction from **CP3** (Lemma 13). So the edge between the two vertices must be o—o in $\mathcal{P}_4$. $\square$

Lemma 26. *Let u be an uncovered circle path in $\mathcal{P}_4$. If A and B are two non-consecutive vertices on u, then A and B are not adjacent in $\mathcal{P}_4$.*

Proof. It follows from Lemma 25 and the fact that $\mathcal{P}_4^c$ is chordal. $\square$

The next a couple of lemmas establish two useful facts for the endpoints of the edges in $\mathbf{REL}(J\circ\!\!\rightarrow K)$.

Lemma 27. *For any $A\circ\!\!\rightarrow B \in \mathbf{REL}(J\circ\!\!\rightarrow K)$, there is an uncovered p.d. path u from J to B in $\mathcal{P}_4$ such that for every vertex V on u other than B, there is an edge $V\circ\!\!\rightarrow K$.*

Proof. By Definition 13, there is a p.d. path from J to A in $\mathcal{P}_4$ such that no vertex on the path (including the endpoints) is a parent of K. This path concatenated with $A\circ\!\!\rightarrow B$ constitutes a p.d. path from J to B which is into B. Lemma 20 implies 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. This path, by Lemma 23, is into B. We now argue that for every vertex V on u other than B, there is an edge $V\circ\!\!\rightarrow K$ in $\mathcal{P}_4$. By Definition 13, either $B = K$ or B is a parent of K. We consider the two cases separately:

Case 1: $B = K$. Let X be the vertex adjacent to K (B) on u. Since u is into K, and X is not a parent of K (because no vertex on u is a parent of B), the edge between X and K must be $X\circ\!\!\rightarrow K$. We prove by induction that for every vertex V between J and X on u, there is an edge $V\circ\!\!\rightarrow K$ in $\mathcal{P}_4$. The base case is trivial, because for the first vertex on u, J, obviously we have $J\circ\!\!\rightarrow K$. For the inductive step, suppose the n'th vertex, V_n, on u satisfies the claim, namely $V_n\circ\!\!\rightarrow K$ is in $\mathcal{P}_4$. Then the $n+1^{st}$ vertex, V_{n+1}, must be adjacent to

K, otherwise $V_n \circ\!\!\rightarrow K$ could be oriented by $\mathcal{R}10$, because u is uncovered (and hence the subpath of u between V_n and K is also uncovered). Since there is a p.d. path from V_{n+1} to K which is into K, by Corollary 24, the edge between V_{n+1} and K is either $V_{n+1} \circ\!\!\rightarrow K$ or $V_{n+1} \rightarrow K$. Since V_{n+1} is on u and hence not a parent of K, we have $V_{n+1} \circ\!\!\rightarrow K$ in $\mathcal{P}_4$.

Case 2: B is a parent of K, namely $B \rightarrow K$ is in $\mathcal{P}_4$. Let X be the vertex adjacent to B on u. If X is not adjacent to K, the path $u \oplus B \rightarrow K$ is an uncovered p.d. path from J to K which is into K. So we can do the exactly same induction as in *Case 1*. If X is adjacent to K, then by Corollary 24, it is either $X \circ\!\!\rightarrow K$ or $X \rightarrow K$. Since X is not a parent of K, it must be $X \circ\!\!\rightarrow K$ in u. Then, again, we are back to *Case 1*. □

Lemma 28. *If $A \circ\!\!\rightarrow B \in \mathbf{REL}(J \circ\!\!\rightarrow K)$, then there is an edge $A \circ\!\!\rightarrow K$ in $\mathcal{P}_4$.*

Proof. If $A = J$ or $B = K$, there is obviously an edge $A \circ\!\!\rightarrow K$ in $\mathcal{P}_4$. Suppose $A \neq J$ and $B \neq K$. Since $A \circ\!\!\rightarrow B \in \mathbf{REL}(J \circ\!\!\rightarrow K)$, by Lemma 27, there is an uncovered p.d. path u from J to B in $\mathcal{P}_4$ such that for every vertex V on u other than B, there is an edge $V \circ\!\!\rightarrow K$. By Lemma 23, we know that u is also into B. Let X be the vertex adjacent to B on u. We have $X \circ\!\!\rightarrow K$ in $\mathcal{P}_4$. Also, because $B \neq K$, $B \rightarrow K$ is in $\mathcal{P}_4$, so the edge between X and B can't be $X \rightarrow B$, for otherwise $X \circ\!\!\rightarrow K$ could be oriented by $\mathcal{R}8$. It follows that $X \circ\!\!\rightarrow B$ is in $\mathcal{P}_4$, because u is into B.

Now, suppose for contradiction that A is not adjacent to K. 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 24, the edge between A and K is either $A \rightarrow K$ or $A \circ\!\!\rightarrow K$. But by definition (Definition 13), A is not a parent of K, so it must be $A \circ\!\!\rightarrow K$ in $\mathcal{P}_4$. □

We are now ready to make important steps towards the proof that in the course of the *Orientation Algorithm*, no violation of $\mathbf{C_1} - \mathbf{C_3}$ (Definition 14) would occur, and hence the output DAG orientation of $\mathcal{P}_4^c$ is agreeable to $J\circ\!\!\rightarrow K$. For this purpose, we assume, without loss of generality, that $\mathbf{UR}_1$ has priority over $\mathbf{UR}_2$ and $\mathbf{UR}_3$ in the sense that whenever two or more different rules can be fired, $\mathbf{UR}_1$ will always be applied first, if applicable. The following series of lemmas will 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. Notice that the stereotype of a chain of $\mathbf{UR}_1$ firings is that the first edge on an uncovered circle path $\circ\!-\!\circ \cdots \circ\!-\!\circ$ is oriented out of the first vertex, which triggers repeated applications of $\mathbf{UR}_1$ that orient the whole circle path. That is why most of the next block of lemmas are concerned with an uncovered circle path.

Lemma 29. *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 $\mathcal{P}_4$.*

Proof. If one of B and C is K, it is manifest in the definition of relevance that there is a directed edge between them, and hence there is no circle path between them, as implied by Lemma 6. So we only need to consider the case where neither of them is K, that is, both of them are parents of K. Suppose for contradiction that in $\mathcal{P}_4$ there is an uncovered circle path u between B and C that includes two or more $\circ\!\!-\!\!\circ$ edges. It follows, by Lemma 26, that B and C are not adjacent. Let A be such a vertex that $A\circ\!\!\rightarrow B \in \mathbf{REL}(J\circ\!\!\rightarrow K)$. It follows from Lemma 6 that either $A\circ\!\!\rightarrow C$ or $A \rightarrow C$ is in $\mathcal{P}_4$. Furthermore, because A is not a parent of K, it must be $A\circ\!\!\rightarrow C$. Now consider the edge $A\circ\!\!\rightarrow K$, which is shown to be present by Lemma 28. It could be oriented by $\mathcal{R}11$, because $A\circ\!\!\rightarrow B$ is an uncovered p.d. path from A to B, a parent of K; $A\circ\!\!\rightarrow C$ is an uncovered p.d. path from A to C, a parent of K; B and C are not adjacent. Hence a contradiction. □

Lemma 30. *Suppose $A\circ\!\!\rightarrow B \in \mathbf{REL}(J\circ\!\!\rightarrow K)$. If $A \circ\!\!-\!\!\circ C$ and C is a parent* *of B in $\mathcal{P}_4$ (i.e. the edge A ∘—∘C is required by condition $\mathbf{C_2}$ to be oriented as $A \leftarrow C$), then C is a parent of K.*

Proof. If $B = K$, it is trivial that C is a parent of K. Suppose $B \neq K$. Since A∘→ $B \in \mathbf{REL}(J$∘→ $K)$, B is a parent of K. By Lemma 28, A∘→ K is present in $\mathcal{P}_4$. It follows that C is adjacent to K, otherwise A∘→ K could be oriented by $\mathcal{R}9$. The edge between C and K must be $C \rightarrow K$, as required by $\mathcal{R}8$. Hence C is a parent of K. □

Lemma 31. *Suppose A∘→ $B \in \mathbf{REL}(J$∘→ $K)$, A ∘—∘C and C is a parent of B in $\mathcal{P}_4$ (i.e. the edge A ∘—∘C is required by condition $\mathbf{C_2}$ to be oriented as $A \leftarrow C$). Then*

(1) if for some $D \in \mathbf{AR}(J$∘→ $K)$, C ∘—∘D is in $\mathcal{P}_4$, then $C \in \mathbf{AR}(J$∘→ $K)$ (so that the edge C ∘—∘D is not subject to $\mathbf{C_1}$);

(2) If $u = \langle C, A, \ldots\rangle$ is an uncovered circle path, no vertex (except possibly C) on u is in $\mathbf{AR}(X$∘→ $Y)$.

Proof. To show (1), note that if $D \in \mathbf{AR}(J$∘→ $K)$, then there is some vertex X such that X∘→ $D \in \mathbf{REL}(J$∘→ $K)$. By **CP1** (Lemma 5), X∘→ C or $X \rightarrow C$ is in $\mathcal{P}_4$. By Lemma 30, C is a parent of K. So it is not $X \rightarrow C$ in $\mathcal{P}_4$, otherwise X∘→ K, which is shown to be present by Lemma 28, could be oriented as $X \rightarrow K$ by $\mathcal{R}8$. So it must be X∘→ C in $\mathcal{P}_4$. Since X∘→ $D \in \mathbf{REL}(J$∘→ $K)$ and C is a parent of K, X∘→ C obviously satisfies Definition 13, which means $C \in \mathbf{AR}(J$∘→ $K)$.

To prove (2), suppose for contradiction that some vertex $E \neq C$ on u is in $\mathbf{AR}(J$∘→ $K)$. Obviously $E \neq K$, otherwise A∘→ E would be present in $\mathcal{P}_4$ by Lemma 27, which contradicts Lemma 6. So E is a parent of K. Now consider the edge A∘→ K, which is implied to exist by Lemma 27. A ∘—∘C constitutes an uncovered p.d. path from A to C, a parent of K, as implied by Lemma 30; $u(A, E)$ is an uncovered p.d. path from A to E, a parent of K. Since u is uncovered, A∘→ K could be oriented as $A \rightarrow K$ by $\mathcal{R}11$, a contradiction. □

Lemma 32. *For any uncovered circle path $u = \langle A, \cdots E\rangle$, 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 30, both A and E are parents of K. Let B be the vertex adjacent to A on u. By our supposition, $A \circ\!\!-\!\!\circ B$ is required by $\mathbf{C_2}$ to be oriented as $A \to B$. This means, by Definition 14, that there is a vertex C such that $B \circ\!\!\to C \in \mathbf{REL}(J \circ\!\!\to K)$ (and A is a parent of C). Consider $B \circ\!\!\to K$, which is shown to be present by Lemma 28. $B \circ\!\!-\!\!\circ A$ 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. Thus it is easy to see that $B \circ\!\!\to K$ could be oriented as $B \to K$ by $\mathcal{R}11$, a contradiction. □

Lemma 33. *If $A \circ\!\!\to B \in \mathbf{REL}(J \circ\!\!\to K)$, and $u = \langle A, C, \cdots\rangle$ is an uncovered circle path such that C is not adjacent to B in $\mathcal{P}_4$ (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 $\mathcal{P}_4$.*

Proof. Since $A \circ\!\!\to B \in \mathbf{REL}(J \circ\!\!\to K)$, by Lemma 28, $A \circ\!\!\to K$ is present in $\mathcal{P}_4$. Suppose for contradiction that a vertex D (which could be C) on u is a parent of K. By definition (Definition 13), either $B = K$ or B is a parent of K. We consider the two cases separately and derive a contradiction in each.

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 24, is either $E \circ\!\!\to K$ or $E \to K$. It follows that $\langle A, C, \cdots, E, K\rangle$ forms an uncovered p.d. path from A to K such that C and K are not adjacent. Hence $A \circ\!\!\to K$ could be oriented as $A \to K$ by $\mathcal{R}10$, a contradiction.

Case 2: $B \to K$ is in $\mathcal{P}_4$. 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 $\mathcal{R}11$, a contradiction. $\square$

Lemma 34. *Suppose $A \circ\!\!\rightarrow B, C \circ\!\!\rightarrow D \in \mathbf{REL}(J \circ\!\!\rightarrow K)$, $A \neq C$ and $u = \langle A, \cdots, C \rangle$ is an uncovered circle path in $\mathcal{P}_4$. 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 vertex next to A (which could be C) is not adjacent to B, and the vertex next to C (which could be A) is not adjacent to D. We consider three cases separately and derive a contradiction in each.

Case 1: $B = D$. In this case, obviously $u \oplus C \circ\!\!\rightarrow B$ 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 $\mathcal{R}10$ 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 $C \circ\!\!\rightarrow D \in \mathbf{REL}(X \circ\!\!\rightarrow Y)$, and $D \neq K$, by definition (Definition 13), 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 exactly the same situation as *Case 1* in the proof of Lemma 33, which implies that $A \circ\!\!\rightarrow B$ could be oriented as $A \to B$ by $\mathcal{R}10$, a contradiction.

Case 3: $B \neq D$ and neither of them is K. By definition (Definition 13, both B and D are parents of Y. Consider the edge $A \circ\!\!\rightarrow K$, which is shown to be present by Lemma 28. 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 $\mathcal{R}11$, a contradiction. $\square$

Notice that in our *Orientation Algorithm*, some $\circ\!\!-\!\!\circ$ edges are explicitly oriented to satisfy one of $\mathbf{C_1} - \mathbf{C_3}$. Lemmas 29, 31, 32, 33, 34 ensure that such orientations will not at the same time violate $\mathbf{C_1} - \mathbf{C_3}$ (and hence $\mathbf{C_1}$, $\mathbf{C_2}$ and $\mathbf{C_3}$ are consistent in themselves and with each other). Furthermore, these lemmas imply that if we propagate such orientations with $\mathbf{UR}_1$ alone, no violation of $\mathbf{C_1} - \mathbf{C_3}$ would occur. (These claims will be formally demonstrated in Lemma 35 and Lemma 38.)

However, it is not yet clear whether propagations with $\mathbf{UR}_1 - \mathbf{UR}_3$ together will create violations of $\mathbf{C_1} - \mathbf{C_3}$. We resolve this worry in Lemma 35 and Lemma 38, with which we establish the key fact that no violation of $\mathbf{C_1} - \mathbf{C_3}$ would occur in the *Orientation Algorithm*. Note that if any violation occurs, it must occur by the end of the third stage of the *Orientation Algorithm*, namely before all $\circ\!\!-\!\!\circ$ edges in $\mathbf{E_1} \cup \mathbf{E_2} \cup \mathbf{E_3}$ get oriented. Let $\mathcal{D}^*$ be the resulting graph at the end of the third stage of the *Orientation Algorithm* — a partial orientation of $\mathcal{P}_4^c$. Clearly the $\circ\!\!-\!\!\circ$ edges left in $\mathcal{D}^*$, if any, do not belong to $\mathbf{E_1} \cup \mathbf{E_2} \cup \mathbf{E_3}$, and hence are not relevant to $\mathbf{C_1} - \mathbf{C_3}$. The next lemma states two important properties of $\mathcal{D}*$. (We assume, without loss of generality, that $\mathbf{UR}_1$ has priority over $\mathbf{UR}_2$ and $\mathbf{UR}_3$.)

Lemma 35. *Let $\mathcal{D}^*$ be the resulting graph at the end of the third stage of the Orientation Algorithm.*

(i) for any vertex $W \in \mathbf{AR}(J\circ\!\!\rightarrow K)$, there is no directed edge into W in $\mathcal{D}^*$;

(ii) for any three vertices X, Y, Z, if $X\circ\!\!\rightarrow Y \in \mathbf{REL}(J\circ\!\!\rightarrow K)$, $X \circ\!\!-\!\!\circ Z$ and Z is a parent of Y in $\mathcal{P}_4$, then there is no directed edge into Z in $\mathcal{D}^*$.

Proof. We first demonstrate (i). Suppose for contradiction that some $\circ\!\!-\!\!\circ$ edge is oriented into a vertex in $\mathbf{AR}(J\circ\!\!\rightarrow K)$ by the end of the third stage of the *Orientation Algorithm*. Let the first occurrence of such an orientation 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.

Case 1: $A \circ\!\!-\!\!\circ B$ is oriented as $A \to B$ to satisfy one of $\mathbf{C_1} - \mathbf{C_3}$. Since B is in $\mathbf{AR}(J \circ\!\!\to K)$, $\mathbf{C_1}$ does not dictate this orientation. It can't be $\mathbf{C_2}$, as entailed by (2) in Lemma 31. So it must be $\mathbf{C_3}$, which means there is a vertex E such that $A \circ\!\!\to E \in \mathbf{REL}(J \circ\!\!\to K)$ and E, B are not adjacent. Then Lemma 33 implies that B is not a parent of K. Furthermore, by Lemma 28, $A \circ\!\!\to K$ is present in $\mathcal{P}_4$, which implies that $B \neq K$ (because the edge between A and B is $A \circ\!\!-\!\!\circ B$ in $\mathcal{P}_4$). It follows that B is not in $\mathbf{AR}(J \circ\!\!\to K)$, which is a contradiction.

Case 2: $A \circ\!\!-\!\!\circ B$ is oriented as $A \to B$ by an application of $\mathbf{UR}_2$. That is, there is an C such that $A \circ\!\!-\!\!\circ B \circ\!\!-\!\!\circ C$ is in $\mathcal{P}_4^c$, 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.

Case 4: $A \circ\!\!-\!\!\circ B$ is oriented as $A \to B$ by an application of $\mathbf{UR}_1$. Then there is a chain of applications of $\mathbf{UR}_1$ (which could consist of just one application) that leads to $A \to B$ where the first edge on the chain is *not* oriented by $\mathbf{UR}_1$. So there are three subcases to consider:

Case 4.1: the first edge is oriented to satisfy one of $\mathbf{C_1} - \mathbf{C_3}$. If it is $\mathbf{C_1}$, then in $\mathcal{P}_4^c$ there is an uncovered circle path with more than one edge between two vertices in $\mathbf{AR}(J \circ\!\!\to K)$, which contradicts Lemma 29. It can't be $\mathbf{C_2}$, as entailed by (2) in Lemma 31. So it must be $\mathbf{C_3}$, but in that case Lemma 33 implies that B is not a parent of K and Lemma 28 implies that $B \neq K$, which contradict the membership of B in $\mathbf{AR}(J \circ\!\!\to K)$.

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 $\mathcal{P}_4^c$, and is oriented as $X \rightarrow Y \rightarrow Z$, which in turn orients the edge $X \circ\!\!-\!\!\circ Z$ as $X \rightarrow Z$. And $X \rightarrow Z$ initiates a chain of $\mathbf{UR}_1$ applications on an uncovered circle path $u = \langle X, Z, \cdots, B \rangle$ that eventually leads to the orientation of $A \rightarrow B$. Now we argue that for every vertex V on u between Z and B, there is an edge between Y and V already oriented as $Y \rightarrow V$ before $X \rightarrow Z$ is thus oriented. The argument is by induction. 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 $\mathcal{P}_4^c$, for otherwise $Z \circ\!\!-\!\!\circ V_1$ would be oriented as $Z \rightarrow V_1$ by $\mathbf{UR}_1$ *before* $X \circ\!\!-\!\!\circ Z$ is oriented by $\mathbf{UR}_2$, according to our convention of 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 $Y \rightarrow V_1$ by $\mathbf{UR}_1$ before $X \rightarrow Z$ is thus oriented. In the inductive step, suppose $Y \rightarrow V_n$ is oriented as such before $X \rightarrow Z$ is thus oriented, where V_n is the n'the vertex after Z on u. Consider the $n + 1^{st}$ vertex V_{n+1}. Again, it must be adjacent to Y, otherwise the edge $V_n \circ\!\!-\!\!\circ V_{n+1}$ should be oriented by $\mathbf{UR}_1$ before $X \circ\!\!-\!\!\circ Z$ is oriented by our convention of the priority of $\mathbf{UR}_1$. Furthermore, by Lemma 26, X and V_{n+1} are not adjacent, so the edge $Y \circ\!\!-\!\!\circ V_{n+1}$ should be oriented as $Y \rightarrow V_{n+1}$ by $\mathbf{UR}_1$ before $X \circ\!\!-\!\!\circ Z$ gets oriented. Hence, in particular, $Y \rightarrow B$ 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 $\mathcal{P}_4^c$, and that W, Z are not adjacent. Furthermore, $W \circ\!\!-\!\!\circ Y \circ\!\!-\!\!\circ Z$ is oriented as $W \rightarrow Y \rightarrow Z$, which in turn orients the edge $X \circ\!\!-\!\!\circ Z$ as $X \rightarrow Z$. This then initiates a chain of $\mathbf{UR}_1$ applications on an uncovered circle path $u = \langle X, Z, \cdots, B \rangle$ that eventually leads to the orientation of $A \rightarrow B$. Notice that W, Z are not adjacent, so $\langle W, X, Z, \cdots, B \rangle$ is also an uncovered path. By the exact same argument as in *Case 4.2*, we can show that for every vertex V between Z and B on u, there is an edge between Y and V already oriented as

$Y \to V$ before $X \to Z$ is thus oriented. So 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 $A \circ\!\!-\!\!\circ B$.

Thus we have established (i).

The proof of (ii) is completely parallel to the proof of (i). The only notable difference is that in the counterparts of *Case 1* and *Case 4.1*, we need to cite some different lemmas. Take *Case 1* for example. We need to argue that an orientation to satisfy one of $\mathbf{C_1} - \mathbf{C_3}$ will not be an orientation that violates (ii). For $\mathbf{C_1}$, it suffices to cite (1) in Lemma 31; for $\mathbf{C_2}$, we need to cite Lemma 32; for $\mathbf{C_3}$, we need Lemma 33. Other details are virtually the same as the arguments for (i). ☐

Corollary 36. *In the course of the Orientation Algorithm, no violation of* $\mathbf{C_1}$ *occurs.*

Proof. This follows trivially from (i) in Lemma 35. ☐

Corollary 37. *In the course of the Orientation Algorithm, no violation of* $\mathbf{C_2}$ *occurs.*

Proof. This follows trivially from (ii) in Lemma 35. ☐

Lemma 38. *In the course of the Orientation Algorithm, no violation of* $\mathbf{C_3}$ *occurs.*

Proof. Suppose for contradiction that such an violation occurs. Let the first occurrence be $A \circ\!\!-\!\!\circ C$ oriented as $A \leftarrow C$. This means there is a vertex B such that $A \circ\!\!\to B \in \mathbf{REL}(J \circ\!\!\to K)$, but C, B are not adjacent. Again, this orientation must occur by the end of the third stage of the *Orientation Algorithm*, so the following are all the possible ways in which this orientation could occur. We derive a contradiction in each.

Case 1: $A \circ\!\!-\!\!\circ C$ is oriented as $A \leftarrow C$ to satisfy one of $\mathbf{C_1} - \mathbf{C_3}$. Lemma 33 implies that it is not $\mathbf{C_1}$ or $\mathbf{C_2}$. So it must be $\mathbf{C_3}$, which, however, contradicts Lemma 34.

Case 2: $A \circ\!\!-\!\!\circ C$ is oriented as $A \leftarrow C$ by an application of $\mathbf{UR}_2$, which means there is a D such that $C \circ\!\!-\!\!\circ D \circ\!\!-\!\!\circ A$ is in $\mathcal{P}_4^c$ and is already oriented as $C \rightarrow D \rightarrow A$ (before $A \leftarrow C$ is thus oriented). Then D must be adjacent to B, otherwise $A \leftarrow D$ would be an earlier violation of $\mathbf{C_3}$. Furthermore, because $D \circ\!\!-\!\!\circ A \circ\!\!\rightarrow B$ is in $\mathcal{P}_4$, the edge between D and B is either $D \rightarrow B$ or $D \circ\!\!\rightarrow B$ by Corollary 24. It can't be the former, for otherwise (ii) of Lemma 35 implies that there should not be any orientation into D (by the end of the third stage of the *Orientation Algorithm*), which contradicts $C \rightarrow D$. In the latter case, we argue that D is not a parent of K, and hence $D \circ\!\!\rightarrow B \in \mathbf{REL}(J \circ\!\!\rightarrow K)$. Suppose on the contrary that D is a parent of K. Obviously $A \circ\!\!\rightarrow K$, which is shown to be present in $\mathcal{P}_4$ by Lemma 28, belongs to $\mathbf{REL}(J \circ\!\!\rightarrow K)$. Since $A \circ\!\!-\!\!\circ D \rightarrow K$, (ii) of Lemma 35 implies that there should not be any orientation into D (by the end of the third stage of the *Orientation Algorithm*), which contradicts $C \rightarrow D$. Therefore, D is not a parent of K, and hence $D \circ\!\!\rightarrow B \in \mathbf{REL}(J \circ\!\!\rightarrow K)$. But then $C \rightarrow D$ is an earlier violation of $\mathbf{C_3}$ than $C \rightarrow A$, a contradiction.

Case 3: $A \circ\!\!-\!\!\circ C$ is oriented as $A \leftarrow C$ by an application of $\mathbf{UR}_3$. That is, there are two vertices D, E such that $D \circ\!\!-\!\!\circ E \circ\!\!-\!\!\circ A$, $D \circ\!\!-\!\!\circ C \circ\!\!-\!\!\circ A$, $C \circ\!\!-\!\!\circ E$ are in $\mathcal{P}_4^c$ and D, A are not adjacent. Furthermore, $D \circ\!\!-\!\!\circ E \circ\!\!-\!\!\circ A$ is already oriented as $D \rightarrow E \rightarrow A$ (before $A \leftarrow C$ is thus oriented). By the same argument as in *Case 2*, there must be an edge $E \circ\!\!\rightarrow B$ in $\mathcal{P}_4$. Furthermore, D and B must be adjacent, otherwise $D \rightarrow E$ would contradict (ii) of Lemma 35. Corollary 24 implies that the edge between D and B is either $D \rightarrow B$ or $D \circ\!\!\rightarrow B$. But then the edge $A \circ\!\!\rightarrow B$ could be oriented as $A \rightarrow B$ by $\mathcal{R}10$ because $\langle A, C, D, B \rangle$ is an uncovered p.d. path from A to B such that C and B are not adjacent. Hence a contradiction.

Case 4: $A \circ\!\!-\!\!\circ C$ is oriented as $A \leftarrow C$ by an application of $\mathbf{UR}_1$. Then there is a chain of applications of $\mathbf{UR}_1$ (which could consist of just one application) that leads to $C \rightarrow A$ where the first edge on the chain is *not* oriented by $\mathbf{UR}_1$. So there are three subcases to consider:

Case 4.1: the first edge is oriented to satisfy one of $\mathbf{C_1} - \mathbf{C_3}$. Lemma 33 implies that it is not $\mathbf{C_1}$ or $\mathbf{C_2}$. So it must be $\mathbf{C_3}$, which, however, contradicts Lemma 34.

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 C) such that $X \circ\!\!-\!\!\circ Y \circ\!\!-\!\!\circ Z$ is in $\mathcal{P}_4^c$, and is oriented as $X \rightarrow Y \rightarrow Z$, which in turn orients the edge $X \circ\!\!-\!\!\circ Z$ as $X \rightarrow Z$. And $X \rightarrow Z$ initiates a chain of $\mathbf{UR}_1$ applications on an uncovered circle path $u = \langle X, Z, \cdots, A\rangle$ that eventually leads to the orientation of $C \rightarrow A$. By the same induction as in Lemma 35, it is easy to show that for every vertex V on u after Z, there is an edge $Y \circ\!\!-\!\!\circ V$ in $\mathcal{P}_4^c$, oriented as $Y \rightarrow V$ before $X \circ\!\!-\!\!\circ Z$ is oriented. So in particular, Y is adjacent to A in $\mathcal{P}_4^c$ (and hence the edge between them is $Y \circ\!\!-\!\!\circ A$ in $\mathcal{P}_4$), and the edge between them is oriented as $Y \rightarrow A$ before $X \circ\!\!-\!\!\circ Z$ is oriented. Then Y must be adjacent to B in $\mathcal{P}_4$, for otherwise $Y \rightarrow A$ would be an earlier violation of $\mathbf{C_3}$ than $C \rightarrow A$. By Corollary 24, the edge between Y and B is either $Y \rightarrow B$ or $Y \circ\!\!\rightarrow B$ in $\mathcal{P}_4$. If it is $Y \rightarrow B$, then according to (ii) of Lemma 35, there should not be any orientation into Y (by the end of the third stage of the *Orientation Algorithm*), which contradicts $X \rightarrow Y$. So it must be $Y \circ\!\!\rightarrow B$ in $\mathcal{P}_4$. Furthermore, Y is not a parent of K, for otherwise there should not be any orientation into Y by (ii) of Lemma 35 (because $A \circ\!\!\rightarrow K \in \mathbf{REL}(J \circ\!\!\rightarrow K)$), which contradicts $X \rightarrow Y$. Furthermore, since $A \circ\!\!\rightarrow B \in \mathbf{REL}(J \circ\!\!\rightarrow K)$, there is a p.d. path from J to A such that no vertex on the path is a parent of K. This path appended by $A \circ\!\!-\!\!\circ Y$ is a p.d. path from J to Y with no parent of K on it. Hence $Y \circ\!\!\rightarrow B$ is in $\mathbf{REL}(J \circ\!\!\rightarrow K)$. This implies that X and B are adjacent in $\mathcal{P}_4$, for otherwise $X \rightarrow Y$ would be an earlier violation of $\mathbf{C_3}$. The edge between X and B, furthermore, is either $X \rightarrow B$ or $X \circ\!\!\rightarrow B$ by Corollary 24. Then consider the path $\langle A, C, \cdots, X, B\rangle$, which is a p.d. path from A to B such that C is not adjacent to B and the segment between A and X is uncovered. It is easy to see that $A \circ\!\!\rightarrow B$ could be oriented as $A \rightarrow B$ by $\mathcal{R}10$, a contradiction.

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 C) such that $W \circ\!\!-\!\!\circ Y \circ\!\!-\!\!\circ Z$, $W \circ\!\!-\!\!\circ X \circ\!\!-\!\!\circ Z$, $X \circ\!\!-\!\!\circ Y$ are in $\mathcal{P}_4^c$, and that W, Z are not adjacent. Furthermore, $W \circ\!\!-\!\!\circ Y \circ\!\!-\!\!\circ Z$ is oriented as $W \rightarrow Y \rightarrow Z$, which in turn orients the edge $X \circ\!\!-\!\!\circ Z$ as $X \rightarrow Z$. This then initiates a chain of $\mathbf{UR}_1$ applications on an uncovered circle path $u = \langle X, Z, \cdots, A\rangle$ that eventually leads to the orientation of $C \rightarrow A$. Notice that W, Z are not adjacent, so $\langle W, X, Z, \cdots, B\rangle$ is also an uncovered path. The rest of the argument is extremely similar to that of *Case 4.2.* □

Let $\mathcal{D}_{J\circ\rightarrow K}$ be the DAG output of the **Orientation Algorithm**. We have thus proved the following proposition:

Corollary 39. *$\mathcal{D}_{J\circ\rightarrow K}$ is a DAG orientation of $\mathcal{P}_4^c$ free of unshielded colliders and agreeable to $J \circ\!\!\rightarrow K$.*

Proof. It follows from Corollary 36, Corollary 37, Lemma 38 and the correctness of Meek's algorithm. □

Let $\mathcal{H}_{J\circ\rightarrow K}$ be the graph resulting from orienting $\mathcal{P}_{4aag}^c$ — the circle component of the arrowhead augmented graph of $\mathcal{P}_4$, which is the same as the circle component of $\mathcal{P}_4$ — into $\mathcal{D}_{J\circ\rightarrow K}$. By Lemma 16 and Corollary 39, $\mathcal{H}_{J\circ\rightarrow K}$ is a MAG equivalent to $\mathcal{G}$. Note that in $\mathcal{H}_{J\circ\rightarrow K}$ there is the edge $J \rightarrow K$. As planned earlier, what is left to show is that $\mathcal{H}_{J\circ\rightarrow K}$ can be transformed into a MAG where $J \leftrightarrow K$ appears through a sequence of equivalence-preserving changes of $\rightarrow$ to $\leftrightarrow$ (recall Lemma 19).

First we mention two simple facts about $\mathcal{P}_4$.

Lemma 40. *For any $A \circ\!\!\rightarrow B$ in $\mathcal{P}_4$, 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 induction on the length of u. If u consists of two edges, the interior vertex on u (i.e., other than A or B) is obviously adjacent to both A and B. Suppose u consists of three edges. If it is covered, then obviously one of the two interior vertices is adjacent to both A and B. If it is uncovered, then the vertex adjacent to A on u must also be adjacent to B, for otherwise $A \circ\!\!\rightarrow B$ could be oriented by $\mathcal{R}10$. In the inductive step, suppose the proposition holds if u consists of less than n edges. Consider the case where u consists of n edges. If it is covered, then a subsequence of u constitutes a p.d. path from A to B with less than n edges, and hence by the inductive hypothesis, a vertex on u is adjacent to both A and B. If u is uncovered, then the vertex adjacent to A on u must also be adjacent to B, for otherwise $A \circ\!\!\rightarrow B$ could be oriented by $\mathcal{R}10$. $\square$

Lemma 41. *Suppose* $C \leftarrow\!\!\circ A \circ\!\!\rightarrow B$ *is in* $\mathcal{P}_4$. *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 28, $A \circ\!\!\rightarrow K$ is in $\mathcal{P}_4$. However, by Definition 13, both B and C are parents of K, which implies that $A \circ\!\!\rightarrow K$ could be oriented by $\mathcal{R}11$ because C and B are not adjacent, a contradiction. $\square$

Now we present the key lemma, of which we provide an informal explanation here. Note that in $\mathcal{H}_{J \circ \rightarrow K}$ all $\circ\!\!\rightarrow$ edges in $\mathcal{P}_4$ are oriented as $\rightarrow$. So in particular, all edges in $\mathbf{REL}(J \circ\!\!\rightarrow K)$ are oriented as $\rightarrow$. Let $\mathcal{M}$ be any MAG identical to $\mathcal{H}_{J \circ \rightarrow K}$ except possibly that some $\circ\!\!\rightarrow$ edges in $\mathbf{REL}(J \circ\!\!\rightarrow K)$ are oriented as $\leftrightarrow$ (instead of $\rightarrow$). The lemma below shows that if all edges in $\mathbf{REL}(J \circ\!\!\rightarrow K)$ are not oriented as $\leftrightarrow$ in $\mathcal{M}$, then some $\rightarrow$ in $\mathcal{M}$ corresponding to some $\circ\!\!\rightarrow$ edge in $\mathbf{REL}(J \circ\!\!\rightarrow K)$ satisfies the conditions in Lemma 19, and hence can be changed into $\leftrightarrow$ while preserving equivalence. As a special case, for example, in $\mathcal{H}_{J \circ \rightarrow K}$ some $\rightarrow$ edge corresponding to a $\circ\!\!\rightarrow$ edge in $\mathbf{REL}(J \circ\!\!\rightarrow K)$ can be changed into $\leftrightarrow$. After this change, some remaining $\rightarrow$ corresponding to a $\circ\!\!\rightarrow$

edge, if any, can be further changed to $\leftrightarrow$ while preserving equivalence. This process can be continued until every edge in $\mathbf{REL}(J\circ\!\!\rightarrow K)$, and in particular $J\circ\!\!\rightarrow K$, can be oriented as $J \leftrightarrow K$ while preserving the Markov equivalence with $\mathcal{G}$.

Lemma 42. *Let $\mathcal{M}$ be any MAG identical to $\mathcal{H}_{J\circ\to K}$ except possibly that some $\circ\!\!\rightarrow$ edges in $\mathbf{REL}(J\circ\!\!\rightarrow K)$ are oriented as $\leftrightarrow$ (instead of $\rightarrow$). Let*

$$\mathbf{RREL} = \{A \rightarrow B \textit{ in } \mathcal{M} | A\circ\!\!\rightarrow B \textit{ is in } \mathcal{P}_4 \textit{ and } A\circ\!\!\rightarrow B \in \mathbf{REL}(J\circ\!\!\rightarrow K)\}$$

If $\mathbf{RREL}$ is not empty, then some edge therein can be changed to $\leftrightarrow$ while preserving Markov equivalence with $\mathcal{M}$.

Proof. Suppose $\mathbf{RREL}$ is not empty. Let

$$\mathbf{W} = \{B | \exists A \ s.t. A \rightarrow B \in \mathbf{RREL}\}$$

Let Y be a minimal vertex in $\mathbf{W}$, that is, $Y \in \mathbf{W}$ and no proper ancestor of D in $\mathcal{M}$ belongs to $\mathbf{W}$. Let X be a vertex such that $X \rightarrow Y \in \mathbf{RREL}$ and no proper descendant of X in $\mathcal{M}$ has this property. We show that $X \rightarrow Y$ satisfies the conditions (t1)-(t4) of Lemma 19.

Suppose, contrary to (t1), that X is an endpoint of an undirected edge $X - V$ in $\mathcal{M}$. Since any undirected edge in $\mathcal{M}$ is also in $\mathcal{H}_{J\circ\to K}$, $X - V$ is also in $\mathcal{P}_4$ (see Definition 12). On the other hand, since $X \rightarrow Y \in \mathbf{RREL}$, $X\circ\!\!\rightarrow Y$ is in $\mathcal{P}_4$. But then $X\circ\!\!\rightarrow Y$ could be oriented by $\mathcal{R}6$, a contradiction.

Suppose, contrary to (t2), that there is a directed path from X to Y in $\mathcal{M}$ that does not contain $X \rightarrow Y$. The corresponding path in $\mathcal{P}_4$ must be potentially directed. It follows from Lemma 40 that some vertex Z on the path is adjacent to both X and Y. Since $\mathcal{M}$ is a MAG, it must be the case that $X \rightarrow Z \rightarrow Y$ is in $\mathcal{M}$, and so the corresponding path $\langle X, Z, Y\rangle$ in $\mathcal{P}_4$ is potentially directed. Notice that the edge between Z and Y can't be $Z -\!\!\circ Y$ in $\mathcal{P}_4$ according to Lemma 7, 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 —o Z, and the edge between Z and Y is either Z o—oY or $Z \rightarrow Y$ or Zo→ Y. We enumerate the possibilities below and derive a contradiction in each:

Case 1: X o—oZ o—oY appears in $\mathcal{P}_4$. This contradicts property **CP1** (Lemma 5) because Xo→ Y is present in $\mathcal{P}_4$.

Case 2: X o—o$Z \rightarrow Y$ appears in $\mathcal{P}_4$. Because Xo→ $Y \in$ **REL**(Jo→ K), and X o—oZ is oriented as $X \rightarrow Z$, $\mathcal{D}_{J\text{o}\rightarrow K}$ is not agreeable to Jo→ K, which contradicts Corollary 39.

Case 3: X o—oZo→ Y appears in $\mathcal{P}_4$. If Z is not a parent of K, then Zo→ $Y \in$ **REL**(Jo→ K). But Z is a proper descendant of X in $\mathcal{M}$, which contradicts our choice of X. So Z must be a parent of K. Notice then that Xo→ K — which is shown to be present in $\mathcal{P}_4$ by Lemma 28 — belongs to **REL**(Jo→ K), but X o—oZ is oriented as $X \rightarrow Z$, which means that $\mathcal{D}_{J\text{o}\rightarrow K}$ is not agreeable to Jo→ K. This contradicts Corollary 39.

Case 4: $X \rightarrow Z$ o—oY appears in $\mathcal{P}_4$. Then Z is not a parent of K, for otherwise Xo→ K — which is implied to be present by Lemma 28 — could be oriented as $X \rightarrow K$ by $\mathcal{R}8$. Furthermore, since Xo→ K is shown to be present in $\mathcal{P}_4$ by Lemma 28, $Z \neq K$. So $Z \notin$ **AR**(Jo→ K). It follows that $\mathcal{D}_{J\text{o}\rightarrow K}$ is not agreeable to Jo→ K, because Z o—oY is oriented as $Z \rightarrow Y$, which contradicts Corollary 39.

Case 5: $X \rightarrow Z \rightarrow Y$ appears in $\mathcal{P}_4$. Then Xo→ Y could be oriented by $\mathcal{R}8$, a contradiction.

Case 6: $X \rightarrow Z$o→ Y appears in $\mathcal{P}_4$. Then Z is not a parent of K, for otherwise Xo→ K could be oriented by $\mathcal{R}8$. It follows that Zo→ $Y \in$ **REL**(Jo→ K). But Z is a proper descendant of X in $\mathcal{M}$, which contradicts our choice of X.

Case 7: Xo→ Z o—oY appears in $\mathcal{P}_4$. Then $Z \notin$ **AR**(Jo→ K), for otherwise Xo→ $Z \in$ **REL**(Jo→ K), but Z is a proper ancestor of Y in $\mathcal{M}$, which contradicts our choice of Y. However, Zo–oY is oriented as $Z \rightarrow Y$, which means that $\mathcal{D}_{J\circ\!\!\rightarrow K}$ is not agreeable to $J \circ\!\!\rightarrow K$. This contradicts Corollary 39.

Case 8: $X \circ\!\!\rightarrow Z \rightarrow Y$ appears in $\mathcal{P}_4$. Then Z must be adjacent to K, otherwise the edge $X \circ\!\!\rightarrow K$ could be oriented by $\mathcal{R}9$. Furthermore, since $Z \rightarrow Y \rightarrow K$ is in $\mathcal{P}_4$, the edge between Z and K is $Z \rightarrow K$ in $\mathcal{P}_4$. So $X \circ\!\!\rightarrow Z \in \mathbf{REL}(J \circ\!\!\rightarrow K)$. But Z is a proper ancestor of Y in $\mathcal{M}$, which contradicts our choice of Y.

Case 9: $X \circ\!\!\rightarrow Z \circ\!\!\rightarrow Y$ appears in $\mathcal{P}_4$. If Z is not a parent of K, then $Z \circ\!\!\rightarrow Y \in \mathbf{REL}(J \circ\!\!\rightarrow K)$. But Z is a proper descendant of X in $\mathcal{M}$, which contradicts our choice of X. So Z must be a parent of K. But then $X \circ\!\!\rightarrow Z \in \mathbf{REL}(J \circ\!\!\rightarrow K)$, and Z is a proper ancestor of Y in $\mathcal{M}$, which contradicts our choice of Y.

Case 10: $X \!-\!\!\circ Z \circ\!\!-\!\!\circ Y$ appears in $\mathcal{P}_4$. This contradicts Lemma 13, because $X \circ\!\!\rightarrow Y$ is present.

Case 11: $X \!-\!\!\circ Z \rightarrow Y$ appears in $\mathcal{P}_4$. Then $X \circ\!\!\rightarrow K$ could be oriented as $X \rightarrow K$ by either $\mathcal{R}8$ or $\mathcal{R}9$, a contradiction.

Case 12: $X \!-\!\!\circ Z \circ\!\!\rightarrow Y$ appears in $\mathcal{P}_4$. Z is not a parent of K, for otherwise $X \circ\!\!\rightarrow K$ could be oriented by $\mathcal{R}8$. So $Z \circ\!\!\rightarrow Y \in \mathbf{REL}(J \circ\!\!\rightarrow K)$. But Z is a proper descendant of X in $\mathcal{M}$, which contradicts our choice of X.

Next, we show that condition (t3) holds as well. For any $W \rightarrow X$ in $\mathcal{M}$, it corresponds to either $W \rightarrow X$ or $W \circ\!\!\rightarrow X$ or $W \circ\!\!-\!\!\circ X$ or $W \!-\!\!\circ X$ in $\mathcal{P}_4$. We argue that in any case W and Y are adjacent. In the former two cases, by Lemma 5, W and Y are adjacent. In the case of $W \circ\!\!-\!\!\circ X$, since it is oriented as $W \rightarrow X$ in $\mathcal{M}$, W must be adjacent to Y, for otherwise $\mathcal{D}_{J\circ\!\!\rightarrow K}$ is not agreeable to $J \circ\!\!\rightarrow K$, which contradicts Corollary 39. In the case of $W \!-\!\!\circ X$, by Lemma 13, W and Y are adjacent. Furthermore, the edge between W and Y must be $W \rightarrow Y$ in $\mathcal{M}$, because $W \rightarrow X \rightarrow Y$ is in $\mathcal{M}$ and $\mathcal{M}$ is a MAG.

For any $W \leftrightarrow X$ in $\mathcal{M}$, it corresponds to either $W {*\!\!\rightarrow} X$ or $W \leftarrow\!\!\circ X$ in $\mathcal{P}_4$. In the former case, W and Y are adjacent by Lemma 5. In the latter case, $W \leftarrow\!\!\circ X \in \mathbf{REL}(J \circ\!\!\rightarrow K)$ by our assumption. It then follows from Lemma 41 that W and Y are adjacent. So W and Y are adjacent in $\mathcal{M}$. Furthermore, since $\mathcal{M}$ is a MAG, the edge between W and Y is either $W \to Y$ or $W \leftrightarrow Y$ in $\mathcal{M}$.

Lastly, we show that condition (t4) in Lemma 19 is also satisfied. Suppose otherwise, that is, in $\mathcal{M}$ there is a path $u = (W, U, \cdots, X, Y)$ which is discriminating for X. We derive a contradiction below.

We first argue that if the edge between W and U is not $W{*\!\!\to} U$ in $\mathcal{P}_4$ (i.e., the arrowhead at U is not already in $\mathcal{P}_4$), then it (together with the next edge on u) can be substituted by a $*\!\!\to$ edge such that the resulting path is still discriminating for X in $\mathcal{M}$.

Here is the argument. First of all, the edge between W and U can't be $W \leftarrow\!\circ U$ in $\mathcal{P}_4$. Suppose otherwise; then in $\mathcal{M}$ the edge between W and U must be $W \leftrightarrow U$ by the definition of discriminating path (Definition 7). According to our assumption about $\mathcal{M}$, $W \leftarrow\!\circ U \in \mathbf{REL}(J{\circ\!\!\to} K)$. It follows that both W and Y are parents of K, and $U{\circ\!\!\to} K$ is present in $\mathcal{P}_4$ by Lemma 28. Furthermore, notice that $U \to Y$ is in $\mathcal{M}$ by the definition of discriminating path, which means the edge between U and Y in $\mathcal{P}_4$ constitutes an (uncovered) p.d. path from U to Y. Since W and Y are not adjacent by the definition of discriminating path, it is easy to see that $U{\circ\!\!\to} K$ could be oriented as $U \to K$ by $\mathcal{R}11$, a contradiction.

So, if the edge between W and U is not $W{*\!\!\to} U$ in $\mathcal{P}_4$, it is either $W \!-\!\!\circ U$ or $W \circ\!\!-\!\!\circ U$. By the definition of discriminating path, the next edge on u in $\mathcal{M}$ must be bi-directed, say $U \leftrightarrow V$. If it is $W \!-\!\!\circ U$ that appears in $\mathcal{P}_4$, then $U \leftrightarrow V$ is not in $\mathcal{P}_4$ by Lemma 7. So it must be $U{\circ\!\!\to} V$ in $\mathcal{P}_4$. It then follows from Lemma 13 that $W{*\!\!\to} V$ is in $\mathcal{P}_4$. So substituting $W{*\!\!\to} V$ for $\langle W, U, V\rangle$ yields another discriminating path for X (on which Y is the endpoint adjacent to X) in $\mathcal{M}$. On the other hand, suppose it is $W \circ\!\!-\!\!\circ U$ that appears in $\mathcal{P}_4$. If $U \leftrightarrow V$ is already in $\mathcal{P}_4$, then by Lemma 6, $W \leftrightarrow V$ also appears in $\mathcal{P}_4$ (and hence also in $\mathcal{M}$). So $\langle W, U, V\rangle$ could be replaced by $W \leftrightarrow V$. If $U \leftrightarrow V$ is not already in $\mathcal{P}_4$, then by our assumption about bi-directed edges in $\mathcal{M}$, either $U \circ\!\!\rightarrow V$ or $V \circ\!\!\rightarrow U$ appears in $\mathcal{P}_4$ and belongs to $\mathbf{REL}(J \circ\!\!\rightarrow K)$. In the former case, W must be adjacent to V, otherwise the orientation of $W \circ\!\!-\!\!\circ U$ (into $W \rightarrow U$) is not agreeable. By Corollary 24, the edge between W and V is either $W \rightarrow V$ or $W \circ\!\!\rightarrow V$ in $\mathcal{P}_4$, and so $\langle W, U, V \rangle$ could be replaced by $W {*\!\!\rightarrow} V$. In the latter case, by Lemma 6, either $V \rightarrow W$ or $V \circ\!\!\rightarrow W$ is in $\mathcal{P}_4$. Now if W is not a parent of K, which means $W \notin \mathbf{AR}(J \circ\!\!\rightarrow K)$ ($W \neq K$ because Y belongs to $\mathbf{AR}(J \circ\!\!\rightarrow K)$ but is not adjacent to W), then the orientation of $W \circ\!\!-\!\!\circ U$ (into $W \rightarrow U$) is not agreeable. So W is a parent of K, but then the edge $V \circ\!\!\rightarrow K$ — which is implied to be present in $\mathcal{P}_4$ by Lemma 28 — could be oriented as $V \rightarrow K$ by $\mathcal{R}11$, because W and Y are not adjacent (and the edge between V and Y constitutes an uncovered p.d. path in $\mathcal{P}_4$), a contradiction.

Therefore, without loss of generality, we can safely assume that the edge between W and U is $W {*\!\!\rightarrow} U$ in $\mathcal{P}_4$, i.e., the arrowhead at U is already in $\mathcal{P}_4$.

Now consider the subpath between W and X, $u(W, X)$. Let the vertex adjacent to X on $u(W, X)$ be Q. By the definition of discriminating path, $Q \rightarrow Y$ is in $\mathcal{M}$, and Q is a collider on u. Since we have shown that (t2) holds of $X \rightarrow Y$ in $\mathcal{M}$, the edge between Q and X is not $Q \leftarrow X$. So it must be $Q \leftrightarrow X$. Therefore, every edge on $u(W, X)$ other than $W {*\!\!\rightarrow} U$ is bi-directed.

It is easy to see that not all of these bi-directed edges are in $\mathcal{P}_4$, for otherwise u is already a discriminating path for X in $\mathcal{P}_4$, and hence $X \circ\!\!\rightarrow Y$ could be oriented by $\mathcal{R}4$. Let $P_1 \leftrightarrow P_2$ be the closest edge to W on $u(W, X)$ such that $P_1 \leftrightarrow P_2$ does not appear in $\mathcal{P}_4$. Then by our assumption about the bi-directed edges in $\mathcal{M}$, it is either $P_1 \circ\!\!\rightarrow P_2$ or $P_2 \circ\!\!\rightarrow P_1$ in $\mathcal{P}_4$. Without loss of generality, suppose it is $P_1 \circ\!\!\rightarrow P_2$, which, according to our assumption, belongs to $\mathbf{REL}(J \circ\!\!\rightarrow K)$. Note that, by our choice of $P_1 \leftrightarrow P_2$, all the arrowheads between P_1 and W are already in $\mathcal{P}_4$, so the edge between P_1 and Y should be oriented as $P_1 \rightarrow Y$ by either $\mathcal{R}1$ (if P_1 is U) or $\mathcal{R}5$. Since Y is a parent of K, $P_1 \circ\!\!\rightarrow K$, which is shown to be present in $\mathcal{P}_4$ by Lemma 28, could be oriented by $\mathcal{R}8$, a contradiction.

Therefore, all the conditions in Lemma 19 are met. Thus changing $X \rightarrow Y$ to $X \leftrightarrow Y$ will yield a MAG Markov equivalent to $\mathcal{M}$. □

Corollary 43. *$\mathcal{G}_{J\circ\!\rightarrow K}$ can be transformed via a series of equivalence-preserving changes into a MAG where $J \leftrightarrow K$ appears.*

Proof. Using Lemma 42, a simple induction on the number of edges in $\mathbf{REL}(J\circ\!\rightarrow K)$ would do. □

Theorem 3. *$\mathcal{P}_4$ is complete with respect to invariant tails. That is, for every circle in $\mathcal{P}_4$, there is a member of $[\mathcal{G}]$ in which the circle is oriented as an arrowhead.*

Proof. It follows readily from Lemma 16, Corollary 39 and Corollary 43. □

The main result of this paper thus follows.

Theorem 4. *$\mathcal{P}_4 = \mathcal{P}_{\mathcal{G}}$, i.e., $\mathcal{P}_4$ is the CPAG for the Markov equivalence class of $\mathcal{G}$.*

Proof. It follows from Theorems 1, 2 and 3. □

3.3 A Characterization of CPAGs

The completeness result leads to a syntactic characterization of CPAGs by the orientation rules. To borrow a term from Andersson et al. (1997), we say a non-circle mark in a partial mixed graph is *protected* by an orientation rule if it could be introduced by that orientation rule, given all other marks in the graph. The next theorem gives the necessary and sufficient conditions for a partial mixed graph — that is, a graph consisting of $\rightarrow$, $\leftrightarrow$, $--$, $\circ\!\rightarrow$, $\circ\!\!-\!\!\circ$, $\circ\!-\!-$ to be a CPAG for some Markov equivalence class of MAGs.

Theorem 5. *A partial mixed graph is a CPAG for a Markov equivalence class of MAGs if and only if* *(i) (a1)-(a3) (in Definition 1) and* **CP**1 − **CP**4 *hold; and there is no inducing path between two non-adjacent vertices;*

(ii) the circle component is chordal;

(iii) it is closed under $\mathcal{R}8 - \mathcal{R}11$*; and*

(iv) every non-circle mark is protected by one of $\mathcal{R}0 - \mathcal{R}11$.

Note that the characterization of essential graphs — graphs that represent Markov equivalence classes of DAGs — given in Andersson et al. (1997) is essentially of the same sort. A proof of the theorem is not hard to construct given what we have shown in the last section. In particular, we can construct a MAG by tail augmenting (or arrowhead augmenting) the given partial mixed graph and orienting the circle component as a DAG with no unshielded colliders. The resulting MAG is a member of the Markov equivalence class of which the given graph is the CPAG.

4 Conclusion

In this paper we provided a characterization of Markov equivalence classes of ancestral graphical models. We did this by defining a complete representation of Markov equivalence classes of MAGs — CPAGs, and introduced a set of orientation rules by which one can construct a CPAG from a given MAG. This work is thus analogous to, and can be regarded as an extension of, the results presented in Meek (1995) and Andersson et al. (1997), since DAGs are special cases of MAGs.

As discussed earlier, two existing representations of equivalence classes of MAGs in the literature are PAGs and JGs. The former is simply a less informative version of CPAGs, which only requires to include non-circle marks enough to capture all the m-separation features. The latter ignores the distinction between circles and tails, and hence only aims to represent the common arrowheads shared by all the members of an equivalence class. Interestingly, to capture all the m-separation features of an equivalence class, it is not necessary to make the tails explicit. So, as shown in Ali (2002), a global Markov property can be defined in a JG that corresponds exactly to the m-separations of the equivalence class of MAGs represented. Therefore, a JG is automatically a PAG, save the difference in symbols. It is thus clear that to characterize PAGs or JGs, $\mathcal{R}0 - \mathcal{R}4$ (or a slightly modified version in the case of JGs) would do.

Although the tails do not contribute to represent m-separations, they do have very intuitive causal interpretations, which renders CPAGs a more desirable formalism for the purpose of causal inference. Under the standard causal interpretations of MAGs (Richardson and Spirtes 2003), invariant tails can signify qualitative causal relationships between variables, and some of them are even crucial for making quantitative predictions about the strength of causal effects. In fact, the foremost reason for dealing with equivalence classes is the need of causal discovery and inference.

The bearing of the results presented here on causal inference is obvious. There are two major approaches to search of causal models: independence-based search and score-based search. The canonical algorithms of the former sort are the PC algorithm (Spirtes et al. 1993) and the FCI algorithm (Spirtes et al. 1999); the canonical algorithm of the latter sort is the GES algorithm (Meek 1996, Chickering 2002). PC and GES both assume no latent confounding and selection bias, while FCI does not need the assumption. The current paper shows how to make the FCI algorithm complete. We speculate that it may also prove important in the design of a GES algorithm in the presence of latent confounding and selection bias.

We end with noting an open problem at this point. It is the one of causal discovery given background knowledge. More specifically, how can we construct a CPAG with some orientations given as "invariant", that is, a CPAG for a subset of a Markov equivalence class of MAGs? This is of course closely related to the task of characterizing an arbitrary set of Markov equivalent MAGs, for which Ali (2002) presented some interesting results.

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