Sound and Complete Causal Identification with Latent Variables Given Local Background Knowledge

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Abstract

Great efforts have been devoted to causal discovery from observational data, and it is well known that introducing some background knowledge attained from experiments or human expertise can be very helpful. However, it remains unknown that *what causal relations are identifiable given background knowledge in the presence of latent confounders*. In this paper, we solve the problem with sound and complete orientation rules when the background knowledge is given in a *local* form. Furthermore, based on the solution to the problem, this paper proposes a general active learning framework for causal discovery in the presence of latent confounders, with its effectiveness and efficiency validated by experiments.

1 Introduction

Causality has attracted tremendous attention in recent years, for its application on explainability [1], fairness [2, 3, 4], decision [5, 6, 7, 8, 9], and so on. In Pearl's causality framework [10], one important problem is *causal discovery*, *i.e.*, learning a causal graph to denote the causal relations among all the variables [11, 12, 13, 14, 15, 16]. Generally, we cannot identify all the causal relations from observational data, unless we make some additional functional assumptions [17, 18, 19] or exploit the abundant information in multiple or dynamic environments [20, 21].

In light of the uncertainty of the causal relations, a common practice to reveal them is introducing *background knowledge*, which is called *BK* for short. BK can be attained from *experiments* or *human expertise*. When experiments are available, we can collect interventional data to learn additional causal relations [22, 23, 24, 25, 26, 27, 28, 29, 30, 31]. And if in the causal discovery task, there are some variables familiar to humans, it is also possible that the human expertise can be helpful [32]. For example, if we study the causal relations among some variables including sales and prices, the causal relations such as price causes sales can be obtained directly according to human expertise.

When BK is available in addition to observational data, a fundamental problem is: *what causal relations are identifiable in the presence of latent variables*? This problem is fundamental for its implication on the maximally identifiable causal knowledge with the observational data and BK. Its difficulty results from the fact that, in addition to the BK itself, some other causal relations can also be learned when incorporating BK. For example, they can be identified on the basis of some restrictions, such as the causal relations are acyclic. It is quite challenging to find the *complete* characterization for such additional causal knowledge in the presence of latent variables, and the complete characterization is necessarily accompanied with theoretical guarantee for the existence of causal graphs consistent to the observational data and local BK that have *exactly different* causal relations for the unidentifiable ones. Unfortunately, the problem remains open.

In this paper, we solve the problem with *sound* and *complete* orientation rules when the background knowledge is given in a *local* form. In the presence of latent variables, a partial ancestral graph (PAG)

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can be learned by FCI algorithm from observational data [33, 34, 35]. PAG can imply the *existence* of causal relation between any two variables but not necessarily imply the causal *direction*. We say *BK is local*, if when the BK contains the causal information with respect to a variable X, for each variable adjacent to X in the PAG, the BK implies whether X causes it or not. The local BK is common in real tasks no matter it is from experiments or human expertise. For example, when we make experiments and collect the data under intervention on X, for each variable V that has a causal relation with X, the interventional data can tell whether X causes V; and businessman often has enough domain knowledge about price, thus they usually know whether price causes other variables or not, such as price causes sales and number of customers, and price is not caused by stocks. Given a PAG and local BK, we propose a set of orientation rules to determine some causal directions in the PAG. We prove that the rules are sound and complete, which state that all the causal relations that are identifiable given available information are *exactly* those determined by the proposed rules, thus closing the problem given local BK.

The establishment of orientation rules compatible with local BK makes causal discovery by interventions possible in the presence of latent variables. We propose the first general active learning framework for causal discovery, with the target of identifying a *maximal ancestral graph (MAG)*, which implies the causal relations when there are latent variables. Considering that intervention is expensive in reality, we hope to achieve the target with as few interventions as possible. Hence we present a baseline maximal entropy criterion, equipped with Metropolis-Hastings sampling, to select the intervention variable such that we can learn more causal relations by each intervention. Our contributions in this paper are twofold:

(1) We show what causal relations are identifiable given local background knowledge in the presence of latent confounders with sound and complete orientation rules.

(2) We give the first active learning framework for causal discovery that is applicable when latent variables exist, where maximal entropy criterion equipped with Metropolis-Hastings sampling is introduced to select intervention variables.

Related works. In the literature, Meek [36] established sound and complete rules, generally called *Meek rules*, for causal identification given BK under the causal sufficiency assumption. The assumption requires that there are no latent variables that cause more than one observed variable simultaneously. However, causal sufficiency is untestable in practice. When we apply causality in subjects such as biology, sociology, and economics, it is quite often that there are latent variables. For example, the macroeconomic policy influences purchase price, the population of customers, and advertising cost, but it is hard to evaluate it, thereby a latent confounder. Andrews et al. [37] showed that FCI algorithm is complete given *tiered* BK, where all variables are partitioned into disjoint sets with explicit causal order. While in many cases, e.g., when BK is revealed by interventions, BK is not tiered. And Jaber et al. [28] investigated the complete algorithm to learn a graph when there are additional interventional distribution, while such knowledge is not needed in our paper.

2 Preliminary

A graph $G = (\mathbf{V}, \mathbf{E})$ consists of a set of vertices $\mathbf{V} = \{V_1, \cdots, V_p\}$ and a set of edges $\mathbf{E}$. For any subset $\mathbf{V}' \subseteq \mathbf{V}$, the *subgraph induced by* $\mathbf{V}'$ is $G_{\mathbf{V}'} = (\mathbf{V}', \mathbf{E}_{\mathbf{V}'})$, where $\mathbf{E}_{\mathbf{V}'}$ is the set of edges in $\mathbf{E}$ whose both endpoints are in $\mathbf{V}'$. For a graph G, $\mathbf{V}(G)$ denotes the set of vertices in G. G is a complete graph if there is an edge between any two vertices. The subgraph induced by an empty set is also a complete graph. $G[-\mathbf{V}']$ denotes the subgraph $G_{\mathbf{V}\backslash\mathbf{V}'}$ induced by $\mathbf{V}\backslash\mathbf{V}'$. Usually, bold letter (*e.g.*, $\mathbf{V}$) denotes a set of vertices and normal letter (*e.g.*, V) denotes a vertex. A graph is *chordal* if any cycle of length four or more has a chord, which is an edge joining two vertices that are not consecutive in the cycle. If $G = (\mathbf{V}, \mathbf{E})$ is chordal, the subgraph of G induced by $\mathbf{V}' \subseteq \mathbf{V}$ is chordal.

A graph G is *mixed* if the edges in G are either directed $\rightarrow$ or bi-directed $\leftrightarrow$. The two ends of an edge are called *marks* and have two types *arrowhead* or *tail*. A graph is a *partial mixed graph* (*PMG*) if it contains directed edges, bi-directed edges, and edges with *circles* ($\circ$). The circle implies that the mark here could be either arrowhead or tail but is indefinite. V_i is *adjacent* to V_j in G if there is an edge between V_i and V_j. A path in a graph G is a sequence of distinct vertices $\langle V_0, \cdots, V_n\rangle$ such that for $0 \leq i \leq n-1$, V_i and V_{i+1} are adjacent in G. An edge in the form of $V_i \circ\!\!-\!\!\circ V_j$ is a *circle edge*. The circle component in G is the subgraph consisting of all the $\circ\!\!-\!\!\circ$ edges in G. Denote the set of vertices adjacent to V_i in G by $\text{Adj}(V_i, G)$. A vertex V_i is a *parent* of a vertex V_j if there is $V_i \rightarrow V_j$. A *directed path* from V_i to V_j is a path comprised of directed edges pointing to the direction of V_j. A *possible directed path* from V_i to V_j is a path without an arrowhead at the mark near V_i on every edge in the path. V_i is an *ancestor/possible ancestor* of V_j if there is a *directed path/possible directed path* from V_i to V_j or $V_i = V_j$. V_i is a *descendant/possible descendant* of V_j if there is a *directed path/possible directed path* from V_j to V_i or $V_j = V_i$. Denote the set of *parent/ancestor/possible ancestor/descendant/possible descendant* of V_i in G by Pa(V_i, G)/Anc(V_i, G)/PossAn(V_i, G)/De(V_i, G)/PossDe(V_i, G). If $V_i \in$ Anc(V_j, G) and $V_i \leftarrow V_j$/$V_i \leftrightarrow V_j$, it forms a *directed cycle/almost directed cycle*. $*$ is a wildcard that denotes any of the marks (arrowhead, tail, and circle). We make a convention that when an edge is in the form of $\circ\!\!\rightarrow\!*$, the $*$ here cannot be a tail since in this case the circle can be replaced by an arrowhead due to the assumption of no selection bias.

A non-endpoint vertex V_i is a collider on a path if the path contains $*\!\!\rightarrow V_i \leftarrow\!\!*$. A path p from V_i to V_j is a *collider path* if V_i and V_j are adjacent or all the passing vertices are colliders on p. p is a *minimal path* if there are no edges between any two non-consecutive vertices. A path p from V_i to V_j is a *minimal collider path* if p is a collider path and there is not a proper subset $\mathbf{V}'$ of the vertices in p such that there is a collider path from V_i to V_j comprised of $\mathbf{V}'$. A triple $\langle V_i, V_j, V_k \rangle$ on a path is unshielded if V_i and V_k are not adjacent. p is an *uncovered path* if every consecutive triple on p is unshielded. A path p is a *minimal possible directed path* if p is minimal and possible directed.

A mixed graph is an *ancestral graph* if there is no directed or almost directed cycle (since we assume no selection bias, we do not consider undirected edges in this paper). An ancestral graph is a *maximal ancestral graph (MAG, denoted by $\mathcal{M}$)* if it is *maximal*, *i.e.*, for any two non-adjacent vertices, there is a set of vertices that *m-separates* them [33]. A path p between X and Y in an ancestral graph G is an *inducing path* if every non-endpoint vertex on p is a collider and meanwhile an ancestor of either X or Y. An ancestral graph is maximal if and only if there is no inducing path between any two non-adjacent vertices [33].

In an MAG, a path $p = \langle X, \cdots, W, V, Y \rangle$ is a *discriminating path for V* if (1) X and Y are not adjacent, and (2) every vertex between X and V on the path is a collider on p and a parent of Y. Two MAGs are *Markov equivalent* if they share the same *m-separations*. A class comprised of all Markov equivalent MAGs is a *Markov equivalence class (MEC)*. We use a *partial ancestral graph (PAG, denoted by $\mathcal{P}$)* to denote an MEC, where a tail/arrowhead occurs if the corresponding mark is tail/arrowhead for all Markov equivalent MAGs, and a circle occurs otherwise.

For a PMG $\mathbb{M}$ that is obtained from a PAG $\mathcal{P}$ by orienting some circles to either arrowheads or tails, an MAG $\mathcal{M}$ is *consistent to the PMG* $\mathbb{M}$ if (1) the non-circle marks in $\mathbb{M}$ are also in $\mathcal{M}$, and (2) $\mathcal{M}$ is in the MEC represented by $\mathcal{P}$. Sometimes we will omit the PAG $\mathcal{P}$ and just directly say a PMG $\mathbb{M}$ (obtained from the PAG $\mathcal{P}$) since in this paper we study the rules to incorporate local BK to a PAG. We say an MAG $\mathcal{M}$ *is consistent to the BK* if $\mathcal{M}$ is with the orientations dictated by the BK.

3 Sound and Complete Rules

In this section, we present the sound and complete orientation rules to orient a PAG $\mathcal{P}$ with local background knowledge (BK), where $\mathcal{P}$ is learned by observational data [11, 35] and $\mathbf{V}(\mathcal{P}) = \{V_1, V_2, \cdots, V_d\}$. The *local BK* regarding X means that the BK directly implies and only directly implies all the true marks at X, denoted by $BK(X)$. We assume the absence of selection bias and that the BK is correct. The correctness indicates that there exists an MAG consistent to $\mathcal{P}$ and the BK. Without loss of generality, we suppose the local BK is regarding $V_1, V_2, \cdots, V_k, 1 \leq k \leq d$. That is, for any vertex $X \in V_1, V_2, \cdots, V_k$, all the marks at X are known according to the local BK; and for any vertex $X \in V_{k+1}, \cdots, V_d$, the local BK does not directly imply any marks at X.

First, we show the orientation rules to incorporate local BK. They follow the rules of Zhang [35] for learning a PAG but with one replacement and one addition. Due to the page limit, we do not list them here but the replaced and additional ones. See Appendix A for the rules proposed by Zhang [35].

$\mathcal{R}'_4$: If $\langle K, \cdots, A, B, R \rangle$ is a discriminating path between K and R for B, and $B \circ\!\!\rightarrow\!* R$, then orient $B \circ\!\!\rightarrow\!* R$ as $B \rightarrow R$.

$\mathcal{R}_{11}$: If $A \rightarrow\!\!* B$, then $A \rightarrow B$.

Algorithm 1: Update a PMG with local background knowledge

Input: A PMG $\mathbb{M}_i$, $BK(X)$

Output: Updated graph $\mathbb{M}_{i+1}$

1 For any $K \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ and any $T \in \mathbf{C}$ such that $K \circ\!\!-\!\!* T$ in $\mathbb{M}_i$, orient $K \leftarrow\!\!* T$ (the mark at T remains); for all $K \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ such that $X \circ\!\!-\!\!* K$, orient $X \rightarrow K$;

2 Orient the subgraph $\mathbb{M}_i[\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])\backslash\{X\}]$ as follows until no feasible updates: for any two vertices V_l and V_j such that $V_l \circ\!\!-\!\!\circ V_j$, orient it as $V_l \rightarrow V_j$ if **(i)** $\mathcal{F}_{V_l}\backslash\mathcal{F}_{V_j} \neq \emptyset$ or **(ii)** $\mathcal{F}_{V_l} = \mathcal{F}_{V_j}$ as well as there is a vertex $V_m \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])\backslash\{X\}$ not adjacent to V_j such that $V_m \rightarrow V_l \circ\!\!-\!\!\circ V_j$;

3 Apply the orientation rules until the graph is closed under the orientation rules.

Prop. 1 implies the soundness of $\mathcal{R}'_4$ to orient a PAG $\mathcal{P}$ or a PMG obtained from $\mathcal{P}$ with local BK. See Appendix A for the proof. $\mathcal{R}_{11}$ is immediate due to no selection bias assumption. In the following, we make a convention that when we say the orientation rules, they refer to $\mathcal{R}_1 - \mathcal{R}_3, \mathcal{R}_8 - \mathcal{R}_{10}$ of Zhang [35] and $\mathcal{R}'_4, \mathcal{R}_{11}$. A PMG is *closed under the orientation rules* if the PMG cannot be oriented further by the orientation rules.

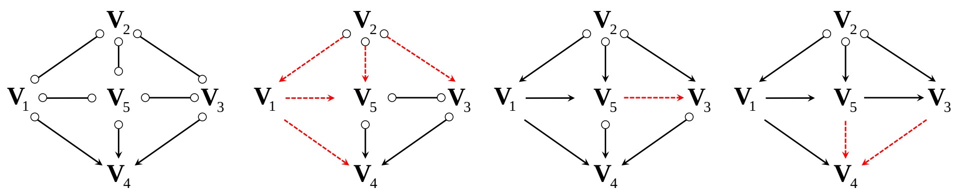
Proposition 1. *Given a PAG $\mathcal{P}$, for any PMG $\mathbb{M}$ that is obtained from $\mathcal{P}$ by orienting some circles in $\mathcal{P}$ (or $\mathbb{M} = \mathcal{P}$), $\mathcal{R}'_4$ is sound to orient $\mathbb{M}$ with local background knowledge.*

Proof sketch: If there is $B \leftarrow\!\!* R$ in an MAG consistent with the case of $\mathcal{R}'_4$, there must be a minimal collider path between K and R across B, in which case $B \leftarrow\!\!* R$ *should have been* identified in the PAG according to Zhao et al. [38], Zhang [35], contradiction. $\square$

Next, we will prove the completeness of the proposed orientation rules. It is somewhat complicated. We first give a roadmap for the proof process. There are mainly two parts. The first is that we present a complete algorithm to orient $\mathcal{P}$ with the local BK regarding $V_1, V_2, \cdots, V_k$. The second part is to prove that the algorithm orient the same marks as the proposed orientation rules. Combining these two parts, we conclude the orientation rules are complete to orient a PAG. The construction of the algorithm and the corresponding proof for the completeness of the algorithm in the first step is the most difficult part. To achieve the construction, we divide the whole process of orienting a PAG with BK regarding $V_1, V_2, \cdots, V_k$ into k steps. Beginning from the PAG $\mathcal{P}$ ($\mathcal{P}$ is also denoted by $\mathbb{M}_0$), in the $(i+1)$-th ($0 \leq i \leq k-1$) step we obtain a PMG $\mathbb{M}_{i+1}$ from $\mathbb{M}_i$ by incorporating $BK(V_{i+1})$ and orienting some other circles further. To obtain the updated graph in each step, we propose an algorithm orienting a PMG with local BK incorporated in this step. Repeat this process by incorporating $BK(V_1), BK(V_2), \ldots, BK(V_k)$ sequentially, we obtain the PMG with incorporated BK regarding $V_1, \cdots, V_k$. We will prove that the k-step algorithm to orient PAG with local BK regarding $V_1, \cdots, V_k$ is complete, by an induction step that if the first i-step algorithm is complete to update the PAG $\mathcal{P}$ with BK regarding $V_1, \cdots, V_i$, then the $(i+1)$-step algorithm is complete to update $\mathcal{P}$ with BK regarding $V_1, \cdots, V_{i+1}$. Hence the proof in the first part completes. In the second part, we show that the k-step algorithm orients the same marks as the proposed orientation rules. We thus conclude that the orientation rules are sound and complete for causal identification in the presence of latent variables given local BK.

We present Alg. 1 to obtain $\mathbb{M}_{i+1}$ from $\mathbb{M}_i$ by incorporating $BK(V_{i+1})$. For brevity, we denote V_{i+1} by X, and introduce a set of vertices $\mathbf{C}$ defined as $\mathbf{C} = \{V \in \mathbf{V}(\mathcal{P}) \mid V *\!\!\rightarrow X \in BK(X)\}$ to denote the vertices whose edges with X will be oriented to ones with arrowheads at X according to $BK(X)$ directly. In $\mathbb{M}_{i+1}$, there is $X \leftarrow\!\!* V$ for $V \in \mathbf{C}$ and $X -\!\!* V$ for $V \in \{V \in \mathbf{V}(\mathcal{P}) \mid V *\!\!-\!\!\circ X \text{ in } \mathbb{M}_i\}\backslash\mathbf{C}$ oriented directly according to $BK(X)$. We define $\mathcal{F}^{\mathbb{M}_i}_{V_l} = \{V \in \mathbf{C} \cup \{X\} \mid V *\!\!-\!\!\circ V_l \text{ in } \mathbb{M}_i\}$ for any $V_l \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])\backslash\{X\}$, which is denoted by $\mathcal{F}_{V_l}$ for short. $\mathcal{F}_{V_l}$ denotes the vertices in $\mathbf{C} \cup \{X\}$ whose edges with V_l are oriented to ones with arrowheads at V_l in the first step of Alg. 1.

In the first step of Alg. 1, the orientation at X follows $BK(X)$, and the orientation at the vertices apart of X is motivated as the necessary condition for the ancestral property. Speaking roughly, if there is an oriented edge $K \rightarrow T$ in the case of the first step, then no matter how we orient the other circles, there will be a directed or almost directed cycle, unless we introduce new unshielded colliders (which takes new conditional independences relative to those in $\mathcal{P}$), both of which are evidently



(a) PMG $\mathbb{M}_i$ (b) After Step 1 (c) After Step 2 (d) After Step 3

Figure 1: An example to demonstrate the implementation of each step of Alg. 1. Fig. 1(a) depicts a PMG $\mathbb{M}_i$. Suppose the local BK is in the form of $V_1 \leftarrow\!\!* V_2, V_1 -\!\!* V_5, V_1 -\!\!* V_4$. The Fig. 1(b)/1(c)/1(d) displays the graph obtained after the first/second/third step of Alg. 1. The edges oriented by each step are denoted by red dashed lines.

invalid to obtain an MAG in the MEC represented by $\mathcal{P}$. And the orientation in the second step is motivated as the necessary condition for that there are no new unshielded colliders in the oriented graph relative to the PAG $\mathcal{P}$. If there is an MAG where there is an inconsistent edge with the edge oriented in this step, then there must be new unshielded colliders relative to $\mathcal{P}$, which implies that the MAG is not consistent to $\mathcal{P}$. The third step orients some other circles based on the updated structure.

Example 1. *See the example in Fig. 1. Suppose the input PMG $\mathbb{M}_i$ in Alg. 1 is the graph shown in Fig. 1(a). And there is local BK regarding $X = V_1$, which is in the form of $V_1 \leftarrow\!\!* V_2, V_1 -\!\!* V_5, V_1 -\!\!* V_4$. Hence $\mathbf{C} = \{V_2\}$. In this case, PossDe$(X, \mathbb{M}_i[-\mathbf{C}]) = \mathrm{PossDe}(V_1, \mathbb{M}_i[-V_2]) = \{V_1, V_3, V_4, V_5\}$. And $\mathcal{F}_{V_3} = \{V_2\}$, $\mathcal{F}_{V_4} = \{V_1\}$, $\mathcal{F}_{V_5} = \{V_1, V_2\}$. When we implement Alg. 1, in the first step, the edges denoted by red dashed lines in Fig. 1(b) are oriented. Among them, $V_1 \circ\!\!-\!\!\circ V_2$/$V_1 \circ\!\!-\!\!\circ V_5$/$V_1 \circ\!\!\rightarrow V_4$ is transformed to $V_1 \leftarrow\!\!\circ V_2$/$V_1 \rightarrow V_5$/$V_1 \rightarrow V_4$ due to $V_1 = X, V_2 \in \mathbf{C}, V_4, V_5 \in \{V \in \mathbf{V}(\mathcal{P}) \mid V \ast\!\!-\!\!\circ X \text{ in } \mathbb{M}_i\} \backslash \mathbf{C}$; and $V_2 \circ\!\!\rightarrow V_5$/$V_2 \circ\!\!\rightarrow V_3$ is oriented due to $V_2 \in \mathbf{C}$ and $V_3, V_5 \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$. In the second step of Alg. 1, the edge denoted by red dashed line in Fig. 1(c) is oriented due to (1) a circle edge $V_3 \circ\!\!-\!\!\circ V_5$ after the first step, where $V_3, V_5 \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$; (2) $\mathcal{F}_{V_3} = \{V_2\} \subset \{V_1, V_2\} = \mathcal{F}_{V_5}$. In the third step of Alg. 1, the edges denoted by red dashed lines in Fig. 1(d) is oriented by $\mathcal{R}_1$ of the orientation rules.*

Then, we present the key induction result in Thm. 1 for the graph obtained by Alg. 1 in each step. Due to the page limit, we only show a proof sketch, with a detailed version in Appendix B. Then with Thm. 1, we directly conclude that k-step algorithm is complete to orient the PAG with the local BK regarding $V_1, \ldots, V_k$ in Cor. 1.

Theorem 1. *Given i, suppose $\mathbb{M}_s, \forall s \in \{0, 1, \ldots, i\}$ satisfies the five following properties:*

(Closed) *$\mathbb{M}_s$ is closed under the orientation rules.*

(Invariant) *The arrowheads and tails in $\mathbb{M}_s$ are invariant in all the MAGs consistent to $\mathcal{P}$ and BK regarding $V_1, \ldots, V_s$.*

(Chordal) *The circle component in $\mathbb{M}_s$ is chordal.*

(Balanced) *For any three vertices A, B, C in $\mathbb{M}_s$, if $A \ast\!\!\rightarrow B \circ\!\!-\!\!\ast C$, then there is an edge between A and C with an arrowhead at C, namely, $A \ast\!\!\rightarrow C$. 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 $A \leftrightarrow C$).*

(Complete) *For each circle at vertex A on any edge $A \circ\!\!-\!\!\ast B$ in $\mathbb{M}_s$, there exist MAGs $\mathcal{M}_1$ and $\mathcal{M}_2$ consistent to $\mathcal{P}$ and BK regarding $V_1, \ldots, V_s$ with $A \leftarrow\!\!* B \in \mathbf{E}(\mathcal{M}_1)$ and $A \rightarrow B \in \mathbf{E}(\mathcal{M}_2)$.*

Then the PMG $\mathbb{M}_{i+1}$ obtained from $\mathbb{M}_i$ with $BK(V_{i+1})$ by Alg. 1 also satisfies the five properties.

Proof sketch: For brevity, we denote V_{i+1} by X. **(A)** The closed property holds due to the third step of Alg. 1.**(B)** The invariant property holds because all the orientations in Alg. 1 either follow $BK(X)$ or are motivated as the necessary condition for the ancestral property and the fact that there cannot be new unshielded colliders introduced relative to $\mathbb{M}_i$. **(C)** The chordal property is proved based on the fact that only the first two steps of Alg. 1 possibly introduce new arrowheads, while the third step will only transform the edges as $A \circ\!\!\rightarrow B$ to $A \rightarrow B$, which is proved in Lemma 12 in Appendix B. With this fact, it suffices to prove that the circle component in the graph obtained after the first two steps is chordal. Denote the graph after the first two steps by $\bar{\mathbb{M}}_{i+1}$. We can prove that the circle components in $\bar{\mathbb{M}}_{i+1}[\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])]$ and in $\bar{\mathbb{M}}_{i+1}[-\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])]$ are chordal, respectively. Since there are no circle edges connecting $\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ and $\mathbf{V}\backslash\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ (otherwise it has been oriented in the first step of Alg. 1), we conclude the desired result. **(D)** The balanced property of $\mathbb{M}_{i+1}$ is proved based on three facts that (1) in Alg. 1, if we transform a circle to arrowhead at V, then $V \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$; (2) if there is $A \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ and $A \circ\!\!-\!\!* B$, $B \notin \mathbf{C}$, in $\mathbb{M}_{i+1}$, then $B \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$; (3) $\mathbb{M}_i$ satisfies the balanced property. We can prove that it is impossible that there is a sub-structure $V_i {*\!\!\rightarrow} V_j \circ\!\!-\!\!* V_k$ where V_i is not adjacent to V_k or there is $V_i *\!\!-\!\!\circ V_k$ in $\mathbb{M}_{i+1}$ by discussing whether V_i, V_j, V_k belongs to $\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$. **(E)** The completeness property is proved by showing two results: (1) for edge circle edge $A \circ\!\!-\!\!\circ B$ and $C \circ\!\!\rightarrow D$ in $\mathbb{M}_{i+1}$, $C \circ\!\!\rightarrow D$ can be transformed to $C \rightarrow D$ and the circle edge can be oriented as both $A \rightarrow B$ and $A \leftarrow B$ in the MAGs consistent to $\mathcal{P}$ and local BK regarding $V_1, \cdots, V_{i+1}$; (2) in $\mathbb{M}_{i+1}$, each edge $A \circ\!\!\rightarrow B$ can be oriented as $A \leftrightarrow B$ in an MAG consistent to $\mathcal{P}$ and local BK regarding $V_1, \cdots, V_{i+1}$. In this part, the most difficult part is to prove the first result, with which the second result can be proved directly following the proof process of Thm. 3 of Zhang [35]. In the proof for the first result, we show that any MAG obtained from $\mathbb{M}_{i+1}$ by transforming the edges as $A \circ\!\!\rightarrow B$ to $A \rightarrow B$ and the circle component into a DAG without new unshielded colliders is consistent to $\mathcal{P}$ and local BK regarding $V_1, \ldots, V_{i+1}$. If not, we can always find an MAG obtained from $\mathbb{M}_i$ by transforming the edges as $A \circ\!\!\rightarrow B$ to $A \rightarrow B$ and the circle component into a DAG without new unshielded colliders that is not consistent to $\mathcal{P}$ and local BK regarding $V_1, \ldots, V_i$. By induction, there is an MAG obtained from $\mathcal{P}$ by transforming the edges as $A \circ\!\!\rightarrow B$ to $A \rightarrow B$ and the circle component into a DAG without new unshielded colliders that is not consistent to $\mathcal{P}$, contradiction with Thm. 2 of Zhang [35]. We conclude the first result. □

Corollary 1. The k-step algorithm from $\mathbb{M}_0 (= \mathcal{P})$ to $\mathbb{M}_k$ is sound and complete. That is, the non-circle marks in $\mathbb{M}_k$ are invariant in all the MAGs consistent to $\mathcal{P}$ and BK regarding $V_1, \ldots, V_k$. And for each circle in $\mathbb{M}_k$, there exist both MAGs with an arrowhead and MAGs with a tail here that are consistent to $\mathcal{P}$ and BK regarding $V_1, \ldots, V_k$.

Proof. Previous studies [34, 35] show that the last four properties in Thm. 1 are fulfilled in PAG, the case in $\mathcal{R}_4'$ will never happen in $\mathcal{P}$ because such circles have been oriented by $\mathcal{R}_4$ in the process of learning $\mathcal{P}$, and the case in $\mathcal{R}_{11}$ is never triggered by the rules to learn $\mathcal{P}$. Hence $\mathcal{P}$ satisfies the five properties. With the induction step implied by Thm 1, we directly conclude that $\mathbb{M}_k$ satisfies the five properties, thereby satisfying the invariant and complete property. □

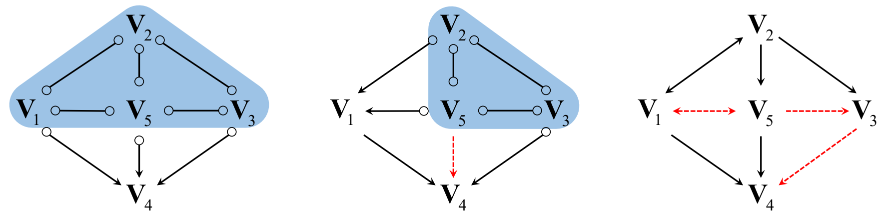
Theorem 2. *The orientation rules are sound and complete to orient a PAG with the local background knowledge regarding $V_1, \ldots, V_k$.*

Proof. The soundness of $\mathcal{R}_4'$ is shown by Prop. 1. The soundness of other rules immediately follows Thm. 4.1 of Ali et al. [34] and Thm. 1 of Zhang [35]. We do not show the details. Roughly speaking, the violation of these rules will lead to that there are new unshielded colliders or directed or almost directed cycles in the oriented graph relative to $\mathcal{P}$. The main part is to prove the completeness.

According to Cor. 1, it suffices to prove that in each step by Alg. 1 to incorporate $BK(X)$ into a PMG $\mathbb{M}_i$, the orientations in Alg. 1 either follow $BK(X)$ directly, or can be achieved by the proposed orientation rules. The orientation in the second step of Alg. 1 can be achieved by $\mathcal{R}_1$, because no matter $\mathcal{F}_{V_l} \backslash \mathcal{F}_{V_j} \neq \emptyset$ or $V_m \rightarrow V_l \circ\!\!-\!\!\circ V_j$, there is $F \in \mathcal{F}_{V_l} \backslash \mathcal{F}_{V_j}$ or $F = V_m$ respectively such that $F {*\!\!\rightarrow} V_l \circ\!\!-\!\!\circ V_j$ where F is not adjacent to V_j. The orientation in the third step naturally follows the orientation rules. For the orientation in the first step, $X \leftarrow\!\!* V$ for $V \in \mathbf{C}$ is dictated by $BK(X)$, and $X \rightarrow V$ for $V \in \{V \in \mathbf{V}(\mathcal{P}) \mid X \circ\!\!-\!\!* V\} \backslash \mathbf{C}$ is obtained from $X -\!\!* V$ dictated by $BK(X)$ and $\mathcal{R}_{11}$. The remaining part is to prove for $K \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}]) \backslash \{X\}$ and $T \in \mathbf{C}$, if there is $K \circ\!\!-\!\!* T$ in $\mathbb{M}_i$, $K \leftarrow\!\!* T$ can be oriented by the proposed orientation rules when we incorporate $BK(X)$.

Due to $K \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}]) \backslash \{X\}$, there is a possible directed path from X to K that does not go through $\mathbf{C}$. According to Lemma 2 in Appendix B, there is a minimal possible directed path $p = \langle X(= F_0), F_1, \ldots, K(= F_t) \rangle, t \geq 1$ where each vertex does not belong to $\mathbf{C}$. Hence $X \rightarrow F_1$ is oriented by $BK(X)$ and $\mathcal{R}_{11}$ unless $X \rightarrow F_1$ has been in $\mathbb{M}_i$. Hence, $X \rightarrow F_1 \rightarrow \cdots \rightarrow F_t$ can be oriented by $\mathcal{R}_1$ after incorporating $BK(X)$ unless they have been in $\mathbb{M}_i$. If $t = 1$, there is $T {*\!\!\rightarrow} X \rightarrow K$, thus $K \leftarrow\!\!* T$ can be oriented by $\mathcal{R}_2$. Next, we consider the case when $t \geq 2$.

We first prove that for any $F_m \in F_1, \ldots, F_t, t \geq 2$, F_m is adjacent to T, and there is not $F_m \rightarrow T$ in $\mathbb{M}_i$. Suppose F_m is not adjacent to T, there must be a sub-structure of $\mathbb{M}_i$ induced by



(a) PAG $\mathcal{P}$(=$\mathbb{M}_0$) (b) $\mathbb{M}_1$ (c) $\mathbb{M}_2$

Figure 2: Fig. 2(a) depicts a PAG $\mathcal{P}$, with the local BK regarding V_1 in the form of $V_1 \leftarrow\!\!\ast V_2, V_1 \leftarrow\!\!\ast V_5, V_1 \multimap\!\!\ast V_4$ and the local BK regarding V_2 in the form of $V_2 \leftarrow\!\!\ast V_1, V_2 -\!\!\ast V_3, V_2 -\!\!\ast V_5$. The connected circle components are denoted by shaded area. The edges oriented by the orientation rules are denoted by red dashed lines.

$F_{m-s}, F_{m-s+1}, \ldots, F_{m+l}, T, 1 \leq s \leq m, 1 \leq l \leq t-m$, such that T is only adjacent to F_{m-s} and F_{m+l} in this sub-structure. There are at least four vertices in this sub-structure. Hence there must be an unshielded collider (denoted by UC for short) in this sub-structure in $\mathcal{P}$, otherwise no matter how we orient the circle there is either a new UC relative to $\mathcal{P}$ or a directed or almost directed cycle there. Since p is possibly directed, the UC is at either F_{m+l} or T (*i.e.*, $\ast\!\!\rightarrow F_{m+l}($ or $T) \leftarrow\!\!\ast$). If there is a UC at F_{m+l}, $T\ast\!\!\rightarrow F_{m+l}$ and $F_{m+l-1}\ast\!\!\rightarrow F_{m+l}$ are identified in $\mathcal{P}$. Thus $F_{m+l} \rightarrow F_{m+l+1} \cdots \rightarrow F_t$ is identified in $\mathcal{P}$. Due to the completeness of FCI algorithm to learn $\mathcal{P}$, there is $K \leftarrow\!\!\ast T$ in $\mathcal{P}$, because there is not an MAG with $K \rightarrow T$ (there has been $T\ast\!\!\rightarrow F_{m+l} \rightarrow \cdots \rightarrow K$ in $\mathcal{P}$). Hence there is $K \leftarrow\!\!\ast T$ in $\mathbb{M}_i$, contradicting with $K \circ\!\!\!\ast\, T$ in $\mathbb{M}_i$. If there is not a UC at F_{m+l}, UC can only be at T. Thus $F_{m-s}\ast\!\!\rightarrow T \leftarrow\!\!\ast F_{m+l}$ is identified in $\mathcal{P}$. Since p is possibly directed, F_{m+l-1} is not adjacent to T, and there is not a UC at F_{m+l} in the sub-structure, there cannot be $F_{m+l} \leftrightarrow T$ in $\mathcal{P}$. Hence the path $\langle F_{m-s}, F_{m-s+1}, \ldots, F_{m+l}, T\rangle$ in $\mathcal{P}$ is an uncovered possible directed path, $F_{m-s} \rightarrow T$ is identified in $\mathcal{P}$ (otherwise $\mathcal{R}_9$ applies). When incorporating $BK(X)$, there is a (almost) directed cycle $T\ast\!\!\rightarrow X \rightarrow \cdots \rightarrow F_{m-s} \rightarrow T$, contradicting with the correctness of BK. Hence, F_m is adjacent to T. Similarly, if $F_m \rightarrow T$ in $\mathbb{M}_i$, there is $T\ast\!\!\rightarrow X \rightarrow \cdots \rightarrow F_m \rightarrow T$, impossibility.

Finally, since F_1 is adjacent to T, and $T\ast\!\!\rightarrow X \rightarrow F_1$ is oriented according to $BK(X)$, there is $T\ast\!\!\rightarrow F_1$ oriented by $\mathcal{R}_2$ unless $T\ast\!\!\rightarrow F_1$ has been in $\mathbb{M}_i$. Hence there is always $T\ast\!\!\rightarrow F_1$ by the orientation rules. Consider $T\ast\!\!\rightarrow F_1 \rightarrow F_2$, there is $T\ast\!\!\rightarrow F_2$ oriented by $\mathcal{R}_2$ unless $T\ast\!\!\rightarrow F_2$ has been in $\mathbb{M}_i$. Repeat the process for $F_3, F_4, \ldots, F_t(= K)$, we can prove that if there is $F_t(= K) \circ\!\!\!\ast\, T$ in $\mathbb{M}_i$, there is $T\ast\!\!\rightarrow F_t(= K)$ oriented by $\mathcal{R}_2$. The rules thus orient the same marks as Alg. 1. $\square$

Example 2. *We give an example in Fig. 2. Suppose we obtain a PAG as Fig. 2(a) with observational data and have the local BK regarding V_1, V_2. We divide the whole process of obtaining a PMG from $\mathcal{P}$ with the local BK into obtaining $\mathbb{M}_1$ from $\mathcal{P}$ with $BK(V_1)$ by Alg. 1 and then obtaining $\mathbb{M}_2$ from $\mathbb{M}_1$ with $BK(V_2)$ by Alg. 1. $\mathbb{M}_1$ and $\mathbb{M}_2$ are shown in Fig. 2(b) and 2(c), respectively. It is not hard to verify that all of $\mathcal{P}$, $\mathbb{M}_1$, $\mathbb{M}_2$ satisfy the closed, chordal, and balanced properties defined in Thm 1. Note if we do not consider $\mathcal{R}'_4$, the edge colored red in Fig. 2(b) cannot be oriented. Fig. 2(a) also shows a case where $BK(V_1)$ is not tiered [37]. The reason is that the vertices V_1, V_4, V_5 cannot partitioned into disjoint subsets with explicit causal order because V_1 and V_4 belong to different subsets according to $BK(V_1)$ but V_5 has ancestor relation with neither V_1 nor V_4.*

4 Active Causal Discovery Framework

The establishment of the orientation rules for causal identification with local BK makes causal discovery by interventions possible in the presence of latent variables. Hence, on the basis of the theoretical results, we propose an active learning framework for causal discovery in the presence of latent variables, with the target of learning the MAG with as fewer interventions as possible. The framework is comprised of three stages. In Stage 1, we learn a PAG with observational data. In Stage 2, we select a singleton variable $X \in V_1, \ldots, V_d$ to intervene and collect the interventional data. In Stage 3, we learn causal relations with the data. For each edge $X \circ\!\!\!\ast\, V_i$, the circle at X can be learned by a two-sample test on whether the interventional distribution of V_i equals to the observational one. There is $X \leftarrow\!\!\ast V_i$ learned if they are equal, and $X -\!\!\ast V_i$ otherwise. Hence, the knowledge taken by the

Algorithm 2: Intervention variable selection based on maximum entropy criterion with MH alg.

Input: A PMG $\mathbb{M}_i$ oriented based on $\mathcal{P}$ and BK regarding $V_1, \ldots, V_i$, number of MAGs L
Output: The selected intervention variable X

Obtain an MAG $\mathcal{M}_0$ based on $\mathbb{M}_i$ by transforming $\circ\!\!\rightarrow$ to $\rightarrow$ and the circle component into a DAG without new unshielded colliders;
for $t = 1, 2, \ldots, L'$ **do**
  Sample an MAG $\mathcal{M}'$ from $S(\mathcal{M}_{t-1})$;
  $\rho = \min(1, \frac{|S(\mathcal{M}_{t-1})|}{|S(\mathcal{M}')|})$;
  Sample u from uniform distribution $U[0, 1]$;
  if $u \leq \rho$ **then** $\mathcal{M}_t = \mathcal{M}'$ **else** $\mathcal{M}_t = \mathcal{M}_{t-1}$;
$\mathcal{S} = \{\mathcal{M}_{t,1 \leq t \leq L'} \mid \mathcal{M}_t$ has the non-circle marks in $\mathbb{M}_i\}$ ▷ The set of MAGs consistent to $\mathbb{M}_i$;
$s \leftarrow 0, X \leftarrow \emptyset$;
for $V_j = V_{i+1}, \ldots, V_d$ **do**
  Denote $\mathbf{V}(V_j) = \{V \in \mathbf{V}(\mathbb{M}_i) \mid V_j \circ\!\!-\!\!* V$ in $\mathbb{M}_i\}$, $L = |\mathcal{S}|$;
  For each possible local structure $\mathcal{L}_k$ of V_j, $1 \leq k \leq 2^{|\mathbf{V}(V_j)|}$, we count the number $\mathcal{N}_k$ of the appearance of $\mathcal{L}_k$ in the L MAGs from $\mathcal{S}$;
  $s' = -\sum_{k=1}^{2^{|\mathbf{V}(V_j)|}} \frac{\mathcal{N}_k}{L} \log \frac{\mathcal{N}_k}{L}$;
  if $s \leq s'$ **then** $X \leftarrow V_j$, $s \leftarrow s'$;
return X.

interventional data is local. We repeat the second and third stages until we identify the MAG. Since the orientation rules are complete, the graph can be updated completely by each intervention. The only remaining problem is how to select the intervention variable in Stage 2.

Considering that the whole process is sequential, we only focus on the intervention variable selection in one round. Without loss of generality, suppose we have obtained a PMG $\mathbb{M}_i$ by i interventions on $V_1, V_2, \ldots, V_i$, and will select a variable from $\{V_{i+1}, \ldots, V_d\}$ to intervene. We adopt the maximum entropy criterion [22]. For $\mathbb{M}_i$, we select the variable X that maximizes

$$H_X = -\sum_{j=1}^{M} \frac{l_j}{L} \log \frac{l_j}{L}, \tag{1}$$

where j is an index for a local structure of X (a local structure of X denotes a definite orientation of the marks at X), M denotes the number of different local structures, l_j denotes the number of MAGs consistent to $\mathbb{M}_i$ which has the j-th local structure of X, and L denotes the total number of MAGs consistent to $\mathbb{M}_i$. Intuitively, the maximum entropy criterion is devoted to selecting the intervention variable X such that there is a similar number of MAGs with each local structure of X and as more as possible local structures of X. A justification for intervening on such a variable is that we hope to have a small space of MAGs after the intervention no matter what the true local structure of X is.

However, it is hard to count the number of MAGs consistent to $\mathbb{M}_i$ with each definite local structure. Even in causal sufficiency setting, implementing such operation (generally called *counting maximally oriented partial DAGs*) is #P-complete [39]. Considering DAG is a special case for MAG, the counting of MAGs is harder. Hence, we adopt a sampling method based on Metropolis-Hastings (MH) algorithm [40], to uniformly sample from the space of MAGs. The algorithm begins from an MAG consistent to $\mathbb{M}_i$, and in each round we transform the MAG to a candidate MAG and decide to accept or reject it with some probability. Here, we introduce an important result of Zhang and Spirtes [41] for MAGs transformation in Prop. 2.

Proposition 2 (Zhang and Spirtes [41], Tian [42])**.** *Let $\mathcal{M}$ be an arbitrary MAG, and $A \rightarrow B$ an arbitrary directed edge in $\mathcal{M}$. Let $\mathcal{M}'$ be the graph identical to $\mathcal{M}$ except that the edge between A and B is $A \leftrightarrow B$. $\mathcal{M}'$ is an MAG Markov equivalent to $\mathcal{M}$ if and only if*

(1) there is no directed path from A to B other than $A \rightarrow B$ in $\mathcal{M}$;

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

(3) there is no discriminating path for A on which B is the endpoint adjacent to A in $\mathcal{M}$.

In the MAG sampling algorithm, in each step we transform the current MAG to a new MAG by *converting a directed edge to bi-directed edge or a bi-directed one to directed one*, where we use Prop. 2 to determine whether an MAG Markov equivalent to the current MAG can be obtained by the conversion. For MH algorithm, a stationary distribution equal to the desired distribution can be obtained if any two states can be transformed to each other in limited steps [43]. As implied by Theorem 3 of Zhang and Spirtes [41], any MAG can be transformed to another Markov equivalent MAG in a limited number of transformations above. Hence, MH algorithm is valid to sample MAGs uniformly from the space of MAGs consistent to $\mathcal{P}$. Then, we only remain the MAGs that have the same non-circle marks as $\mathbb{M}_i$. In this way, we obtain a set of MAGs which are uniformly sampled from the space of MAGs consistent to $\mathbb{M}_i$.

Given an MAG $\mathcal{M}$, let $S(\mathcal{M})$ denote the set of MAGs that can be obtained from $\mathcal{M}$ by transforming one bi-directed edge to directed edge or one directed edge to bi-directed edge according to Prop. 2. Denote the cardinality of $S(\mathcal{M})$ by $|S(\mathcal{M})|$. We set the probability $Q(\mathcal{M}' \mid \mathcal{M})$ of an MAG $\mathcal{M}$ transformed to another MAG $\mathcal{M}' \in S(\mathcal{M})$ as $1/|S(\mathcal{M})|$. Hence, the acceptance ratio ρ that is used to decide whether to accept or reject the candidate is

$$\rho = \min\left(1, \frac{p(\mathcal{M}')Q(\mathcal{M} \mid \mathcal{M}')}{p(\mathcal{M})Q(\mathcal{M}' \mid \mathcal{M})}\right) = \min\left(1, \frac{|S(\mathcal{M})|}{|S(\mathcal{M}')|}\right).$$

We propose Alg. 2 to select the intervention variable X. As shown by Lemma 15.1 in Appendix B, the graph $\mathcal{M}_0$ is an MAG consistent to $\mathbb{M}_i$. From Line 2-Line 6, we execute MH algorithm to sample L' MAGs. Then, we select the MAGs among them which are consistent to $\mathbb{M}_i$ on Line 7. Finally, we estimate the entropy by (1) and select X from Line 9-Line 14.

5 Experiments

In this section, we conduct a simple simulation of the three-stage active learning framework. We generate 100 Erdös-Rényi random DAGs for each setting, where the number of variables $d = 10$ and the probability of including each edge $p \in \{0.1, 0.15, 0.2, 0.25, 0.3\}$. The weight of each edge is drawn from $\mathcal{U}[1, 2]$. We generate 10000 samples from the linear structural equations, and take three variables as latent variables and the others as observed ones. In the implementation of the MH algorithm in Alg. 2, we discard the first 500 sampled MAGs and collect the following 1000 MAGs. For each intervention variable X, we collect 10000 samples under $do(X = 2)$, and learn the circles at X by two-sample test with a significance level of 0.05.

We compare the maximum entropy criterion with a baseline random criterion where we randomly select one variable with circles to intervene in each round. We show the results in Tab. 1. # int. denotes the number of interventions to achieve MAG identification. The effectiveness of the maximum entropy criterion is verified by noting that the number of interventions with maximum entropy criterion is fewer than that with random criterion. Further, we evaluate the three stages respectively. In Stage 1, we obtain a PAG by running FCI algorithm with a significance level of 0.05. In Stage 2, we adopt the two criteria to select intervention variables. In Stage 3, we learn the marks with corresponding interventional data and orientation rules. We evaluate the performance of Stage 1 by # correct PAG/# wrong PAG. # correct PAG/# wrong PAG denotes the number of edges that are correctly/wrongly identified by FCI. An edge is correctly/wrongly identified by FCI if the edge learned by FCI is identical/not identical to the true PAG. The performance of Stage 2 is evaluated by # int.. And we evaluate the performance of Stage 3 by # correct int./# wrong int., where # correct int./# wrong int. denotes the number of edges whose direction are correctly/wrongly identified by interventions. An edge is correctly/wrongly identified by interventions if its existence is correctly identified in $\mathcal{P}$ but the direction is uncertain, and after interventions we learn its direction correctly/wrongly. We evaluate the performance of the whole process by Norm. SHD and F1. Norm. SHD denotes the normalized structural hamming distance (SHD), which is calculated by dividing SHD by $d(d-1)/2$. F1 score is calculated by the confusion matrix to indicate whether the edge between any two vertices is correctly learned. According to the SHD and F1 score, the active framework can learn the MAG accurately when p is not large. And as shown by the evaluations of Stage 1 and Stage 3, the marks are learned accurately in Stage 3, and most of the mistakes are generated in Stage 1. Hence, in the active learning framework, the PAG estimation in the first stage is the bottleneck of having a good performance.

Table 1: Number of interventions, normalized SHD, F1 score, number of correctly/ wrongly learned marks by interventions, and number of correctly/wrongly learned marks in PAG over 100 simulations with $d = 10$ and varying p in the format of mean $\pm$ std.

Strategy-p	# int.	Norm. SHD	F1	# correct int.	# wrong int.	# correct PAG	# wrong PAG
Random-0.10	2.88 ± 1.28	0.02 ± 0.04	0.85 ± 0.29	3.92 ± 2.40	0.11 ± 0.53	4.78 ± 3.11	0.39 ± 0.82
MCMC-0.10	2.77 ± 1.19	0.02 ± 0.04	0.85 ± 0.29	4.00 ± 2.40	0.03 ± 0.22		
Random-0.15	3.30 ± 1.15	0.02 ± 0.05	0.91 ± 0.17	5.17 ± 2.62	0.10 ± 0.41	7.21 ± 3.85	0.40 ± 0.92
MCMC-0.15	3.20 ± 1.03	0.02 ± 0.04	0.92 ± 0.16	5.25 ± 2.66	0.02 ± 0.14		
Random-0.20	3.59 ± 1.22	0.04 ± 0.06	0.91 ± 0.15	6.26 ± 2.75	0.19 ± 0.61	9.26 ± 3.94	0.59 ± 1.30
MCMC-0.20	3.42 ± 1.16	0.03 ± 0.06	0.92 ± 0.15	6.38 ± 2.70	0.07 ± 0.33		
Random-0.25	3.47 ± 1.34	0.08 ± 0.14	0.89 ± 0.18	7.08 ± 3.37	0.06 ± 0.34	11.92 ± 4.01	1.59 ± 2.85
MCMC-0.25	3.22 ± 1.19	0.08 ± 0.14	0.89 ± 0.18	7.05 ± 3.39	0.09 ± 0.35		
Random-0.30	3.64 ± 1.32	0.14 ± 0.15	0.83 ± 0.18	7.03 ± 3.33	0.36 ± 1.01	12.59 ± 4.08	2.63 ± 3.19
MCMC-0.30	3.55 ± 1.37	0.14 ± 0.15	0.83 ± 0.18	7.25 ± 3.50	0.14 ± 0.43		

6 Conclusion

In this paper, we show what causal relations are identifiable in the presence of latent variables given local background knowledge with sound and complete orientation rules. Based on the theoretical results, we give the first active learning framework for causal discovery in the presence of latent variables. In the future, we will investigate the causal relations identifiability with general background knowledge. It is also worthy to study how our research may help some recent novel decision-making methodology [44].

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Checklist

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes]
   (b) Did you describe the limitations of your work? [Yes]
   (c) Did you discuss any potential negative societal impacts of your work? [No] It is mainly a theoretical paper.
   (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]
2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [Yes]
   (b) Did you include complete proofs of all theoretical results? [Yes]
3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [No] It will be publicly available later.
   (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [Yes]
   (c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [Yes]
   (d) Did you include the total amount of compute and the type of resources used (e.g., type of GPUs, internal cluster, or cloud provider)? [No]
4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...
   (a) If your work uses existing assets, did you cite the creators? [N/A]
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   (d) Did you discuss whether and how consent was obtained from people whose data you're using/curating? [N/A]

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5. If you used crowdsourcing or conducted research with human subjects...

    (a) Did you include the full text of instructions given to participants and screenshots, if applicable? [N/A]

    (b) Did you describe any potential participant risks, with links to Institutional Review Board (IRB) approvals, if applicable? [N/A]

    (c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [N/A]

A Orientation Rules for Causal Discovery with Observational Data

In this section, we show the complete orientation rules proposed by Zhang [35] for causal discovery with observational data in the presence of latent variables and selection bias. There are eleven rules ($\mathcal{R}_0 - \mathcal{R}_{11}$). Since selection bias is not considered in this paper, we do not show the cases ($\mathcal{R}_5 - \mathcal{R}_7$) that happen only when there is selection bias. $\mathcal{R}_0$ is triggered according to the conditional independence relationship at the beginning of learning a PAG. It is evidently not triggered after, hence we do not show it as well.

$\mathcal{R}_1$: If $A{*\!\!\rightarrow} B \circ\!\!-\!\!* R$, and A and R are not adjacent, then orient the triple as $A{*\!\!\rightarrow} B \rightarrow R$.

$\mathcal{R}_2$: If $A \rightarrow B{*\!\!\rightarrow} R$ or $A{*\!\!\rightarrow} B \rightarrow R$, and $A *\!\!-\!\!\circ R$, then orient $A *\!\!-\!\!\circ R$ as $A{*\!\!\rightarrow} R$.

$\mathcal{R}_3$: If $A{*\!\!\rightarrow} B \leftarrow\!\!* R$, $A *\!\!-\!\!\circ D \circ\!\!-\!\!* R$, A and R are not adjacent, and $D *\!\!-\!\!\circ B$, then orient $D *\!\!-\!\!\circ B$ as $D{*\!\!\rightarrow} B$.

$\mathcal{R}_4$: If $\langle K, \dots, A, B, R\rangle$ is a discriminating path between K and R for B, and $B \circ\!\!-\!\!* R$; then if $B \in \text{Sepset}(K, R)$, orient $B \circ\!\!-\!\!* R$ as $B \rightarrow R$; otherwise orient the triple $\langle A, B, R\rangle$ as $A \leftrightarrow B \leftrightarrow R$.

$\mathcal{R}_8$: If $A \rightarrow B \rightarrow R$, and $A {\circ\!\!\rightarrow} R$, orient $A {\circ\!\!\rightarrow} R$ as $A \rightarrow R$.

$\mathcal{R}_9$: If $A {\circ\!\!\rightarrow} R$, and $p = \langle A, B, D, \dots, R\rangle$ is an uncovered possible directed path from A to R such that R and B are not adjacent, then orient $A {\circ\!\!\rightarrow} R$ as $A \rightarrow R$.

$\mathcal{R}_{10}$: Suppose $A {\circ\!\!\rightarrow} R$, $B \rightarrow R \leftarrow D$, p_1 is an uncovered possible directed path from A to B, and p_2 is an uncovered possible directed path from A to D. Let U be the vertex adjacent to A on p_1 (U could be B), and W be the vertex adjacent to A on p_2 (W could be D). If U and W are distinct, and are not adjacent, then orient $A {\circ\!\!\rightarrow} R$ as $A \rightarrow R$.

In this paper, when we orient the PAG $\mathcal{P}$ with local BK, we replace $\mathcal{R}_4$ by $\mathcal{R}_4'$. We will show the soundness of $\mathcal{R}_4'$ in Prop. 1. Before that, we present a fact in Lemma 1.

Lemma 1. *If there exists a minimal collider path in an MAG $\mathcal{M}$ consistent to a PAG $\mathcal{P}$, then it is also a collider path in $\mathcal{P}$.*

Proof. Suppose a minimal collider path p in $\mathcal{M}$, we consider its corresponding path in $\mathcal{P}$. If there exists a circle or tail at the non-endpoint vertex on this path, according to the completeness of FCI [35], there exists an MAG Markov equivalent to $\mathcal{M}$ that has a tail there, which contradicts Theorem 2.1 of Zhao et al. [38] that Markov equivalent MAGs have the same minimal collider paths. Hence the corresponding path of p in $\mathcal{P}$ is also a collider path. □

Proposition 1. *Given a PAG $\mathcal{P}$, for any PMG $\mathbb{M}$ that is obtained from $\mathcal{P}$ by orienting some circles in $\mathcal{P}$ (or $\mathbb{M} = \mathcal{P}$), $\mathcal{R}_4'$ is sound to orient $\mathbb{M}$ with local background knowledge.*

Proof. Suppose there is a discriminating path $\langle K, \dots, A, B, R\rangle$ between K and R for B, and $B \circ\!\!-\!\!* R$ in a PMG $\mathbb{M}$ such that there exists an MAG $\mathcal{M}$ consistent to $\mathbb{M}$. According to the definition of discriminating path and the soundness of $\mathcal{R}_2$, there is $B {\circ\!\!\rightarrow} R$. Suppose the violation of $\mathcal{R}_4'$, that is, in $\mathcal{M}$ there is $B \leftrightarrow R$. Since there is $A \rightarrow R$, the edge between A and B can only be $A \leftrightarrow B$ due to the ancestral property. Hence, there is a collider path between K and R as $K{*\!\!\rightarrow} \cdots \leftrightarrow A \leftrightarrow B \leftrightarrow R$. If this collider path is a minimal one, then according to Lemma 1 the collider path is identifiable in $\mathcal{P}$, thus there is $A \leftrightarrow B \leftarrow\!\!* R$ in $\mathbb{M}$, contradiction. Hence the collider path is not a minimal collider path from K to R, there is a path p_1 comprised of a subset of these vertices that is a minimal collider path from K to R. Note **(1)** for any vertex V in the non-endpoint from K to B, there is $V \rightarrow R$. And **(2)** K is not adjacent to R. Hence the only vertex that can be adjacent to R in p_1 is B. Hence the minimal path is as $\langle K, \dots, B, R\rangle$. According to Lemma 1 again, $B \leftarrow\!\!* R$ is identifiable in $\mathcal{P}$, thus there is $B \leftarrow\!\!* R$ in $\mathbb{M}$, contradiction. We conclude the impossibility of the violation of $\mathcal{R}_4'$. □

B Proof of Theorem 1

For brevity, when we introduce a set of vertices $\mathbf{C}$ defined as $\mathbf{C} = \{V \in \mathbf{V}(\mathcal{P}) \mid V{*\!\!\rightarrow} X \in BK(X)\}$ to denote the vertices whose edges with X will be oriented to ones with arrowheads at X according to $BK(X)$, we call the BK (of X) is *dictated by* $\mathbf{C}$.

We first show two definitions. A vertex A of G is called *simplicial* if its adjacency set $\text{Adj}(A, G)$ induces a complete subgraph of G. A *perfect elimination order* of a graph G is an ordering $\sigma = (V_1, \ldots, V_n)$ of its vertices, so that each vertex V_i is a simplicial vertex in the induced subgraph $G_{V_i,\ldots,V_n}$.

Proposition 3 (Ali et al. [45], Zhang [35])**.** *In a PAG $\mathcal{P}$, 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 $A \leftrightarrow C$).*

Proposition 4 (Spirtes and Richardson [46])**.** *Two MAGs over the same set of vertices are Markov equivalent if and only if*

(1) They have the same adjacencies;

(2) They have the same unshielded colliders;

(3) If a path is a discriminating path for a vertex V in both graphs, then V is a collider on the path in one graph if and only if it is a collider on the path in the other.

Lemma 2. *Consider $\mathbb{M}_i$ in Thm. 1 that satisfies the five properties. If there is a possible directed path from A to B in $\mathbb{M}_i$, then there is a minimal possible directed path from A to B in $\mathbb{M}_i$.*

Proof. If the path is minimal, then it trivially holds. If not, suppose the path comprised of $V_0(= A), V_1, \ldots, V_m(= B)$. As long as the path is not minimal, we can always find a sub-path comprised of $V_i, V_{i+1}, \ldots, V_j, j - i \geq 2$ such that any non-consecutive vertices in $V_i, \cdots, V_j$ are not adjacent except for an edge between V_i and V_j. We will show that it is impossible that there is $V_i \leftarrow\!\!* V_j$ in $\mathbb{M}_i$. If $j - i = 2$, when there is an edge $V_i \leftarrow\!\!* V_j$ and an edge between V_i and V_{i+1} with a circle or tail at V_i, according to the balanced property and closed property of $\mathbb{M}_i$ under the orientation rules ($\mathcal{R}_2$ is triggered here) respectively, there is always an edge $V_{i+1} \leftarrow\!\!* V_j$, contradicting the possible directed path comprised of an edge from V_{i+1} to V_j. If $j - i > 2$ and $V_i \leftarrow\!\!* V_j$, due to the non-adjacency of the vertices, there is either $V_i \rightarrow V_{i+1} \rightarrow \ldots V_j$ or $V_i \leftarrow\!\!* V_{i+1}$ identified in $\mathcal{P}$. The latter case is impossible due to the possible directed path. For the former case, there is an almost directed or directed cycles, contradiction. Hence, we can find a shorter possible directed path comprised of $V_0, V_1, \ldots, V_i, V_j, V_{j+1}, \ldots, V_m$ in $\mathbb{M}_i$. Repeat this process until we obtain a possible directed path that there is not a proper sub-structure where any non-consecutive vertices are not adjacent except for an edge between endpoints. This path is a minimal possible directed path. □

Lemma 3. *Consider $\mathbb{M}_i$ in Thm. 1 that satisfies the five properties. If there is $A{*\!\!\rightarrow} B$ in $\mathbb{M}_i$, then there is an edge as $A{*\!\!\rightarrow} V$ for any V in a connected circle component with B in $\mathbb{M}_i$, and A and B are not in a connected circle component.*

Proof. It is a direct conclusion according to the balanced property of $\mathbb{M}_i$. We first consider any one vertex V_1 that is with a circle edge with B. That is, there is $A{*\!\!\rightarrow} B \circ\!\!-\!\!\circ V_1$ in $\mathbb{M}_i$. According to the balanced property of $\mathbb{M}_i$, there is an edge $A{*\!\!\rightarrow} V_1$. Similarly, we can conclude that the result holds for all the vertices in a connected circle component with B. Hence there cannot be a circle edge linking A and any one vertex in a connected circle component with B. Thus A and B are not in a connected circle component. □

Lemma 4. *Consider $\mathbb{M}_i$ in Thm. 1 that satisfies the five properties. Suppose an MAG $\mathcal{M}$ consistent to $\mathbb{M}_i$ and the local BK of X dictated by $\mathbf{C}$. Then $V \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ if and only if $V \in \text{De}(X, \mathcal{M})$.*

Proof. Suppose $\mathcal{M}$ an MAG consistent to $\mathbb{M}_i$ with the local BK of X dictated by $\mathbf{C}$.

We prove the "only if" statement. If $V \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$, by Lemma 2, there is a minimal possible directed path p from X to V comprised of $X, F_1, \ldots, F_m(= V)$. Due to $F_1 \notin \mathbf{C}$ and local BK, the edge between X and V_1 can only be $X \rightarrow V_1$ in $\mathcal{M}$. Hence the path can only be directed in $\mathcal{M}$, otherwise there is at least one unshielded collider $F_{i-1}{*\!\!\rightarrow} F_i \leftarrow\!\!* F_{i+1}$ in $\mathcal{M}$, thus unshielded collider are identified in $\mathcal{P}$ and $\mathbb{M}_i$, contradicting with that p is a minimal possible directed path from X to F_m in $\mathbb{M}_i$.

We then prove the "if" statement. There must be a minimal directed path $X \rightarrow F_1 \cdots \rightarrow F_{m-1}, F_m(= V)$ from X to V in $\mathcal{M}$. It is evident that X cannot be adjacent to $F_2, \ldots, F_m$.

The corresponding path in $\mathbb{M}_i$ of this path is a minimal possible directed path from X to V. If $V \notin \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$, there can only be $F_1 \in \mathbf{C}$ (since the vertices $F_2, F_3, \dots, F_m$ are not adjacent to X). In this case $X \leftarrow\!\!* F_1$ should be dictated by $\mathbf{C}$ in $\mathcal{M}$, which contradicts the edge $X \to F_1$ in $\mathcal{M}$. The proof completes. □

Lemma 5. *The PMG $\mathbb{M}_{i+1}$ in Thm. 1 satisfies the closed property.*

Proof. It is due to the third step of Alg. 1. □

Lemma 6. *The PMG $\mathbb{M}_{i+1}$ in Thm. 1 satisfies the invariant property.*

Proof. We denote the oriented graph based on $\mathbb{M}_i$ and the local BK of X dictated by $\mathbf{C}$ after the first two steps of Alg. 1 by $\bar{\mathbb{M}}_{i+1}$. Note in the third step of Algorithm 1 we just update the $\bar{\mathbb{M}}_{i+1}$ with the orientation rules. It is easy to prove the orientation rules are sound to orient $\bar{\mathbb{M}}_{i+1}$ referring to the results of Ali et al. [45], Zhang [35] because new unshielded colliders, or directed or almost directed cycles will be introduced otherwise, we thus do not present the details here. It suffices to show that the non-circle marks in $\bar{\mathbb{M}}_{i+1}$ are invariant in all MAGs consistent to $\mathbb{M}_i$ with the local BK of X dictated by $\mathbf{C}$.

Consider $\forall K \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ and $\forall T \in \mathbf{C}$. As shown by Lemma 4, for any MAG $\mathcal{M}$ consistent to $\mathbb{M}_i$ and the local BK dictated by $\mathbf{C}$, there is $K \in \text{De}(X, \mathcal{M})$. For brevity, in the following we call such MAG by *the MAG consistent to* $\mathbb{M}_i$ *and* $\mathbf{C}$. Considering $T *\!\!\rightarrow X \to \cdots \to K$, the edge between K and T can only be as $K \leftarrow\!\!* T$ in any MAG $\mathcal{M}$ if $K \neq X$, otherwise there is a directed or almost directed cycle in $\mathcal{M}$, contradiction. If $K = X$, the orientation $X \leftarrow\!\!* T$ in $\mathcal{M}$ just follows the local BK of X dictated by $\mathbf{C}$.

Next we prove that the oriented edges in the second step are consistent to any MAG $\mathcal{M}$ consistent to $\mathbb{M}_i$ and $\mathbf{C}$. Suppose the edge between two vertices V_j and V_l oriented by the second step of Alg. 1 in $\mathbb{M}_i$ is not invariant in MAGs consistent to $\mathbb{M}_i$ and $\mathbf{C}$. That is, there is $V_l \leftarrow\!\!* V_j$ in an MAG $\mathcal{M}$ consistent to $\mathbb{M}_i$ and $\mathbf{C}$. The circle edges are oriented in two cases in the second step. We consider them one by one. **(A)** If $\mathcal{F}_{V_l} \backslash \mathcal{F}_{V_j} \neq \emptyset$ in $\mathbb{M}_i$, there exists some vertex $T \in \mathcal{F}_{V_l} \backslash \mathcal{F}_{V_j}$ forming a collider $V_j *\!\!\rightarrow V_l \leftarrow\!\!* T$ in $\mathcal{M}$. Then we prove the collider is unshielded. If V_j is adjacent to T, we consider the edge in $\mathbb{M}_i$. **(a)** The edge is not $V_j \to T$, otherwise there must be a directed or almost directed cycles $X \to \cdots \to V_j \to T *\!\!\rightarrow X$ in $\mathcal{M}$; **(b)** the edge is not $V_j \circ\!\!-\!* T$, otherwise $T \in \mathcal{F}_{V_j}$; **(c)** the edge is not $V_j \leftarrow\!\!* T$, otherwise in $\mathbb{M}_i$ there is a sub-structure $T *\!\!\rightarrow V_j \circ\!\!-\!\!\circ V_l \circ\!\!-\!* T$, contradicting with the balanced property of $\mathbb{M}_i$. Hence, T cannot be adjacent to V_j. Thus $V_j *\!\!\rightarrow V_l \leftarrow\!\!* T$ is an unshielded collider. Thus $V_j *\!\!\rightarrow V_l$ is identifiable in $\mathcal{P}$. Since $\mathbb{M}_i$ is oriented based on $\mathcal{P}$, there is $V_j *\!\!\rightarrow V_l$ in $\mathbb{M}_i$, contradicting with $V_j \circ\!\!-\!\!\circ V_l$ in $\mathbb{M}_i$. **(B)** If there is $V_m \to V_j \circ\!\!-\!\!\circ V_l$ where $V_m \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}]) \backslash \{X\}$ is not adjacent to V_l, there is an unshielded collider in $\mathcal{M}$ thus $V_l *\!\!\rightarrow V_i$ is identifiable in $\mathcal{P}$ and $\mathbb{M}_i$, contradiction. The proof completes. □

Lemma 7. *Consider $\mathbb{M}_i$ in Thm. 1 that satisfies the five properties. For an edge $J \circ\!\!-\!\!\circ K$ satisfying $\mathcal{F}_J = \mathcal{F}_K$ in $\mathbb{M}_i[\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}]) \backslash \{X\}]$, if it is oriented as $J \to K$ in the second step of Alg. 1 to obtain $\mathbb{M}_{i+1}$ based on $\mathbb{M}_i$ and $\mathbf{C}$, then there is a vertex $V_m \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}]) \backslash \{X\}$ such that there is a minimal path $V_m \circ\!\!-\!\!\circ \dots \circ\!\!-\!\!\circ V_1 (= J) \circ\!\!-\!\!\circ V_0 (= K), m \geq 1$ in $\mathbb{M}_i[\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}]) \backslash \{X\}]$ where $\mathcal{F}_{V_m} \supset \mathcal{F}_{V_{m-1}} = \cdots = \mathcal{F}_{V_0}$.*

Proof. A directed edge $J \to K$ is oriented in the second step only if in two situations: (1) $\mathcal{F}_K \subset \mathcal{F}_J$; (2) $\mathcal{F}_K = \mathcal{F}_J$ and there is another vertex $L \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}]) \backslash \{X\}$ that is not adjacent to K and there is an edge $L \to J$ oriented in the second step (if $L \to J$ is not oriented in the second step, it can only be in $\mathbb{M}_i$. However, the $L \to J \circ\!\!-\!\!\circ K$ in $\mathbb{M}_i$ contradicts with the complete property of $\mathbb{M}_i$ because in this case there is $J \to K$ in any MAG consistent to $\mathbb{M}_i$). If $\mathcal{F}_{V_0} \subset \mathcal{F}_{V_1}$, in this case there is such a path for $m = 1$. If $\mathcal{F}_{V_0} = \mathcal{F}_{V_1}$, Then we could find some vertex $V_2 \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}]) \backslash \{X\}$ that is not adjacent to V_0 and there is an edge $V_2 \to V_1$ oriented in the second step. And similar to the analysis for V_1, we conclude either $\mathcal{F}_{V_1} \subset \mathcal{F}_{V_2}$, in this case there is a path satisfying the result for $m = 2$; or $\mathcal{F}_{V_1} = \mathcal{F}_{V_2}$, in this case there is another vertex $V_3 \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}]) \backslash \{X\}$ that is not adjacent to V_1 and there is an edge $V_3 \to V_2$ oriented. Repeat the process and we can always find an uncovered path $V_m \circ\!\!-\!\!\circ \dots \circ\!\!-\!\!\circ V_1 (= J) \circ\!\!-\!\!\circ V_0 (= K), m \geq 1$ in $\mathbb{M}_i[\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}]) \backslash \{X\}]$ where $\mathcal{F}_{V_0} = \cdots = \mathcal{F}_{V_{m-1}} \subset \mathcal{F}_{V_m}$. If the path is not minimal, then there exists a sub-structure $V_i \circ\!\!-\!\!\circ V_{i+1} \circ\!\!-\!\!\circ \cdots \circ\!\!-\!\!\circ V_j, j > i + 2$ where any two non-consecutive vertices are not adjacent except for an circle edge $V_i \circ\!\!-\!\!\circ V_j$ (the edge between V_i and V_j can only be a circle edge, if it is $V_i{*\!\!\rightarrow} V_j$ or $V_i \leftrightarrow\!\!* V_j$, V_i and V_j cannot be in a connected circle component according to Lemma 3, but there is a circle path comprised of $V_i, V_{i+1}, \dots, V_j$, contradiction). It contradicts with the fact that the circle component in $\mathbb{M}_i$ is chordal. Hence the path is minimal. $\square$

Lemma 8. *Suppose $\mathbb{M}_s, 0 \leq s \leq i$ in Thm. 1 satisfy the five properties, there must exist an MAG consistent to $\mathbb{M}_i$.*

Proof. Suppose there does not exist an MAG consistent to $\mathbb{M}_i$. According to the invariant property of $\mathbb{M}_i$ and the basic assumption that the background knowledge is correct, there is not an MAG consistent to $\mathbb{M}_{i-1}$. Since $\mathbb{M}_s, 0 \leq s \leq i$ satisfies the invariant property, repeat the process above and we can conclude that there is not an MAG consistent to $\mathcal{P}$, contradiction. $\square$

Lemma 9. *Consider $\mathbb{M}_{i+1}$ in Thm. 1. The subgraph of $\mathbb{M}_{i+1}$ induced by $\mathbf{C}$ is a complete graph.*

Proof. If it is not a complete graph, new unshielded colliders are introduced by the local background knowledge of X dictated by $\mathbf{C}$ when obtaining $\mathbb{M}_{i+1}$ by Alg. 1. Hence there does not exist an MAG consistent to $\mathbb{M}_{i+1}$. According to the invariant property of $\mathbb{M}_{i+1}$ implied by Lemma 6 and the basic assumption that the background knowledge is correct, there is not an MAG consistent to $\mathbb{M}_i$, contradicting with Lemma 8. $\square$

Lemma 10. *Suppose $\mathbb{M}_s, 0 \leq s \leq i$ in Thm. 1 satisfy the five properties. Then there is* $\mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}]) \cap \mathrm{Pa}(\mathbf{C}, \mathbb{M}_i) = \emptyset$.

Proof. Suppose there is an edge $V \rightarrow T$ where $V \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ and $T \in \mathbf{C}$ in $\mathbb{M}_i$. According to Lemma 4 and the definition of $\mathbf{C}$, for any graph oriented from $\mathbb{M}_i$ with the local background knowledge of X dictated by $\mathbf{C}$, there will be a directed or almost directed cycle $X \rightarrow \cdots V \rightarrow T{*\!\!\rightarrow} X$. Hence there is not an MAG consistent to $\mathbb{M}_i$, contradicting with Lemma 8. $\square$

Lemma 11. *Suppose $\mathbb{M}_s, 0 \leq s \leq i$ in Thm. 1 satisfy the five properties. In the second step of Alg. 1 to obtain $\mathbb{M}_{i+1}$ based on $\mathbb{M}_i$ and the local background knowledge of X dictated by $\mathbf{C}$, there is not an edge oriented as both $J \leftarrow K$ and $J \rightarrow K$.*

Proof. For simplicity, we use $\mathbb{M}_i^1$ to denote $\mathbb{M}_i[\mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}]) \backslash \{X\}]$. At first, we prove for any distinct vertices $J, K \in \mathbf{V}(\mathbb{M}_i^1)$, there is $\mathcal{F}_J \subseteq \mathcal{F}_K$ or $\mathcal{F}_K \subseteq \mathcal{F}_J$. Otherwise, there must exist at least two vertices $A, B \in \mathbf{C}$ such that there is $A {*\!\!-\!\!\circ}\, J$, $B {*\!\!-\!\!\circ}\, K$, where A is not adjacent to K, and B is not adjacent to K in $\mathbb{M}_i^1$. Lemma 6 implies that the arrowhead added in the first step of Alg. 1 is invariant in all the MAGs consistent to $\mathbb{M}_i$ and local BK of X dictated by $\mathbf{C}$ (we call such MAG by MAG consistent to $\mathbb{M}_i$ and $\mathbf{C}$ for short). Hence the added arrowheads in the first step appear in any MAG $\mathcal{M}$ consistent to $\mathbb{M}_i$ and $\mathbf{C}$. According to the condition, there are $A{*\!\!\rightarrow} J$ and $B{*\!\!\rightarrow} K$ in $\mathcal{M}$. In this case, there are always new unshielded colliders in $\mathcal{M}$ relative to $\mathbb{M}_i$ no matter what the orientation of the edge connecting J and K is in $\mathcal{M}$. Hence there are always new unshielded collider in the oriented graph relative to $\mathcal{P}$. That is, there does not exist an MAG consistent to $\mathbb{M}_i$ and $\mathbf{C}$. Due to the correctness of BK and Lemma 6, there is not an MAG consistent to $\mathbb{M}_i$, which contradicts with Lemma 8. Hence there is $\mathcal{F}_J \subseteq \mathcal{F}_K$ or $\mathcal{F}_K \subseteq \mathcal{F}_J$.

If $\mathcal{F}_J \neq \mathcal{F}_K$, without loss of generality, suppose $\mathcal{F}_J \subset \mathcal{F}_K$. Then $J \leftarrow K$ is oriented in the second step. If there is also $J \rightarrow K$ oriented in the second step, it implies there is $L \rightarrow J$ oriented in the second step where L is not adjacent to K. In this case, no matter we orient $J \rightarrow K$ or $J \leftarrow K$, there is also a new unshielded collider at J or K, hence there does not exist an MAG consistent to $\mathbb{M}_i$ and $\mathbf{C}$, a contradiction similar to the above case. In the following, we only consider the case of $\mathcal{F}_J = \mathcal{F}_K$. Suppose we orient both $J \rightarrow K$ and $J \leftarrow K$ in the second step.

By Lemma 7, if we orient $J \rightarrow K$ in the second step, there is a minimal circle path $V_0 \circ\!\!-\!\!\circ V_1 \circ\!\!-\!\!\circ \cdots \circ\!\!-\!\!\circ V_m(= J)$ where $\mathcal{F}_{V_m} \supset \mathcal{F}_{V_{m-1}} = \cdots = \mathcal{F}_{V_0}$. If we also orient $J \leftarrow K$ in the second step, there is a circle path $V_{m-1}(= J) \circ\!\!-\!\!\circ V_m(= K) \circ\!\!-\!\!\circ \cdots \circ\!\!-\!\!\circ V_n, n > m$ in $\mathbb{M}_i^1$ where $\mathcal{F}_{V_{m-1}} = \mathcal{F}_{V_m} = \cdots = \mathcal{F}_{V_{n-1}} \subset \mathcal{F}_n$. Note V_{m+1} is adjacent to V_m but is not adjacent to V_{m-1}, while V_{m-2} is adjacent to V_{m-1} but not adjacent to V_m, hence $V_{m-2} \neq V_{m+1}$, and $V_{m-2}, V_{m-1}, V_m, V_{m+1}$ are distinct vertices. Also note no circle edges in $\mathbb{M}_i^1$ are oriented in the first step of Alg. 1. Hence the circle component in $\mathbb{M}_i^1$ is still chordal. Hence $V_0 \circ\!\!-\!\!\circ V_1 \circ\!\!-\!\!\circ \cdots \circ\!\!-\!\!\circ V_n$ is also a minimal circle path, otherwise there must be a cycle comprised of circle edges whose length is larger than 3 without a chord because this cycle must contain $V_{m-2}, V_{m-1}, V_m, V_{m+1}$ where V_{m-2} is not adjacent to V_m and V_{m-1} is not adjacent to V_{m+1}, contradiction. Hence we consider the minimal circle path $V_0 \circ\!\!-\!\!\circ V_1 \circ\!\!-\!\!\circ \cdots \circ\!\!-\!\!\circ V_n$. According to Lemma 6, there must be $V_0 \to \cdots \to V_{m-1}$ and $V_m \leftarrow \cdots V_n$ in any MAG $\mathcal{M}$ consistent to $\mathbb{M}_i$ and $\mathbf{C}$. However, in this case there are new unshielded colliders in $\mathcal{M}$ relative to $\mathbb{M}_i$ and $\mathbf{C}$ no matter what the orientation of the edge connecting V_{m-1} and V_m is, that is, $\mathcal{M}$ is always not consistent to $\mathcal{P}$. Hence there does not exist an MAG consistent to $\mathbb{M}_i$ and $\mathbf{C}$, a contradiction similar to the above case. The proof completes. $\square$

Lemma 12. *Consider $\mathbb{M}_i$ in Thm. 1 that satisfies the five properties. In the third step of Alg. 1 to obtain $\mathbb{M}_{i+1}$ based on $\mathbb{M}_i$ and the local BK of X dictated by $\mathbf{C}$, there are only edges as $A \leftarrow\!\circ B$ transformed to $A \leftarrow B$.*

Proof. There are three possible transformations by the orientation rules: there are edges as $A \circ\!\!-\!\!\circ B$ transformed to the edges with arrowheads; there are edges as $A \leftarrow\!\circ B$ transformed to $A \leftrightarrow B$; there are edges as $A \leftarrow\!\circ B$ transformed to $A \leftarrow B$ ($A \circ\!\!\rightarrow B$ is equivalent to $A \leftarrow\!\circ B$ due to the generality of A and B). We will prove the impossibility of the first two cases. We denote the graph obtained from $\mathbb{M}_i$ and BK regarding V_{i+1} after the first two steps of Alg. 1 by $\bar{\mathbb{M}}_{i+1}$. The proof idea is, suppose in the third step we orient some edges as $A \leftrightarrow R$ or orient some circle edges. We can always find the first edge which is transformed from $A \leftarrow\!\circ R$ to $A \leftrightarrow R$ or from circle edges to some directed or bi-directed edges in the third step. If we prove that this edge can be neither an edge as $A \leftarrow\!\circ R$ transformed to $A \leftrightarrow B$ nor a circle edge, we have a contradiction. Hence we can conclude that there are no edges as $A \leftarrow\!\circ R$ transformed to $A \leftrightarrow R$ or circle edges transformed to directed or bi-directed edges in the third step.

If we orient some edges $A \leftarrow\!\circ R$ as $A \leftrightarrow R$ or orient some circle edges in the third step, the first such edge is not as $A \leftarrow\!\circ R$ and transformed to $A \leftrightarrow R$. Suppose $A \leftarrow\!\circ R$ is transformed to $A \leftrightarrow R$ by the third step of Alg. 1. Note that an arrowhead is introduced by the orientation rules. We analyze the orientation rules. $\mathcal{R}_3$ is triggered in only the process of obtaining $\mathcal{P}$. $\mathcal{R}_4'$ does not transform an edge as $A \leftarrow\!\circ R$ to a bi-directed edge. $\mathcal{R}_8 - \mathcal{R}_{10}$ only introduces tails. Hence only $\mathcal{R}_1$ and $\mathcal{R}_2$ possibly introduce arrowheads. $\mathcal{R}_1$ cannot transform an edge $A \leftarrow\!\circ R$ to $A \leftrightarrow R$. Hence it suffices to prove there are no edges $A \leftarrow\!\circ R$ transformed to $A \leftrightarrow R$ by $\mathcal{R}_2$ in the third step of Alg. 1. According to the condition of $\mathcal{R}_2$, when $A \leftarrow\!\circ R$ is transformed to $A \leftrightarrow R$ by $\mathcal{R}_2$, there is **(i)** $A \to B \leftrightarrow R \circ\!\!\rightarrow A$ or **(ii)** $A \leftrightarrow B \to R \circ\!\!\rightarrow A$. We then prove two results: $(\mathbf{1})$ the bi-directed edges in **(i)** or **(ii)** cannot appear in $\mathbb{M}_i$. $(\mathbf{2})$ the bi-directed edges cannot be introduced in the first two steps of Alg. 1 to obtain $\mathbb{M}_{i+1}$ based on the local BK of X dictated by $\mathbf{C}$.

$(\mathbf{1})$ For **(i)**, suppose there is $B \leftrightarrow R$ in $\mathbb{M}_i$. Since after the first two steps there is $A \leftarrow\!\circ R$, there is $A \ast\!\!-\!\!\circ R$ in $\mathbb{M}_i$. According to the balanced property of $\mathbb{M}_i$, there is $A \leftarrow\!\!\ast B$ in $\mathbb{M}_i$, in which case there cannot be an edge $A \to B$ as **(i)**. For **(ii)**, suppose there is $A \leftrightarrow B$ in $\mathbb{M}_i$. Since after the first two steps there is $B \to R$, there must be $B \to R$ or $B \circ\!\!-\!\!\ast R$ in $\mathbb{M}_i$. For the former case, $A \ast\!\!\rightarrow R$ is oriented in $\mathbb{M}_i$ since $\mathbb{M}_i$ is closed under $\mathcal{R}_2$. For the latter case, $A \ast\!\!\rightarrow R$ is oriented in $\mathbb{M}_i$ due to the balanced property of $\mathbb{M}_i$. Both of them contradict with $A \ast\!\!-\!\!\circ R$ in the graph after the first two steps.

$(\mathbf{2})$ For **(i)**, there is $R \circ\!\!-\!\!\ast A$ in $\mathbb{M}_i$. If $B \leftrightarrow R$ is oriented in the first two steps of Alg. 1, there is either $B \circ\!\!\rightarrow R$ or $B \leftarrow\!\circ R$ in $\mathbb{M}_i$. For the former case, according to the balanced property there is $A \leftarrow\!\!\ast B$ in $\mathbb{M}_i$ due to $R \circ\!\!-\!\!\ast A$, which contradicts with the structure $A \to B$ in **(i)**. For the latter case, since $B \leftarrow\!\circ R$ is transformed to $B \leftrightarrow R$ by the first two steps of Alg. 1, there is $R \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ and $B \in \mathbf{C}$. We discuss whether $A \in \mathbf{C}$, if $A \in \mathbf{C}$, there is $A \ast\!\!\rightarrow R$ oriented by the first step of Alg. 1, contradicting with the structure in **(i)**; if $A \notin \mathbf{C}$, since there is $A \ast\!\!-\!\!\circ R$ after the first two steps, there is $A \ast\!\!-\!\!\circ R$ in $\mathbb{M}_i$, there is $A \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$, hence $A \leftarrow\!\!\ast B$ is oriented in the first step, contradicting with the structure in **(i)**. The contradiction for **(ii)** is similar, we thus do not present the details.

Combining the results in $(\mathbf{1})$ and $(\mathbf{2})$, for the first edge in the third step that is transformed from $A \leftarrow\!\circ R$ to $A \leftrightarrow R$ or transformed from a circle edge to a directed or bi-directed edge, the edge cannot be transformed by $\mathcal{R}_2$ as well. Hence the first edge mentioned above is not an edge transformed from $A \leftarrow\!\circ R$ to $A \leftrightarrow R$ because no orientation rules can achieve it.

If we orient some edges $A \leftarrow\!\circ R$ as $A \leftrightarrow R$ or orient some circle edges in the third step, the first such edge is not a circle edge. We prove that the first edge in the third step that is transformed from $A \leftarrow\!\circ R$ to $A \leftrightarrow R$ or transformed from a circle edge to a directed or bi-directed edge cannot be a circle edge. We analyze the orientation rules respectively. The result is evident for $\mathcal{R}_8 - \mathcal{R}_{10}$ since the transformed edge is as $A \circ\!\!\rightarrow R$, which is not a circle edge. $\mathcal{R}_3$ is triggered in only the process of obtaining $\mathcal{P}$. When an edge is oriented by $\mathcal{R}_4'$, it can be seen as that we first transform a circle to an arrowhead by $\mathcal{R}_2$, then transform the other circle to tail by $\mathcal{R}_4'$. Hence it suffices to show that there are no circle edge oriented by $\mathcal{R}_1$ and $\mathcal{R}_2$ in the third step of Alg. 1. We first consider $\mathcal{R}_1$. Suppose there is $A {*\!\!\rightarrow} B \circ\!\!-\!\!\circ R$ where A and R are not adjacent after the first two steps of updating $\mathbb{M}_i$ with the local BK of X dictated by $\mathbf{C}$. Since $\mathbb{M}_i$ satisfies the complete property, the arrowhead at B on the edge $A {*\!\!\rightarrow} B$ can only be oriented in the first two steps, otherwise the arrowhead is in $\mathbb{M}_i$ and there is either $B \rightarrow R$ or $B \leftarrow\!\!* R$ in $\mathbb{M}_i$. Note the fact that in the first two steps of Alg. 1 we only add arrowheads at the vertex in $\mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$. Hence $B \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$. In addition, there is $R \notin \mathbf{C}$, otherwise $B \leftarrow\!\!\circ R$ is oriented in the first step of Alg. 1. Hence there is $R \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ by Lemma 2. The edge $A {*\!\!\rightarrow} B$ is oriented by either the first or the second step. If $A {*\!\!\rightarrow} B$ is oriented by the first step, then $B \rightarrow R$ should be oriented in the second step since $A \in \mathcal{F}_B \backslash \mathcal{F}_R$; if $A {*\!\!\rightarrow} B$ is oriented by the second step, then $B \rightarrow R$ is also oriented by the second step, in both of cases there is not $B \circ\!\!-\!\!\circ R$ after the first two steps. Hence $\mathcal{R}_1$ is not triggered in the third step.

Then we consider that a circle edge is oriented by $\mathcal{R}_2$. Suppose there is $A \rightarrow B {*\!\!\rightarrow} R$ or $A {*\!\!\rightarrow} B \rightarrow R$, and $A \circ\!\!-\!\!\circ R$. We consider the cases: **(i)** the arrowhead at R on the edge connecting B and R appears in $\mathbb{M}_i$; **(ii)** the arrowhead at R on the edge connecting B and R is introduced by the first two steps of Alg. 1 to obtain $\mathbb{M}_{i+1}$ based on $\mathbb{M}_i$ and the local BK of X dictated by $\mathbf{C}$.

(i) For the first case, there is $B {*\!\!\rightarrow} R$ and $A \circ\!\!-\!\!\circ R$ in $\mathbb{M}_i$. According to the balanced property of $\mathbb{M}_i$, there is $A \leftarrow\!\!* B$ in $\mathbb{M}_i$. Hence the only case that $\mathcal{R}_2$ is triggered is that there is $A \leftrightarrow B \rightarrow R \circ\!\!-\!\!\circ A$ after the first two steps, in which case there can only be $A \leftarrow\!\!\circ B$ in $\mathbb{M}_i$ due to the balance property. In this case, $A \leftarrow\!\!\circ B$ is transformed to $A \leftrightarrow B$ in only the first step. It implies that $A \in \mathbf{C}$ and $B \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$. If $R \in \mathbf{C}$, there is $B \leftrightarrow R$ oriented in the first step, contradicting with $B \rightarrow R$ after the first two steps. If $R \notin \mathbf{C}$, since there is $B \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ and $B \rightarrow R$ or $B \circ\!\!\rightarrow\!\!* R$ in $\mathbb{M}_i$, there is $B \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$, thus there is $A {*\!\!\rightarrow} R$ oriented in the first step, contradicting with $A \circ\!\!-\!\!\circ R$ after the first two steps. Hence case **(i)** is impossible.

(ii) For the second case, note in the first two steps of Alg. 1 we only add arrowheads at the vertex in $\mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$, there is thus $R \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$. In this case there is $A \notin \mathbf{C}$, otherwise $A {*\!\!\rightarrow} R$ is oriented by the first step, contradiction. Due to $R \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ and $A \circ\!\!-\!\!\circ R$ in $\mathbb{M}_i$, there is $A \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ according to Lemma 2. We discuss whether $B \in \mathbf{C}$. **(ii.1)** If $B \in \mathbf{C}$, the only case that $\mathcal{R}_2$ is triggered is that $A \leftrightarrow B \rightarrow R$ in $\bar{\mathbb{M}}_{i+1}$, which implies that there is $A {*\!\!\rightarrow} B$ and $B \rightarrow R$ or $B \circ\!\!-\!\!* R$ in $\mathbb{M}_i$. If $B \rightarrow R$ in $\mathbb{M}_i$, according to the closed property of $\mathbb{M}_i$ under $\mathcal{R}_1$, there is $A {*\!\!\rightarrow} R$ in $\mathbb{M}_i$, thus there is $A {*\!\!\rightarrow} R$ in $\bar{\mathbb{M}}_{i+1}$, contradiction. If $A {*\!\!\rightarrow} B \circ\!\!-\!\!* R$ in $\mathbb{M}_i$, according to the balanced property of $\mathbb{M}_i$, there is also $A {*\!\!\rightarrow} R$ in $\mathbb{M}_i$, thus there is $A {*\!\!\rightarrow} R$ in $\bar{\mathbb{M}}_{i+1}$, contradiction. **(ii.2)** If $B \notin \mathbf{C}$, if there exists an edge between A, B, R that is not a circle edge in $\mathbb{M}_i$, due to the balanced property of $\mathbb{M}_i$ and $A \circ\!\!-\!\!\circ R$ in $\mathbb{M}_i$, there can be either $A {*\!\!\rightarrow} B \leftarrow\!\!* R$ or $A \leftarrow\!\!* B {*\!\!\rightarrow} R$ in $\mathbb{M}_i$. We just show the proof for the first case, and that for the other one is similar. If the case in $\mathcal{R}_2$ happens, there can only be $A \rightarrow B \leftrightarrow R$ in $\bar{\mathbb{M}}_{i+1}$. Since we never add a new bi-directed edge between $\mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ in Alg. 1, the edge $B \leftrightarrow R$ is in $\mathbb{M}_i$. However, in this case due to balanced property of $\mathbb{M}_i$ and $A \circ\!\!-\!\!\circ R$ in $\mathbb{M}_i$, there is $A \leftrightarrow B$ in $\mathbb{M}_i$, contradicting with $A \rightarrow B$ in $\bar{\mathbb{M}}_{i+1}$. Hence in $\mathbb{M}_i$ there can only be $A \circ\!\!-\!\!\circ B \circ\!\!-\!\!\circ R \circ\!\!-\!\!\circ A$. Note the edge between $\mathrm{PossDe}(X, \mathcal{P}[-\mathbf{C}])$ is oriented in only the second step of Alg. 1, where we transform circle edges to directed edges, hence there is $A \rightarrow B \rightarrow R$ in $\bar{\mathbb{M}}_{i+1}$. Then we will prove the impossibility of $A \rightarrow B \rightarrow R \circ\!\!-\!\!\circ A$ in $\bar{\mathbb{M}}_{i+1}$. According to Lemma 7 and Lemma 11, if $A \rightarrow B \rightarrow R$ is oriented, then there is $\mathcal{F}_A \supseteq \mathcal{F}_B \supseteq \mathcal{F}_R$. If there is $\mathcal{F}_A \supset \mathcal{F}_B$ or $\mathcal{F}_B \supset \mathcal{F}_R$, then there is $\mathcal{F}_A \supset \mathcal{F}_R$, hence there is $A \rightarrow R$ oriented by the second step of Alg. 1, contradiction. If there is $\mathcal{F}_A = \mathcal{F}_B = \mathcal{F}_R$, we will prove its impossibility. According to Alg. 1, there is another vertex $C \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ such that $C \rightarrow A$ is oriented by the second step of Alg. 1, C is not adjacent to B, and $\mathcal{F}_C \supseteq \mathcal{F}_A$. Hence there is $\mathcal{F}_C \supseteq \mathcal{F}_R$. We can see that R must be adjacent to C, otherwise $A \rightarrow R$ will be oriented to $A \rightarrow R$ in the second step of Alg. 1. Due to Lemma 6, in each MAG $\mathcal{M}$ consistent to $\mathbb{M}_i$ and $\mathbf{C}$, there is $C \rightarrow A \rightarrow B \rightarrow R$, hence there can only be $C \rightarrow R$ in $\mathcal{M}$. In this case there is a new unshielded collider $C \rightarrow R \leftarrow B$ in $\mathcal{M}$ relative to $\mathbb{M}_i$ because there is $B \circ\!\!-\!\!\circ R$ in $\mathbb{M}_i$, hence $\mathcal{M}$ is not consistent to $\mathcal{P}$. Hence there does not exist an MAG consistent to $\mathbb{M}_i$ and $\mathbf{C}$. Due to the correctness of local BK, there does not exist an MAG consistent to $\mathbb{M}_i$, contradicting with Lemma 8. With **(i)** and **(ii)**, it is concluded that $\mathcal{R}_2$ is not triggered in the third step of Alg. 1. Combining the parts above, we conclude that for the first edge in the third step that is transformed from $A \leftarrow\!\!\circ R$ to

$A \leftrightarrow R$ or transformed from a circle edge to a directed or bi-directed edge cannot be a circle edge, the first edge cannot be a circle edge.

Combining the two parts above, we conclude that for the first edge in the third step that is transformed from $A \leftarrow\!\circ R$ to $A \leftrightarrow R$ or transformed from a circle edge to a directed or bi-directed edge, the first edge can be neither an edge transformed from $A \leftarrow\!\circ R$ to $A \leftrightarrow R$, nor a circle edge. Hence we conclude there cannot be an edge in the third step that is transformed from $A \leftarrow\!\circ R$ to $A \leftrightarrow R$ or transformed from a circle edge to a directed or bi-directed edge. Hence, in the third step of Alg. 1, only the transformation as $A \leftarrow\!\circ R$ to $A \leftarrow R$ is possibly triggered by the orientation rules. $\square$

Lemma 13. *The PMG $\mathbb{M}_{i+1}$ in Thm. 1 satisfies the chordal property.*

Proof. We denote the oriented graph based on $\mathbb{M}_i$ and the local BK dictated by $\mathbf{C}$ after the first two steps of Alg. 1 by $\bar{\mathbb{M}}_{i+1}$. As shown by Lemma 12, there are no circle edges oriented in the third step of Alg. 1. Hence, it suffices to prove that the circle component in $\bar{\mathbb{M}}_{i+1}$ is chordal.

Note the edges in $\bar{\mathbb{M}}_{i+1}[-\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])]$ are identical to those in $\mathbb{M}_i[-\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])]$ since we do not orient the edges in this region in the first two steps. Due to chordal property of $\mathbb{M}_i$ and the fact that the subgraph of a chordal graph is also chordal, the circle component in $\bar{\mathbb{M}}_{i+1}[-\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])]$ is chordal. We consider the circle edge connecting $\bar{\mathbb{M}}_{i+1}[\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])]$ and $\bar{\mathbb{M}}_{i+1}[-\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])]$. Suppose an edge of $V_1 \circ\!\!-\!\!\circ V_2$, where $V_1 \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ and $V_2 \in \mathbf{V}(\mathbb{M}_i) \backslash \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$. If there is $V_2 \notin \mathbf{C}$, then there is $V_2 \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ due to $V_1 \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$, $V_1 \circ\!\!-\!\!\circ V_2$, and Lemma 2, contradicting with $V_2 \in \mathbf{V}(\mathbb{M}_i) \backslash \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$. Hence there is $V_2 \in \mathbf{C}$. According to the first step of Alg. 1, $V_1 \circ\!\!-\!\!\circ V_2$ is oriented as $V_1 \leftarrow\!\circ V_2$. Hence after the first step there is not circle edge connecting $\bar{\mathbb{M}}_{i+1}[\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])]$ and $\bar{\mathbb{M}}_{i+1}[-\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])]$. There are not circle edges connecting X with any other vertices in $\bar{\mathbb{M}}_{i+1}$ since the marks at X is definite after the first step. In the following, it suffices to show the circle component in $\bar{\mathbb{M}}_{i+1}[\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}]) \backslash \{X\}]$ is chordal. For simplicity, we denote $\bar{\mathbb{M}}_{i+1}[\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}]) \backslash \{X\}]$ by $\bar{\mathbb{M}}^1_{i+1}$.

We will use three facts in the following: **(i)** each circle edge in $\bar{\mathbb{M}}_{i+1}$ is also a circle edge in $\mathbb{M}_i$; **(ii)** the circle edges in $\mathbb{M}_i[\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}]) \backslash \{X\}]$ are only possibly oriented in the second step in the process of obtaining $\bar{\mathbb{M}}_{i+1}$ from $\mathbb{M}_i$ by the first two steps of Alg. 1; **(iii)** Lemma 11.

Suppose the circle component in $\bar{\mathbb{M}}^1_{i+1}$ is not chordal, there is a circle cycle as $V_0 \circ\!\!-\!\!\circ V_1 \circ\!\!-\!\!\circ \cdots \circ\!\!-\!\!\circ V_n \circ\!\!-\!\!\circ V_0, n \geq 3$, where there is not a circle edge between every two unconsecutive vertices. And there must exist edges between the unconsecutive vertices in this cycle, otherwise it is a cycle of length four or more without a chord in $\mathbb{M}_i$, contradicting with the chordal property of $\mathbb{M}_i$. We can always find a sub-structure $V_k \circ\!\!-\!\!\circ V_{k+1} \circ\!\!-\!\!\circ \cdots \circ\!\!-\!\!\circ V_m \leftarrow V_k, 0 \leq k < m \leq n$ without other directed edges between any two vertices among $V_k, \cdots, V_m$ except for $V_m \leftarrow V_k$ (if there is another directed edge, for instance $V_{k+1} \to V_m$, we can find a proper sub-structure $V_{k+1} \circ\!\!-\!\!\circ \cdots \circ\!\!-\!\!\circ V_m \leftarrow V_{k+1}$ instead. And since the path is symmetric, suppose $V_k \to V_m$ without loss of generality.). According to Lemma 3, the directed edge between V_k and V_m can only be a circle edge in $\mathbb{M}_i$. Hence in $\mathbb{M}_i$ there is $V_k \circ\!\!-\!\!\circ V_{k+1} \circ\!\!-\!\!\circ \cdots \circ\!\!-\!\!\circ V_m \circ\!\!-\!\!\circ V_k$. Since the circle component in $\mathbb{M}_i$ in chordal, the length of the circle cycle can only be three. Hence it holds $m = k + 2$ and there is a sub-structure $V_k \circ\!\!-\!\!\circ V_{k+1} \circ\!\!-\!\!\circ V_{k+2} \leftarrow V_k$ in $\bar{\mathbb{M}}^1_{i+1}$. Next, we will prove its impossibility.

Since there is $V_k \circ\!\!-\!\!\circ V_{k+1} \circ\!\!-\!\!\circ V_{k+2} \leftarrow V_k$ in $\bar{\mathbb{M}}^1_{i+1}$, there is $\mathcal{F}_{V_k} = \mathcal{F}_{V_{k+1}} = \mathcal{F}_{V_{k+2}}$. Considering it is oriented as $V_k \to V_{k+2}$ in the second step, there is another vertex F_1 in $\bar{\mathbb{M}}^1_{i+1}$ such that there is $F_1 \to V_k$ where F_1 is not adjacent to V_{k+2}. Evidently F_1 is adjacent to V_{k+1}, otherwise $V_k \to V_{k+1}$ is also oriented. Next, we consider the relation between $\mathcal{F}_{F_1}$ and $\mathcal{F}_{V_k}$. Since $F_1 \to V_k$, there is $\mathcal{F}_{V_k} \subseteq \mathcal{F}_{F_1}$ (Note $F_1 \to V_k$ is oriented in the second step, if $\mathcal{F}_{V_k} \supset \mathcal{F}_{F_1}$, there can be an another edge oriented as $V_k \to F_1$ in the second step, contradicting with Lemma 11). If $\mathcal{F}_{V_k} \subset \mathcal{F}_{F_1}$, there is also $\mathcal{F}_{V_{k+1}} \subset \mathcal{F}_{F_1}$ since $\mathcal{F}_{V_k} = \mathcal{F}_{V_{k+1}}$. Hence $F_1 \to V_{k+1}$. And due to $\mathcal{F}_{V_{k+1}} = \mathcal{F}_{V_{k+2}}$ and the non-adjacency of F_1 and V_{k+2}, in the second step $V_{k+1} \to V_{k+2}$ is oriented, contradicting with $V_{k+1} \circ\!\!-\!\!\circ V_{k+2}$. Hence, it is only possible that there is $\mathcal{F}_{V_k} = \mathcal{F}_{F_1}$ and $F_1 \circ\!\!-\!\!\circ V_{k+1}$ in $\bar{\mathbb{M}}^1_{i+1}$. Here we find a sub-structure $F_1 \circ\!\!-\!\!\circ V_{k+1} \circ\!\!-\!\!\circ V_k \leftarrow F_1$. Since $F_1 \to V_k$ is oriented, there is another vertex F_2 that is not adjacent to V_k in $\bar{\mathbb{M}}^1_{i+1}$ such that $F_2 \to F_1$ is oriented in the second step. Similar to the previous proof, there is not a contradiction only when $\mathcal{F}_{F_2} = \mathcal{F}_{F_1}$ and $F_2 \circ\!\!-\!\!\circ V_{k+1}$. Repeat this process and we can conclude that if there is not a contradiction, in any uncovered directed path as $F_t \to \cdots \to F_1 \to V_k \to V_{k+2}$, for any a vertex V' on the path, there is $\mathcal{F}_{V'} = \mathcal{F}_{V_k}$ and there is a circle edge between V' and V_{k+1}. It contradicts with Lemma 7. Hence, there cannot be a sub-structure as $V_k \circ\!\!-\!\!\circ V_{k+1} \circ\!\!-\!\!\circ V_{k+2} \leftarrow V_k$ after the first three steps. The proof completes. $\square$

Lemma 14. *The PMG $\mathbb{M}_{i+1}$ in Thm. 1 satisfies the balanced property.*

Proof. If there is $V_i {*\!\!\rightarrow} V_j \circ\!\!\!-\!\!* V_k$, we first prove that V_i is adjacent to V_k. Suppose V_i is not adjacent to V_k. This structure cannot appear in $\mathbb{M}_i$ due to the complete property of $\mathbb{M}_i$. Hence $V_i {*\!\!\rightarrow} V_j$ is oriented in the process of obtaining $\mathbb{M}_{i+1}$ based on $\mathbb{M}_i$. According to Lemma 12, the arrowhead is introduced in only the first two steps of obtaining $\mathbb{M}_{i+1}$. And in the first two steps arrowhead is added at the vertex in $\mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$. Hence there is $V_j \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$. In this case if $V_k \in \mathbf{C}$, there is $V_j \leftarrow\!\!* V_k$ oriented in the first step, contradiction. If $V_k \notin \mathbf{C}$, if there is $V_j \circ\!\!-\!\!\circ V_k$ in $\mathbb{M}_i$, there is $V_k \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$, thus there is always $V_j \rightarrow V_k$ oriented in the second step by discussing whether $V_i \in \mathbf{C}$ (we omit the details), contradiction. If $V_j \circ\!\!\rightarrow V_k$ in $\mathbb{M}_i$, it will be oriented as $V_j \rightarrow V_k$ by $\mathcal{R}_1$ in the third step of Alg. 1, which contradict with $V_j \circ\!\!\!-\!\!* V_k$ in $\mathbb{M}_{i+1}$.

Next we consider the case that V_i is adjacent to V_k. If there is $V_i {*\!\!\rightarrow} V_j \circ\!\!\!-\!\!* V_k$ in $\mathbb{M}_i$, there is $V_i {*\!\!\rightarrow} V_k$ due to the balanced property of $\mathbb{M}_i$, hence there is $V_i {*\!\!\rightarrow} V_k$ in $\mathbb{M}_{i+1}$. Hence it suffices to consider there is $V_i *\!\!-\!\!\circ V_j \circ\!\!\!-\!\!* V_k$ in $\mathbb{M}_i$ while $V_i {*\!\!\rightarrow} V_j \circ\!\!\!-\!\!* V_k$ in $\mathbb{M}_{i+1}$. Note in the process of obtaining $\mathbb{M}_{i+1}$ based on $\mathbb{M}_i$, arrowhead are oriented only at the vertex in $\mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$, thereby $V_j \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$. In addition, $V_k \notin \mathbf{C}$, otherwise there is $V_j \leftarrow\!\!* V_k$ in $\mathbb{M}_{i+1}$. Combining $V_j \circ\!\!\!-\!\!* V_k$ and $V_j \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$, there is $V_k \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$. We discuss whether $V_i \in \mathbf{C}$ in the following.

(i). If $V_i \in \mathbf{C}$, there is $V_i {*\!\!\rightarrow} V_j$ and $V_i {*\!\!\rightarrow} V_k$ after the first step of obtaining $\mathbb{M}_{i+1}$ based on $\mathbb{M}_i$. In this case, when there is $V_i \rightarrow V_j$ in $\mathbb{M}_{i+1}$, there is $V_i \circ\!\!-\!\!\circ V_j$ in $\mathbb{M}_i$, hence there is $V_i \circ\!\!\!-\!\!* V_k$ or $V_i \rightarrow V_k$ in $\mathbb{M}_i$ (if there is $V_i \leftarrow\!\!* V_k \circ\!\!\!-\!\!* V_j \circ\!\!\!-\!\!* V_i$ in $\mathbb{M}_i$, it contradicts with the balanced property of $\mathbb{M}_i$). Therefore there is $V_i \rightarrow V_k$ in $\mathbb{M}_{i+1}$. Balanced property is satisfied for $\mathbb{M}_{i+1}$ when $V_i \in \mathbf{C}$.

(ii). If $V_i \notin \mathbf{C}$, there is $V_i \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ due to $V_i *\!\!-\!\!\circ V_j$ and $V_j \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$. In this case the arrowhead is introduced in the second step of obtaining $\mathbb{M}_{i+1}$ based on $\mathbb{M}_i$. Hence there is $V_i \circ\!\!-\!\!\circ V_j$ in $\mathbb{M}_i$. In this case either $V_i \circ\!\!-\!\!\circ V_j {*\!\!\rightarrow} V_k \leftarrow\!\!* V_i$, or $V_i \circ\!\!-\!\!\circ V_j \circ\!\!-\!\!\circ V_k \circ\!\!-\!\!\circ V_i$ in $\mathbb{M}_i$. For the former case, there is $V_i \rightarrow V_j {*\!\!\rightarrow} V_k \leftarrow\!\!* V_i$ in $\mathbb{M}_{i+1}$. And there cannot be $V_i \leftrightarrow V_k$ in $\mathbb{M}_{i+1}$, otherwise there is $V_j \leftrightarrow V_k$ since $\mathbb{M}_{i+1}$ is closed under $\mathcal{R}_2$, contradicting with $V_j \circ\!\!\!-\!\!* V_k$ in $\mathbb{M}_{i+1}$. Hence the balanced property also holds in $\mathbb{M}_{i+1}$ for the first case. For the latter case, suppose there is $V_i \rightarrow V_j \circ\!\!-\!\!\circ V_k$ oriented after the second step, V_i is adjacent to V_k. According to the proof of Lemma 13, there cannot be a structure $V_i \circ\!\!-\!\!\circ V_k \circ\!\!-\!\!\circ V_j \leftarrow V_i$, thus there is not a circle-edge between V_i and V_k. Since we only transform the circle edges between $\mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ to directed edges in the second step, the edge between V_i and V_k is directed. If there is $V_i \rightarrow V_k$ oriented in the second step, balanced property of $\mathbb{M}_{i+1}$ is satisfied. If there is $V_k \rightarrow V_i$ oriented in the second step, there is $V_k \rightarrow V_j$ oriented by $\mathcal{R}_2$ in the third step, which contradicts with Lemma 12 that there are no circle edges oriented in the third step, impossibility.

As shown above, balanced property also holds in $\mathbb{M}_{i+1}$. $\square$

Lemma 15. *The PMG $\mathbb{M}_{i+1}$ in Thm. 1 satisfies the complete property.*

In $\mathbb{M}_{i+1}$, the edges with circles are either $A \circ\!\!-\!\!\circ B$ or $A \circ\!\!\rightarrow B$. In Lemma 15.1, we show that we can always obtain an MAG consistent to $\mathcal{P}$ and local BK regarding $V_1, \cdots, V_{i+1}$ by transforming $\circ\!\!\rightarrow$ to $\rightarrow$ and the circle component into a DAG without unshielded colliders in $\mathbb{M}_{i+1}$. Due to the chordal property of $\mathbb{M}_{i+1}$, for the edge $A \circ\!\!-\!\!\circ B$ in $\mathbb{M}_{i+1}$, there exist both perfect elimination orders to orient the circle component into DAGs without unshielded colliders where there is $A \rightarrow B$ and $A \leftarrow B$ respectively, as implied by Lemma 5 of Meek [36]; and for the edge $C \circ\!\!\rightarrow D$ in $\mathbb{M}_{i+1}$, the edge can be oriented as $C \rightarrow D$ in some MAG consistent to $\mathcal{P}$ and local BK regarding $V_1, \cdots, V_{i+1}$. For the edge $A \circ\!\!\rightarrow B$ in $\mathbb{M}_{i+1}$, we show the edge can be oriented as $A \leftrightarrow B$ in Lemma 15.2. Here the most difficult part is to prove Lemma 15.1, *i.e.*, we can always obtain an MAG consistent to $\mathcal{P}$ and local BK regarding $V_1, \cdots, V_{i+1}$ by transforming $\circ\!\!\rightarrow$ to $\rightarrow$ and the circle component into a DAG without unshielded colliders in $\mathbb{M}_{i+1}$. With this result, we can prove Lemma 15.2 totally following the procedure of that of Theorem 3 of Zhang [35], with the invariant, chordal, and balanced property of $\mathbb{M}_{i+1}$. Since the proof is too lengthy and completely follow that of Theorem 3 of Zhang [35], we will not show the details but just a sketch in the proof of Lemma 15.2.

Note according to the invariant property of $\mathbb{M}_{i+1}$, there cannot be new unshielded colliders or directed or almost directed cycles introduced in $\mathbb{M}_{i+1}$ relative to $\mathbb{M}_i$, otherwise there does not exist an MAG consistent to $\mathbb{M}_{i+1}$. Given the invariant property of $\mathbb{M}_{i+1}$ by Lemma 6 and the basic assumption that the background knowledge is correct, there is not an MAG consistent to $\mathbb{M}_i$, contradicting with Lemma 8.

Lemma 15.1. *Consider $\mathbb{M}_{i+1}$ in Thm. 1. We orient a graph $\mathcal{H}$ from $\mathbb{M}_{i+1}$ by transforming $\circ\!\!\rightarrow$ to $\rightarrow$ and the circle component in $\mathbb{M}_{i+1}$ into a DAG without unshielded colliders. Then $\mathcal{H}$ is an MAG consistent to $\mathcal{P}$ and local BK regarding $V_1, \cdots, V_{i+1}$.*

Proof. Our proof idea is as follows. We aim to prove if the constructed graph $\mathcal{H}$ by the following orientation process based on $\mathbb{M}_{i+1}$ which transforms all edges $\circ\!\!\rightarrow$ to $\rightarrow$ and orient the circle component into a DAG without unshielded colliders is not an MAG consistent to $\mathcal{P}$ and local BK regarding $V_1, \cdots, V_{i+1}$, then a constructed graph based on $\mathbb{M}_i$ which transform all edges $\circ\!\!\rightarrow$ to $\rightarrow$ and orient the circle component into a DAG without unshielded colliders is not an MAG consistent to $\mathcal{P}$ and local BK regarding $V_1, \cdots, V_i$. Repeat this process until $\mathbb{M}_0$ and we can conclude that a constructed graph based on $\mathbb{M}_0(= \mathcal{P})$ which transforms all edges $\circ\!\!\rightarrow$ to $\rightarrow$ and orient the circle component into a DAG without unshielded colliders is not an MAG consistent to $\mathbb{M}_0(= \mathcal{P})$, which contradicts Theorem 2 of Zhang [35]. Hence we get the desired result. The process of obtaining $\mathcal{H}$ is as follows.

- (Step 1) For all $K \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ and $\forall T \in \mathbf{C}$ such that $K \circ\!\!-\!\!* T$ in $\mathbb{M}_i$, orient $K \leftarrow\!\!* T$ (the mark at T remains); for all $K \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ such that $X \circ\!\!-\!\!* K$, orient $X \rightarrow K$;
- (Step 2) Orient the subgraph $\mathbb{M}_i[\mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])\backslash\{X\}]$ as follows until no feasible updates: for any two vertices V_i and V_j such that $V_i \circ\!\!-\!\!\circ V_j$, orient it as $V_i \rightarrow V_j$ if **(i)** $\mathcal{F}_{V_i}\backslash\mathcal{F}_{V_j} \neq \emptyset$ or **(ii)** $\mathcal{F}_{V_i} = \mathcal{F}_{V_j}$ as well as there is a vertex $V_k \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])\backslash\{X\}$ not adjacent to V_j such that $V_k \rightarrow V_i \circ\!\!-\!\!\circ V_j$, where $\mathcal{F}_{V_l} = \{V \in \mathbf{C} \cup \{X\} \mid V *\!\!-\!\!\circ V_l \text{ in } \mathbb{M}_i\}$;
- (Step 3) Obtain $\mathbb{M}_{i+1}$ by applying the orientation rules until the graph is closed under the rules;
- (Step 4) for the circle component in subgraph $\mathbb{M}_{i+1}[\mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])\backslash\{X\}]$, orient it into a DAG without new unshielded colliders;
- (Step 5) for the circle component in subgraph $\mathbb{M}_{i+1}[-\mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])]$, orient it into a DAG without new unshielded colliders;
- (Step 6) for any edge as $\circ\!\!\rightarrow$, orient it as $\rightarrow$.

Note the first three steps are the process of obtaining $\mathbb{M}_{i+1}$ from $\mathbb{M}_i$ with the local structure of X dictated by $\mathbf{C}$. And in Step 4 - Step 6 we transform the edges as $\circ\!\!\rightarrow$ to $\rightarrow$ and transform the circle component in $\mathbb{M}_{i+1}$ into a DAG without new unshielded colliders. Note X is not in a connected circle component with any other vertices after the first step. Hence when we consider the circle component in $\mathbb{M}_{i+1}$, we do not need to consider X. And we have proven that there is not a circle edge connecting $\mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])\backslash\{X\}$ and $\mathbf{V}(\mathbb{M}_i)\backslash(\mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])\backslash\{X\})$ in the proof of Lemma 13. Hence the circle component in $\mathbb{M}_{i+1}[\mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])\backslash\{X\}]$ is not connected to that in $\mathbb{M}_{i+1}[-(\mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])\backslash\{X\})]$. Hence we can divide the circle component orientation in $\mathbb{M}_{i+1}$ into Step 4 and Step 5. The achievability of Step 4 and Step 5 is due to the chordal property of $\mathbb{M}_{i+1}$ according to Lemma 13.

In the following there are mainly two parts. The first part is that we construct an auxiliary graph $\mathcal{H}_0$ *based on* $\mathcal{H}$, and we show that this constructed graph can also be seen as a graph obtained from $\mathbb{M}_i$ by transforming all edges $\circ\!\!\rightarrow$ to $\rightarrow$ and orienting the circle component into a DAG without new unshielded colliders. The second part is we show that if $\mathcal{H}_0$ is an MAG consistent to $\mathcal{P}$ and local BK regarding $V_1, \cdots, V_i$, then $\mathcal{H}$ is an MAG consistent to $\mathcal{P}$ and local BK regarding $V_1, \cdots, V_{i+1}$.

(A) Auxiliary graph $\mathcal{H}_0$. We construct an auxiliary graph $\mathcal{H}_0$ based on $\mathcal{H}$ by transforming all and only the bi-directed edges $K \leftrightarrow T$ in $\mathbb{M}_{i+1}$ which are $K \circ\!\!\rightarrow T$ in $\mathbb{M}_i$ to $K \rightarrow T$, where $K \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ and $T \in \mathbf{C}$ according to the first step. It is direct that $\mathcal{H}_0$ has the non-circle marks in $\mathbb{M}_i$ and there are no new bi-directed edges in $\mathcal{H}_0$ compared to $\mathbb{M}_i$ because all additional bi-directed edges in $\mathcal{H}$ relative to $\mathbb{M}_i$ are possibly introduced in only the first step of the process of obtaining $\mathcal{H}$ according to the construction process and Lemma 12. Besides, all the circles on $\circ\!\!\rightarrow$ edges in $\mathbb{M}_i$ are oriented as tails in $\mathcal{H}_0$. In the following it suffices to show that $\mathcal{H}_0$ is also a graph oriented from $\mathbb{M}_i$ by orienting the circle component in $\mathbb{M}_i$ into a DAG without new unshielded colliders.

Hence, we only consider the circle component in $\mathbb{M}_i$. We divide it into two parts, one is the circle component in $\mathbb{M}_i[\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])\backslash\{X\}]$, denoted by CC_1; and the other is the circle component in $\mathbb{M}_i[-(\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])\backslash\{X\})]$, denoted by CC_2.

Note the oriented edges of CC_1 in $\mathcal{H}_0$ totally follows those in $\mathcal{H}$, which are oriented by either Step 2 or Step 4. There are no new unshielded colliders or directed or almost directed cycles oriented in the edges of CC_1 by the three following facts. **(1).** There are no new unshielded colliders or directed or almost directed cycles in the edges of CC_1 oriented by Step 2. Otherwise, given the invariant property of $\mathbb{M}_{i+1}$ by Lemma 6 and the basic assumption that the background knowledge is correct, there is not an MAG consistent to $\mathbb{M}_i$, contradicting with Lemma 8. **(2).** There are no unshielded colliders or directed or almost directed cycles in the edges of CC_1 oriented by Step 4 because the circle component in $\mathbb{M}_{i+1}$ is chordal and is oriented to a DAG without new unshielded colliders. **(3).** There are no new unshielded colliders or directed or almost directed cycles in edges of CC_1 oriented by both Step 2 and Step 4 due to the balanced property of $\mathbb{M}_{i+1}$ and the impossibility of the transformation of circle edges to bi-directed edges.

Note the edges in CC_2 also totally follow those in $\mathcal{H}$. Although when $X \circ\!\!\rightarrow T$ in $\mathbb{M}_i$ where $T \in \mathbf{C}$, there is $X \leftrightarrow T$ in $\mathcal{H}$ while $X \rightarrow T$, such edge is not in the circle component CC_2 because it is as $X \circ\!\!\rightarrow T$ in $\mathbb{M}_i$. According to the orientation process, the sub circle component of CC_2 induced by $\mathbf{V}(\text{CC}_2)\backslash\{X\}$, is oriented into a DAG without new unshielded colliders. Hence if there are new unshielded colliders or directed or almost directed cycles in edges of CC_2, they contain X. **(1)** There are not new unshielded colliders as $A {*\!\!\rightarrow} X \leftarrow\!\!* B$ in edges of CC_2 in Step 2. Otherwise, given the invariant property of $\mathbb{M}_{i+1}$ by Lemma 6 and the basic assumption that the background knowledge is correct, there is not an MAG consistent to $\mathbb{M}_i$, contradicting with Lemma 8. **(2)** There are no directed or almost directed cycles in CC_2 containing X because for each vertex V in CC_2 that has a circle edge with X, the edge is oriented as $V \rightarrow X$.

For the circle edge in the circle component connecting $K \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])\backslash\{X\}$ and $T \in \mathbf{V}(\mathbb{M}_i)\backslash(\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])\backslash\{X\})$, there must be $T \in \mathbf{C} \cup \{X\}$, otherwise there is $T \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])\backslash\{X\}$ due to $K \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])\backslash\{X\}$ and $K \circ\!\!-\!\!\circ T$. Hence in $\mathcal{H}$ the circle edge is oriented as $K \leftarrow T$ by the first step and the last step. According to the relation between $\mathcal{H}$ and $\mathcal{H}_0$, there is $K \leftarrow T$ in $\mathcal{H}_0$. Hence, for each circle edge $K \circ\!\!-\!\!\circ T$ where $K \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])\backslash\{X\}$ and $T \in \mathbf{V}(\mathbb{M}_i)\backslash(\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])\backslash\{X\})$, there is $K \leftarrow T$ in $\mathcal{H}_0$ and $T \in \mathbf{C} \cup \{X\}$. Hence it is evident that in $\mathcal{H}_0$ there cannot be a directed or almost directed cycles oriented from the circle component which contain both the vertices in $\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])\backslash\{X\}$ and $\mathbf{V}(\mathbb{M}_i)\backslash(\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])\backslash\{X\})$. If there is a new unshielded collider in $\mathcal{H}_0$ relative to $\mathbb{M}_i$ comprised of the vertices in both $\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])\backslash\{X\}$ and $\mathbf{V}\backslash(\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])\backslash\{X\})$, the unshielded collider can only be as $T_1 \rightarrow K_1 \leftarrow T_2$ or $T_1 \rightarrow K_1 \leftarrow K_2$ where $T_1, T_2 \in \mathbf{C} \cup \{X\}$ and $K_1, K_2 \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])\backslash\{X\}$. We first prove that the first case is impossible. Due to Lemma 6, there is $T_1 {*\!\!\rightarrow} K_1$ and $T_2 {*\!\!\rightarrow} K_2$ in all MAGs consistent to $\mathcal{P}$ and the local BK regarding $V_1, \ldots, V_{i+1}$. If they form a new unshielded collider, it implies that there does not exist MAG consistent to $\mathcal{P}$ and the local BK regarding $V_1, \ldots, V_{i+1}$. Due to the correctness of BK and Lemma 6, there does not exist an MAG consistent to $\mathbb{M}_i$, contradicting with Lemma 8. For the second case, there is $T_1 \in \mathcal{F}_{K_1}\backslash\mathcal{F}_{K_2}$, hence $K_1 \rightarrow K_2$ should be oriented in the second step. While there is also $K_1 \leftarrow K_2$ oriented, it contradicts with Lemma 11. Hence, if there is a new unshielded collider in $\mathcal{H}_0$, there is always a contradiction.

Hence, we prove that the graph $\mathcal{H}_0$ constructed based on $\mathcal{H}$ can also be seen as a graph obtained from $\mathbb{M}_i$ by transforming all edges $\circ\!\!\rightarrow$ to $\rightarrow$ and transforming the circle component into a DAG without new unshielded colliders.

(B) If $\mathcal{H}_0$ is an MAG consistent to $\mathcal{P}$ and local BK regarding $V_1, \cdots, V_i$, then $\mathcal{H}$ is an MAG consistent to $\mathcal{P}$ and local BK regarding $V_1, \cdots, V_{i+1}$. Suppose $\mathcal{H}_0$ is an MAG consistent to $\mathcal{P}$ and local BK regarding $V_1, \cdots, V_i$. We will prove that $\mathcal{H}$ is an MAG Markov equivalent to $\mathcal{H}_0$ by Lemma 1 of Zhang and Spirtes [41]. Because $\mathcal{H}$ has the non-circle marks in $\mathbb{M}_{i+1}$, and $\mathcal{H}_0$ belongs to the MEC represented by $\mathcal{P}$, we can conclude that $\mathcal{H}$ is an MAG consistent to $\mathcal{P}$ and local BK regarding $V_1, \cdots, V_{i+1}$.

Note that the only difference between $\mathcal{H}$ and $\mathcal{H}_0$ is that for $\forall K \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ and $\forall T \in \mathbf{C}$ such that $K \circ\!\!\rightarrow T$ in $\mathbb{M}_i$, there is $K \rightarrow T$ in $\mathcal{H}_0$ but $K \leftrightarrow T$ in $\mathcal{H}$. Denote the set of different edges in $\mathcal{H}_0$ by $Edge(\mathcal{H}_0) = \{K \rightarrow T \text{ in } \mathcal{H}_0 \mid K \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}]), T \in \mathbf{C}, K \circ\!\!\rightarrow T \text{ in } \mathbb{M}_i\}$. We could obtain $\mathcal{H}$ from $\mathcal{H}_0$ by transforming these edges to bi-directed edges. We transform one edge one time. At first, we select the edge $K \rightarrow T$ in $Edge(\mathcal{H}_0)$ according to the selection criterion that (1) we select K that is not an ancestor of any other V_1 such that there is an edge $V_1 \rightarrow V_2$ in $Edge(\mathcal{H}_0)$; and (2) given K selected in the first step, we select T that is not a descendant of any other V_2 such that there is an edge $K \rightarrow V_2$ in $Edge(\mathcal{H}_0)$. Then we obtain $Edge(\mathcal{H}_1)$ by deleting $K \rightarrow T$ from $Edge(\mathcal{H}_0)$. By such operation, we obtain a new graph $\mathcal{H}_1$ and $Edge(\mathcal{H}_1)$. Repeat the process above and we could obtain a series of graphs $\mathcal{H}_0, \mathcal{H}_1, \cdots, \mathcal{H}_m, \mathcal{H}_{m+1}(= \mathcal{H})$. We will prove that for any $\mathcal{H}_j$ and $\mathcal{H}_{j+1}$, where $0 \leq j \leq m$, if $\mathcal{H}_j$ is an MAG, then $\mathcal{H}_{j+1}$ is an MAG Markov equivalent to $\mathcal{H}_j$. According to the conditions, $\mathcal{H}_0$ is an MAG in the MEC represented by $\mathcal{P}$. Suppose the edge that will be transformed in $\mathcal{H}_j$ is $K \rightarrow T$. According to Lemma 1 of Zhang and Spirtes [41], given $\mathcal{H}_j$ is an MAG, it suffices to show that (1) there is no directed path from K to T in $\mathcal{H}_j$ other than $K \rightarrow T$; (2) for any $A \rightarrow K$ in $\mathcal{H}_j$, $A \rightarrow T$ is also in $\mathcal{H}_j$; and for any $B \leftrightarrow K$ in $\mathcal{H}_j$, either $B \rightarrow T$ or $B \leftrightarrow T$ is in $\mathcal{H}_j$; (3) there is no discriminating path for K on which T is the endpoint adjacent to K in $\mathcal{H}_j$. We show the proof in order.

(1) In this part, we prove that there is not a directed path from K to T in $\mathcal{H}_j$. For the sake of contradiction, suppose there is a directed path from K to T in $\mathcal{H}_j$, we suppose the minimal directed path of this path is $K(= F_0) \rightarrow F_1 \rightarrow \cdots \rightarrow F_m \rightarrow T(= F_{m+1})$. Since we only transform directed edges to bi-directed edges in the process, the directed path is also in $\mathcal{H}_0$. We first prove that there must be a vertex $F_n, 1 \leq n \leq m$ such that $F_n \in \mathbf{C}$. Otherwise, all of $F_1, \cdots, F_m$ belong to $\mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ since $F_0 \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ and there is a possible directed path comprised of $F_0, F_1, \cdots, F_m$ in $\mathbb{M}_i$. **(i.)** If there is $F_m \rightarrow T$ in $\mathbb{M}_i$, it contradicts with Lemma 10. **(ii.)** If there is $F_m \circ\!\!-\!\!\circ T$ in $\mathbb{M}_i$, according to the first step of orientation procedure to construct $\mathcal{H}$, there is $F_m \leftarrow T$ in $\mathcal{H}$. Since in the process from $\mathcal{H}_j$ to $\mathcal{H}$ we never transform an edge $A \rightarrow B$ to $A \leftarrow B$, there cannot be an edge $F_m \rightarrow T$ in $\mathcal{H}_j$. **(iii.)** If there is $F_m \circ\!\!\rightarrow T$ in $\mathbb{M}_i$, there is $F_m \rightarrow T$ in $\mathcal{H}_0$. According to the edge selection criterion, when there is both $F_m \rightarrow T$ and $K \rightarrow T$ in $\mathcal{H}_j$, we should transform $F_m \rightarrow T$ ahead of $K \rightarrow T$ due to $K \rightarrow F_1 \rightarrow \cdots \rightarrow F_m$, contradiction. For the other situations for the edge between F_m and T in $\mathbb{M}_i$, there cannot form an edge $F_m \rightarrow T$ in $\mathcal{H}_j$. Hence we conclude there is a vertex $F_n, 1 \leq n \leq m$ such that $F_n \in \mathbf{C}$.

Without loss of generality, we suppose $F_n \in \mathbf{C}$ and $F_l \notin \mathbf{C}, \forall 1 \leq l \leq n-1$. We first prove there is not a vertex $F_l, 1 \leq l \leq n-1$ adjacent to T. If there is, since $F_l \rightarrow \cdots \rightarrow F_m \rightarrow T$ in $\mathcal{H}_0$, there is $F_l \rightarrow T$ in $\mathcal{H}_0$ due to the ancestral property. In this case there is a directed path $F_1 \rightarrow \cdots F_l \rightarrow T$ without vertices in $\mathbf{C}$ in $\mathcal{H}_0$, which implies that there is a possible directed path where the sub-path from F_1 to F_l is minimal and any variables on the path do not belong to $\mathbf{C}$, contradicting the result we prove above. Hence F_l cannot be adjacent to T for $\forall 1 \leq l \leq n-1$. **(i.)** If $n \geq 2$, **(i.a.)** if there $F_n \circ\!\!-\!\!* T$ or $F_n \rightarrow T$ in $\mathbb{M}_i$, there is an uncovered possible directed path comprised of $K, F_1, \cdots, F_n, T$ in $\mathbb{M}_i$ where F_1 is not adjacent to T. In this case $K \circ\!\!\rightarrow T$ has been oriented as $K \rightarrow T$ in $\mathbb{M}_i$ by $\mathcal{R}_9$ of Zhang [35] due to $\mathbb{M}_i$ is closed under the orientation rules, contradiction. **(i.b.)** If there is $F_n \leftarrow\!\!* T$ in $\mathbb{M}_i$, note the non-adjacency of T and F_{n-1}. Due to the edge $T *\!\!\rightarrow F_n$ and the complete property of $\mathbb{M}_i$, the mark at F_n on the edge between F_{n-1} and F_n is identifiable in $\mathbb{M}_i$. And due to the possible directed path, there is $F_{n-1} \rightarrow F_n$ in $\mathcal{H}_0$, there can only be $F_{n-1} \rightarrow F_n$ or $F_{n-1} \circ\!\!\rightarrow F_n$ in $\mathbb{M}_i$. The former case contradicts with Lemma 10 due to $F_{n-1} \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ and $F_n \in \mathbf{C}$. For the latter case, the edge $F_{n-1} \rightarrow F_n$ should be transformed to bi-directed edge ahead of $K \rightarrow T$, hence there cannot be an edge $F_{n-1} \rightarrow F_n$ in $\mathcal{H}_j$, contradiction. **(ii.)** If $n = 1$, there is $K \rightarrow T' \rightarrow T$ in $\mathcal{H}$, where $T' \in \mathbf{C}$. In this case if there is not $K \circ\!\!\rightarrow T'$ in $\mathbb{M}_i$, there cannot be an edge $K \rightarrow T'$ in $\mathcal{H}_j$; if there is $K \circ\!\!\rightarrow T'$ in $\mathbb{M}_i$, there is thus both $K \rightarrow T'$ and $K \rightarrow T$ in $\mathcal{H}_0$, $K \circ\!\!\rightarrow T'$ is transformed to a bi-directed edge ahead of $K \rightarrow T$ due to $T' \rightarrow T$, thereby there is not an edge $K \rightarrow T'$ in $\mathcal{H}_j$. Hence there cannot be a sub-structure $K \rightarrow T' \rightarrow T$ in $\mathcal{H}_j$, contradiction. Hence, there is always a contradiction if there is a directed path from K to T in $\mathcal{H}_j$.

(2) In this part, we prove that if there is an edge $A \rightarrow K$ in $\mathcal{H}_j$, there is $A \rightarrow T$ in $\mathcal{H}_j$; if there is $B \leftrightarrow K$ in $\mathcal{H}_j$, either $B \rightarrow T$ or $B \leftrightarrow T$ is in $\mathcal{H}_j$. Note there is $K \circ\!\!\rightarrow T$ in $\mathbb{M}_i$, where $K \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ and $T \in \mathbf{C}$.

It suffices to show that for vertex A such that $A \rightarrow K$ or $A \leftrightarrow K$ in $\mathcal{H}_j$, A is adjacent to T. Then according to the ancestral property of $\mathcal{H}_i$, we directly get the desired result due to $K \rightarrow T$ in $\mathcal{H}_j$.

We discuss the possible cases of the edge between A and K in $\mathbb{M}_i$. If there is $A{*\!\!\rightarrow} K$ in $\mathbb{M}_i$, due to the circle at K on the edge of K and T and the closed property of $\mathbb{M}_i$, A is adjacent to T. Hence the result evidently holds.

If there is $A \circ\!\!-\!\!\circ K$ in $\mathbb{M}_i$, we discuss whether $A \in \mathbf{C}$. If not, then $A \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ due to $K \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$. Suppose T is not adjacent to A, we will prove its impossibility. In this case, we orient $K \to A$ in the second step due to $T \in \mathcal{F}_K \backslash \mathcal{F}_A$, there is thus $K \to A$ in $\mathcal{H}_0$. Considering we do not transform $\to$ to $\leftarrow$ in the whole procedure, there cannot be an edge $A \to K$ in $\mathcal{H}_j$. And since only the directed edge connecting a vertex in $\mathbf{C}$ and a vertex in $\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ is possibly converted to a bi-directed edge in the process from $\mathcal{H}_0$ to $\mathcal{H}_j$, $A \leftarrow K$ is also not transformed to $A \leftrightarrow K$ due to $A, K \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$, so that $A \leftrightarrow K$ cannot be in $\mathcal{H}_j$. Hence when $A \circ\!\!-\!\!\circ K$ in $\mathbb{M}_i$ and $A \notin \mathbf{C}$, there is not an edge $A \to K$ or $A \leftrightarrow K$ in $\mathcal{H}_j$. If $A \in \mathbf{C}$, A is adjacent to T due to $T \in \mathbf{C}$ and Lemma 9. Hence the result holds when $A \in \mathbf{C}$. We conclude that if there is $A \circ\!\!-\!\!\circ K$ in $\mathbb{M}_i$, the result holds.

If there is $A \leftarrow\!\!\circ K$ in $\mathbb{M}_i$, there is $A \leftarrow K$ in $\mathcal{H}_0$. Since we do not add an arrowhead at a vertex in $\mathbf{C}$ in the process of obtaining $\mathcal{H}$ from $\mathcal{H}_0$, and only the directed edge connecting a vertex in $\mathbf{C}$ and a vertex in $\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ is possibly converted to a bi-directed edge in the process from $\mathcal{H}_0$ to $\mathcal{H}_j$, we only need to consider there is $A \leftrightarrow K$ in $\mathcal{H}_j$, where $A \in \mathbf{C}$. In this case, A is adjacent to T by Lemma 9. The result holds.

For the other cases for the edge between A and K in $\mathbb{M}_i$ except for $A{*\!\!\rightarrow} K$, $A \circ\!\!-\!\!\circ K$, and $A \leftarrow\!\!\circ K$, there cannot be an edge as $A \to K$ or $A \leftrightarrow K$ in $\mathcal{H}_j$. We thus have considered all the possible cases and conclude that if there is an edge $A \to K$ in $\mathcal{H}_j$, there is $A \to T$ in $\mathcal{H}_j$; if there is $A \leftrightarrow K$ in $\mathcal{H}_j$, either $A \to T$ or $A \leftrightarrow T$ is in $\mathcal{H}_j$ according to the balanced property.

(3) In this part, we prove that there is no discriminating path for K on which T is the endpoint adjacent to K in $\mathcal{H}_j$. The proof of this part refers to the proof of (T3) of Theorem 3 by Zhang [35], with modifications due to the additional background knowledge.

Suppose a path $p = (V_0, V_1, \cdots, V_n = K, T)$ which is a discriminating path for K. Without loss of generality, suppose p is the shortest path. According to the construction of $\text{Edge}(\mathcal{H}_0)$, there is $K {\circ\!\!\rightarrow} T$ in $\mathbb{M}_{i+1}$. We derive a contradiction by showing that p is already a discriminating path in $\mathbb{M}_i$. Hence there cannot be an edge $K {\circ\!\!\rightarrow} T$ in $\mathbb{M}_i$, otherwise if $i \geq 1$ it will be oriented as $K \to T$ by $\mathcal{R}_4'$ or if $i = 0$ it will be oriented as $K \to T$ or $K \leftrightarrow T$ by $\mathcal{R}_4$ due to the closed property of $\mathbb{M}_i$. There is $V_{n-1} \leftrightarrow K$ in $\mathcal{H}_j$, for otherwise there would be a directed path $K \to V_{n-1} \to T$ from K to T other than the edge $K \to T$ in $\mathcal{H}_j$. It follows that every edge on the subpath from V_1 to K is bi-directed in $\mathcal{H}_j$.

Next we will prove that there is an edge $V_0{*\!\!\rightarrow} V_1$ in $\mathbb{M}_i$. Suppose for contradiction, the edge is either $V_0 \circ\!\!-\!\!\circ V_1$ or $V_0 \leftarrow\!\!\circ V_1$.

(i). Suppose $V_0 \circ\!\!-\!\!\circ V_1$ in $\mathbb{M}_i$. There cannot be an edge $V_1 \leftrightarrow V_2$ in $\mathbb{M}_i$, for otherwise there is $V_0 \leftrightarrow V_2$ in $\mathbb{M}_i$ by balanced property of $\mathbb{M}_i$, which contradicts with the shortest discriminating path p. Since we do not transform a circle edge in $\mathbb{M}_i$ to a bi-directed edge, the edge between V_1 and V_2 are either $V_1 {\circ\!\!\rightarrow} V_2$ or $V_1 \leftarrow\!\!\circ V_2$. For the former case, V_0 is adjacent to V_2, for otherwise $V_0{*\!\!\rightarrow} V_1 \leftarrow\!\!* V_2$ is identifiable in $\mathcal{P}$ and $\mathbb{M}_i$ since $V_0{*\!\!\rightarrow} V_1 \leftrightarrow V_2$ in $\mathcal{H}_j$ and $\mathcal{H}_j$ is an MAG Markov equivalent to $\mathcal{H}_0$ which belongs to the MEC represented by $\mathcal{P}$, contradicting with $V_0 \circ\!\!-\!\!\circ V_1$ in $\mathbb{M}_i$. According to the balanced property of $\mathbb{M}_i$, there is $V_0{*\!\!\rightarrow} V_2$ in $\mathbb{M}_i$ thus there is $V_0{*\!\!\rightarrow} V_2$ in $\mathcal{H}_j$, in which case there is a shorter discriminating path without V_1, contradiction. For the latter case, there is $V_0 \circ\!\!-\!\!\circ V_1 \leftarrow\!\!\circ V_2$ in $\mathbb{M}_i$. As shown by the orientation procedure, we only add an arrowhead at the vertex in $\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$, and we never orient an edge as bi-directed edge in an edge connecting two vertices from $\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$, hence $V_0{*\!\!\rightarrow} V_1$ and $V_1 \leftrightarrow V_2$ cannot be oriented at the same time in the process of obtaining $\mathcal{H}$ from $\mathcal{H}_0$.

(ii). Suppose $V_0 \leftarrow\!\!\circ V_1$. Due to the fact that a bi-directed edge is oriented in $\mathcal{H}_j$ compared to $\mathbb{M}_i$ only if the edge connects a vertex in $\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ and a vertex in $\mathbf{C}$, and the fact that an arrowhead is added only at the vertex in $\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$, there is $V_0 \in \mathbf{C}$ and $V_1 \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$. And due to $T \in \mathbf{C}$ and the non-adjacency of T and V_0, there is a contradiction with the condition that $\mathbb{M}_i[\mathbf{C}]$ is complete in Lemma 9.

We conclude there is $V_0{*\!\!\rightarrow} V_1$ in $\mathbb{M}_i$. The remaining part is to prove by induction that for every $1 \leq i \leq n-1$, V_i is a collider and a parent of T in $\mathbb{M}_i$. $V_1 \to T$ is evident due to the non-adjacency of V_0 and T. Note $T \in \mathbf{C}$ and $V_1 \to T$ in $\mathbb{M}_i$, thus $V_1 \notin \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ due to $\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}]) \cap \text{Pa}(\mathbf{C}, \mathbb{M}_i) = \emptyset$ as Lemma 10. There cannot be an edge $V_1 \to V_2$ in $\mathbb{M}_i$ because the edge cannot be oriented as $V_1 \leftrightarrow V_2$ in $\mathcal{H}_j$. If there is not a collider at V_1 in $\mathbb{M}_i$, there is $V_1 \circ\!\!\rightarrow V_2$. We orient it to bi-directed edges only if $V_1 \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$, contradiction. Hence the collider is identifiable in $\mathbb{M}_i$. Similarly, we could prove $V_2 \to T$ in $\mathbb{M}_i$. Due to $T \in \mathbf{C}$ and $\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}]) \cap \text{Pa}(\mathbf{C}, \mathbb{M}_i) = \emptyset$, $V_2 \notin \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$, thus $V_1 \leftrightarrow V_2 \leftarrow\!\!* V_3$ is identifiable in $\mathbb{M}_i$ since arrowhead is added at only the vertex in $\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$. By such way, we prove that the path is a discriminating path for K in $\mathbb{M}_i$. Thus there cannot be an edge $K \circ\!\!\rightarrow T$ in $\mathbb{M}_i$, otherwise it will be oriented as $K \to T$ by $\mathcal{R}_4'$ if $i \geq 1$ and oriented as $K \to T$ or $K \leftrightarrow T$ if $i = 0$ since $\mathbb{M}_i$ is closed under the orientation rules, contradicting with the fact that there is $K \circ\!\!\rightarrow T$ in $\mathbb{M}_{i+1}$.

Hence, we conclude that $\mathcal{H}$ is an MAG Markov equivalent to $\mathcal{H}_0$. It is evident that $\mathcal{H}$ has the non-circle marks in $\mathbb{M}_{i+1}$. Since $\mathcal{H}_0$ belongs to the MEC represented by $\mathcal{P}$, $\mathcal{H}$ also belongs to the MEC. We conclude that $\mathcal{H}$ is an MAG consistent to $\mathcal{P}$ and the local BK regarding $V_1, \cdots, V_{i+1}$. The proof in this part completes.

Hence, according to the result (**A**), $\mathcal{H}_0$ can be seen as an MAG obtained from $\mathbb{M}_i$ by transforming $\circ\!\!\rightarrow$ to $\to$ and the circle component into a DAG without new unshielded colliders in $\mathbb{M}_i$. With the inverse negative proposition of the result (**B**), if $\mathcal{H}$ is not an MAG consistent to $\mathcal{P}$ and the local BK regarding $V_1, \cdots, V_{i+1}$, then $\mathcal{H}_0$ is not an MAG consistent to $\mathcal{P}$ and the local BK regarding $V_1, \cdots, V_i$, which can be obtained from $\mathbb{M}_{i-1}$ by transforming $\circ\!\!\rightarrow$ to $\to$ and the circle component into a DAG without new unshielded colliders in $\mathbb{M}_{i-1}$. Repeat the process above, we can conclude that there is a graph obtained from $\mathcal{P}$ by transforming $\circ\!\!\rightarrow$ to $\to$ and the circle component into a DAG without new unshielded colliders that is not MAG consistent to $\mathcal{P}$, which contradicts with Theorem 2 of Zhang [35]. We get the desired result. □

Lemma 15.2. *Suppose there is an edge $A \circ\!\!\rightarrow B$ in the PMG $\mathbb{M}_{i+1}$ in Thm. 1, then there is an MAG $\mathcal{M}_1$ consistent to $\mathcal{P}$ and local BK regarding $V_1, \cdots, V_{i+1}$ with $A \leftrightarrow B$.*

Proof. This part totally follows Theorem 3 of Zhang [35] with the results we have proved before. Hence we only show the sketch. We take $\mathbb{M}_{i+1}$ as the $\mathcal{P}_{AFCI}$ of Zhang [35]. Note we do not consider selection bias in this paper. Hence the cases of $\mathbf{P}_2, \mathbf{P}_3, \mathbf{P}_4$ (Lemma A.2, Lemma A.4, Lemma A.5) of Zhang [35] will not happen. And $\mathbf{P}_1$, *i.e.*, the balanced property, has been proved to hold in $\mathbb{M}_{i+1}$ according to Lemma 14. With the balanced property, Lemma B.1-Lemma B.18 of Zhang [35], which are sufficient to prove Theorem 3 of Zhang [35], also hold in $\mathbb{M}_{i+1}$ because there are not other conditions involved. As proved by Lemma 15.1, we prove that when we transform the $\circ\!\!\rightarrow$ edges to $\to$, and orient the circle component into a DAG without new unshielded colliders based on $\mathbb{M}_{i+1}$, we can always obtain an MAG consistent to $\mathcal{P}$ and local BK regarding $V_1, \cdots, V_{i+1}$. It plays the roles of Theorem 2 of Zhang [35]. We can construct a graph $\mathcal{H}$ with $A \leftrightarrow B$ by the same procedure of Theorem 3 of Zhang [35] and prove $\mathcal{H}$ is an MAG that is Markov equivalent to an MAG $\mathcal{H}_0$ obtained from $\mathbb{M}_{i+1}$ by transforming $\circ\!\!\rightarrow$ edges to $\to$ and transforming the circle component in $\mathbb{M}_{i+1}$ into a DAG $\mathcal{D}_{A \circ\!\rightarrow B}$ defined in Theorem 3. According to Lemma 15.1, $\mathcal{H}_0$ is an MAG in the MEC represented by $\mathcal{P}$. Hence $\mathcal{H}$ is an MAG in the MEC represented by $\mathcal{P}$. And since $\mathcal{H}$ has the non-circle edges in $\mathbb{M}_{i+1}$, $\mathcal{H}$ is an MAG with $A \leftrightarrow B$ consistent to $\mathcal{P}$ and local BK regarding $V_1, \cdots, V_{i+1}$. □

Theorem 1. *Given i, suppose $\mathbb{M}_s, \forall s \in \{0, 1, \ldots, i\}$ satisfies the five following properties:*

(Closed) *$\mathbb{M}_s$ is closed under the orientation rules.*

(Invariant) *The arrowheads and tails in $\mathbb{M}_s$ are invariant in all the MAGs consistent to $\mathcal{P}$ and BK regarding $V_1, \ldots, V_s$.*

(Chordal) *The circle component in $\mathbb{M}_s$ is chordal.*

(Balanced) *For any three vertices A, B, C in $\mathbb{M}_s$, 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 $A \to B$, then the edge between A and C is either $A \to C$ or $A \circ\!\!\rightarrow C$ (i.e., it is not $A \leftrightarrow C$).*

(Complete) *For each circle at vertex A on any edge $A \circ\!\!-\!\!* B$ in $\mathbb{M}_s$, there exist MAGs $\mathcal{M}_1$ and $\mathcal{M}_2$ consistent to $\mathcal{P}$ and BK regarding $V_1, \ldots, V_s$ with $A \leftarrow\!\!* B \in \mathbf{E}(\mathcal{M}_1)$ and $A \to B \in \mathbf{E}(\mathcal{M}_2)$.*

Then the PMG $\mathbb{M}_{i+1}$ obtained from $\mathbb{M}_i$ with $BK(V_{i+1})$ by Alg. 1 also satisfies the five properties.

Proof. The closed, invariant, chordal, balanced, complete properties of $\mathbb{M}_{i+1}$ are proved by Lemma 5, 6, 13, 14, 15. $\square$