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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 two applications that are of independent interests. One is that we give a maximal ancestral graph (MAG) listing algorithm, to output all the MAGs consistent to the observational data in the presence of latent variables. The other application is that we present a general active learning framework for causal discovery in the presence of latent confounders, where we propose a baseline criterion to select the intervention variable with a Metropolis-Hastings MAG-sampling method. Experiments validate the efficiency of the proposed MAG listing method and the effectiveness of the active learning framework.

1. Introduction

Causality has garnered significant attention in recent years due to its applications in various fields such as decision-making [1–4], fairness [5,6], and anomaly diagnosis [7,8]. Moreover, it has also served as a source of inspiration for machine learning studies in open environments [9], given its ability to capture the invariant underlying mechanisms of the physical world [10,11]. In Pearl's causality framework [12], an important problem is *causal discovery*, *i.e.*, learning the causal graph to represent causal relations among the variables [13–17]. However, identifying all causal relations solely from observational data is generally infeasible, unless we make some additional assumptions [18–20] or exploit the abundant information in multiple or dynamic environments [21,22].

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, additional causal relations can be learned from interventional data [23–31]. Also, if certain variables in the causal discovery task are well-understood by humans, their expertise can be helpful [32]. For example, if we are studying the causal relations among some variables including sales and prices, the causal relations such as price causes sales can be obtained directly based on human expertise.

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When BK is available in addition to observational data, a fundamental problem is: *what causal relations are identifiable in the presence of latent variables*? It 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 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, since it must be proved that there does not exist any unidentified "common causal relations" among *all the causal graphs* consistent to the observational data and BK. Unfortunately, the problem remains open.

In this paper, we solve the problem with *sound* and *complete* orientation rules when BK is given in a *local* form. In the presence of latent variables, a partial ancestral graph (PAG) can be learned by FCI algorithm from observational data [33–35]. PAG can imply the *existence* of causal relation between any two variables but not necessarily the causal *direction*. We say *BK is local* given a PAG, 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. For example, when we obtain a PAG $\mathcal{P}$ with observational data that has some indeterminate causal relations, a conventional method to reveal them is to introduce active intervention on some variable X [36,23,25]. In this case, for each edge $X \circ\!\!\to\!* V$ in $\mathcal{P}$, we can determine $X \leftarrow\!* V$ or $X \to\!* V$ by testing whether $P(V|do(X=x)) = P(V)$. Local BK can be obtained from human expertise as well. For instance, if a PAG $\mathcal{P}$ implies the existence of causal relations between price and sales, number of customers, and inventory, it is widely recognized among business professionals that price causes sales and the number of customers, but not inventory. Given a PAG and local BK, we propose a set of orientation rules to determine some causal directions in the PAG. Under the assumption of absence of selection bias, we prove that the rules are sound and complete, which means that all the identifiable causal relations given available information are *exactly* those determined by the proposed rules, thus closing the problem given local BK.

The establishment of complete orientation rules compatible with local BK inspires two (theoretical) applications. One is that we propose a method to list all the *maximal ancestral graphs (MAG)*[1] consistent to a PAG $\mathcal{P}$. The method is useful in many real applications, such as identifying possible causal effects in a PAG [37–39] or causal graph sampling [23,40]. It can also help verifying some PAG-related theoretical results or methods [41–43]. There have been mature methods for efficient *directed acyclic graph* listing [44], but it remains unknown for MAGs. A key result we build is the *necessary and sufficient* conditions for the existence of MAGs consistent to $\mathcal{P}$ with a given local structure, through which we can find all the MAGs efficiently by determining all the local structure of each vertex recursively.

The other application is that we present the first general active learning framework for identifying an MAG with active interventions. Bringing active learning into causal discovery has been shown successful for causal DAGs [23,45,46], but actively discovering MAGs remains untouched due to the lack of complete orientation rules, which are exactly what we present in this paper. Therefore, our work lays the theoretical foundations for, and propose the first active learning framework for discovering MAGs. In light of the expensive cost of interventions, we hope to identify an MAG with as fewer interventions as possible. Hence we present a baseline maximal entropy criterion, equipped with Metropolis-Hastings MAG-sampling, to select the intervention variable.

Overall, our contributions in this paper are threefold:

(1) We present the sound and complete orientation rules for causal identification given local background knowledge in the presence of latent confounders.
(2) We propose an efficient method to list MAGs consistent to a PAG.
(3) We give the first active learning framework for causal discovery that is applicable when latent variables exist.

A preliminary version of this work appeared in a conference paper [40]. Compared with the original version, we propose an additional efficient MAG listing method. We present the necessary and sufficient conditions for the existence of MAGs consistent to a PAG with a given local structure, through which we can find all the MAGs by determining local structure recursively. In addition, we improve the Metropolis-Hastings MAG-sampling method in the active learning framework such that all the sampled MAGs by the method in this paper are valid MAGs. We also conduct more experiments to validate the effectiveness and efficiency of our method.

Related works. In the literature, Meek [47] established sound and complete rules, generally called *Meek rules*, for causal identification given BK under causal sufficiency assumption. The assumption requires that there are no latent variables that cause more than one observed variable simultaneously. Causal sufficiency is untestable in practice. And it is quite often that there are latent variables in many real tasks. Jaber et al. [29] investigated the complete algorithm to learn a graph with solid results when there are additional interventional distribution, where the *exact* interventional distribution is needed. In this paper, BK is in the form of local marks. As shown by Jaber et al. [29], Wang and Zhou [30], the learned marks by exact interventional distribution can be beyond the local marks. Andrews et al. [48] showed that FCI algorithm is complete given *tiered* BK, where all variables can be partitioned into disjoint sets with explicit causal order. Tiered BK is totally different from local BK. We discuss it at the end of Section 3.

[1] MAG is generally used to represent causal relations when there are latent variables.

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 (of G) 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 $G_{\mathbf{V}\setminus\mathbf{V}'}$ induced by $\mathbf{V}\setminus\mathbf{V}'$. 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 $0 \le i \le n-1$, 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. V_i and V_j are in a *connected circle component* in G if they are connected in the circle component in G. A *circle path* is a path comprised of only circle edges. 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 close to V_i and without a tail at the mark close to V_j 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 $\mathrm{Pa}(V_i, G)$/$\mathrm{Anc}(V_i, G)$/$\mathrm{PossAn}(V_i, G)$/$\mathrm{De}(V_i, G)$/$\mathrm{PossDe}(V_i, G)$. If $V_i \in \mathrm{Anc}(V_j, G)$ 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 we say an edge is in the form of $\circ\!\!-\!\!*$, 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. Denote the set of vertices adjacent to V_i in G by $\mathrm{Adj}(V_i, G)$. Consider a graph G comprised of only circle edges, a vertex V_i in G is called *simplicial* if $\mathrm{Adj}(V_i, G)$ induces a complete subgraph of G, and a *perfect elimination order* of G is an ordering $\sigma = (V_1, \ldots, V_n)$ of its vertices such that each vertex V_i is a simplicial vertex in the induced subgraph $G_{\{V_i,\ldots,V_n\}}$.

A non-endpoint V_i is a collider on a path p if p contains $*\!\!\rightarrow V_i \leftarrow\!\!*$. A path p from V_i to V_j is a *collider path* if $p = \langle V_i, V_j\rangle$ or all the non-endpoints are colliders. 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. p is a *minimal possible directed path* if p is minimal and possible directed. p is a *minimal circle path* if p is minimal and a circle path.

A mixed graph is an *ancestral graph* if there is no directed or almost directed cycle (since we assume no selection bias, there are no undirected edges). 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 from X to 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.

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 $\mathbb{M}$ (with respect to $\mathcal{P}$)* if (1) the non-circle marks in $\mathbb{M}$ are also in $\mathcal{M}$, and (2) $\mathcal{M}$ is in the MEC represented by $\mathcal{P}$. Note the PAG $\mathcal{P}$ is needed in the second condition above. We omit $\mathcal{P}$ and just say $\mathcal{M}$ consistent to $\mathbb{M}$ for brevity because in the whole paper a PAG $\mathcal{P}$ is given throughout. An MAG $\mathcal{M}$ *is consistent to the BK* if $\mathcal{M}$ is with the orientations represented 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 BK, where $\mathcal{P}$ can be obtained by, for example, applying the FCI algorithm with observational data [13,35]. Denote $\mathbf{V}(\mathcal{P}) = \{V_1, V_2, \cdots, V_d\}$. We present the definition of local BK in Definition 1.

Definition 1 *(local BK).* Given a PAG $\mathcal{P}$ and BK, a circle in $\mathcal{P}$ is *accessible* if the BK can directly indicate an arrowhead or tail here. BK is *local* if there exists $\mathbf{V} \subseteq \mathbf{V}(\mathcal{P})$ such that for any vertex $V \in \mathbf{V}$, all the circles at V in $\mathcal{P}$ are accessible and for any $V \in \mathbf{V}(\mathcal{P})\setminus\mathbf{V}$, no circle at V is accessible.

In this section, we make a convention that the term BK refers to local BK in Definition 1. We assume the absence of selection bias[2] and the correctness of BK. 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. All the proofs for the results in this section are presented in Section 3.2.

3.1. Our results

First, we show the orientation rules to incorporate local BK into a PAG that has been learned with observational data. They are proposed with one replacement[3] and one addition based on the rules of Zhang [35] for learning a PAG. We do not list all of them here but only 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 $A -\!\!\circ B$, then $A \rightarrow B$.

We present Proposition 1 to imply the soundness of $\mathcal{R}_4'$ to orient a PAG $\mathcal{P}$ or a PMG obtained from $\mathcal{P}$ with local BK incorporated. $\mathcal{R}_{11}$ is immediate from no selection bias assumption. In this paper, we make a convention that when we say the orientation rules, they refer to $\mathcal{R}_1 - \mathcal{R}_3, \mathcal{R}_8 - \mathcal{R}_{10}$[4] 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.

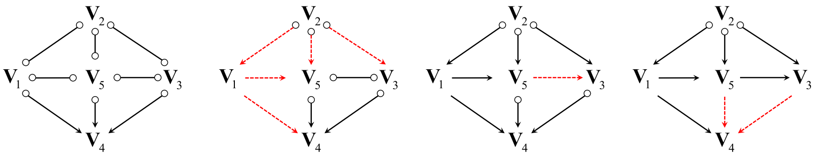
Proposition 1. *Given a PAG $\mathcal{P}$, for any PMG $\mathbb{M}$ that is obtained from $\mathcal{P}$ with part of local BK incorporated (or $\mathbb{M} = \mathcal{P}$), $\mathcal{R}_4'$ is sound to orient $\mathbb{M}$.*

Next, we will prove the completeness of the proposed orientation rules. It is somewhat complicated. We first give a roadmap for the proof idea. 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 complete algorithm orients the same marks as the proposed orientation rules. Combining these two parts, we conclude that the orientation rules are sound and complete to orient a PAG with local BK. The construction of the algorithm along with the proof of the algorithm completeness in the first step is the most difficult part. In this part, 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, where $BK(V_{i+1})$ denotes all the marks at V_{i+1} indicated by BK. To obtain the updated graph in each step, we propose an algorithm orienting a PMG with local BK regarding one variable. Repeat this process of 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.

We present Algorithm 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 $\mathbf{C}(X) = \{V \in \mathbf{V}(\mathcal{P}) \mid V *\!\!\rightarrow X \in BK(X)\}$ to denote the vertices whose edges with X will be oriented to ones with arrowheads at X according to $BK(X)$. For simplicity, and considering that the variable which the local BK is regarding will always be specified in the following, we will use $\mathbf{C}$ to represent $\mathbf{C}(X)$ hereafter. It is direct that $\mathbf{C}$ can represent the local BK regarding X. In $\mathbb{M}_{i+1}$, there is $X \leftrightarrow\!* V$ for $V \in \mathbf{C}$ and $X -\!* V$ for $V \in \{V \in \mathbf{V}(\mathcal{P}) \mid V *\!\!-\!\circ X \text{ in } \mathbb{M}_i\} \backslash \mathbf{C}$ according to $BK(X)$. Since some marks of X are incorporated as local BK regarding X, we can orient some edges further.

In the first step of Algorithm 1, the orientation of the marks at X follows $BK(X)$, and the orientation of the vertices apart of X is motivated as the necessary condition for the ancestral property. Speaking roughly, we orient $K \leftrightarrow\!* T$ in the first step for otherwise no matter how we orient the other circles, there will be a directed or almost directed cycle if there is $K \rightarrow T$, unless we introduce new unshielded colliders which take new conditional independence relative to $\mathcal{P}$, both of which are evidently invalid to obtain an MAG in the MEC represented by $\mathcal{P}$. Since some additional arrowheads are introduced in the first step, they can lead to some other circles identification. To characterize them, we define $\mathcal{F}_{V_l}^{\mathbb{M}_i} = \{V \in \mathbf{C} \cup \{X\} \mid V *\!\!-\!\circ V_l \text{ in } \mathbb{M}_i\}$ for any $V_l \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}]) \backslash \{X\}$, 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. 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 $\mathcal{P}$. The third step orients some other circles based on the updated structure.

[2] In general, MAG can contain undirected edges in the case of selection bias. Since in this paper we assume the absence of such bias, the term MAG only refers to *directed MAG*, which does not contain undirected edges.
[3] $\mathcal{R}_4$ is necessary for learning a PAG with observational data. We replace $\mathcal{R}_4$ with $\mathcal{R}_4'$ when we incorporate local BK *after* we have learned a PAG.
[4] $\mathcal{R}_5 - \mathcal{R}_7$ are not considered as they are not triggered in the absence of selection bias.



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

Fig. 1. An example to demonstrate the implementation of each step of Algorithm 1. Fig. 1(a) depicts a PMG $\mathbb{M}_i$. Suppose the local BK is in the form of $V_1 \leftarrow\!\ast V_2, V_1 -\!\ast V_5, V_1 -\!\ast V_4$. The Fig. 1(b)/ 1(c)/ 1(d) displays the graph obtained after the first/second/third step of Algorithm 1. The edges oriented by each step are denoted by red dashed lines. (For interpretation of the colors in the figure(s), the reader is referred to the web version of this article.)

Algorithm 1 Update a PMG with local BK of X represented by $\mathbf{C}$.

input: A PMG $\mathbb{M}_i$, $BK(X)$ represented by $\mathbf{C}$

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

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

Example 1. Consider the example in Fig. 1. Suppose the input PMG $\mathbb{M}_i$ in Algorithm 1 is the graph in Fig. 1(a). And there is local BK regarding $X = V_1$ in the form of $V_1 \leftarrow\!\ast V_2, V_1 -\!\ast V_5, V_1 -\!\ast V_4$. Hence $\mathbf{C} = \{V_2\}$. In this case, $\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}]) = \text{PossDe}(V_1, \mathbb{M}_i[-V_2]) = \{V_1, V_3, V_4, V_5\}$. And $\mathcal{F}_{V_3} = \{V_2\}$, $\mathcal{F}_{V_4} = \emptyset$, $\mathcal{F}_{V_5} = \{V_1, V_2\}$. We will first illustrate the implementation of each step of Algorithm 1, then discuss the reasons behind these orientations. When implementing Algorithm 1, in the first step, the edges denoted by red dashed lines in Fig. 1(b) are oriented. $V_1 \leftarrow\!\circ V_2/V_1 \rightarrow V_5/V_1 \rightarrow V_4$ is oriented due to $V_1 = X, V_2 \in \mathbf{C}, \{V_4, V_5\} \subseteq \{V \in \mathbf{V}(\mathcal{P}) \mid V \ast\!\!-\!\!\circ X \text{ in } \mathbb{M}_i\} \backslash \mathbf{C}$. $V_2 \circ\!\!\rightarrow V_5/V_2 \circ\!\!\rightarrow V_3$ is oriented due to $V_2 \in \mathbf{C}$ and $V_3, V_5 \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$. In the second step of Algorithm 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 $V_3, V_5 \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$; (2) $\mathcal{F}_{V_3} = \{V_2\} \subset \{V_1, V_2\} = \mathcal{F}_{V_5}$. In the third step of Algorithm 1, the edges denoted by red dashed lines in Fig. 1(d) are oriented by $\mathcal{R}_1$.

We next briefly discuss the reasons behind the orientations in the first two steps of Algorithm 1. The explanations are not strictly chronological. It is direct that $V_1 \leftarrow\!\circ V_2/V_1 \rightarrow V_5/V_1 \rightarrow V_4$ is oriented in the first step according to the local BK and $\mathcal{R}_{11}$. In this case, as there is $V_1 \in \mathcal{F}_{V_5} \backslash \mathcal{F}_{V_3}$, if $V_3 \ast\!\!\rightarrow V_5$, they form an additional unshielded collider with $\mathcal{F}_{V_5} \backslash \mathcal{F}_{V_3}$, *i.e.*, $V_1 \rightarrow V_5 \leftarrow\!\ast V_3$, which is not allowed. Hence there can only be $V_5 \rightarrow V_3$, which is oriented in the second step of Algorithm 1. The orientation $V_2 \circ\!\!\rightarrow V_5/V_2 \circ\!\!\rightarrow V_3$ follows the ancestral property. We take $V_2 \circ\!\!\rightarrow V_3$ for an example. If there is $V_2 \leftarrow V_3$, there is $V_2 \circ\!\!\rightarrow V_1 \rightarrow V_5 \rightarrow V_3 \rightarrow V_2$, which violates the ancestral property.

Then, we present the key induction result in Theorem 1 for the graph obtained by Algorithm 1 in each step. Based on Theorem 1, we conclude the completeness of the k-step algorithm to orient the PAG with the local BK regarding $V_1, \ldots, V_k$ in Corollary 1.

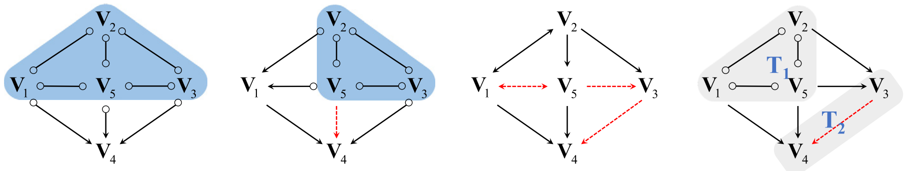
Theorem 1. *Given a positive integer i, for any $s \in \{0, 1, \ldots, i\}$, we iteratively obtain $\mathbb{M}_{s+1}$ from $\mathbb{M}_s$ by incorporating $BK(V_{s+1})$ with Algorithm 1 ($\mathbb{M}_0 = \mathcal{P}$). Suppose $\mathbb{M}_s, \forall s \in \{0, 1, \ldots, i\}$, satisfies the five following 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 $A \leftarrow\!\ast B \in \mathbf{E}(\mathcal{M}_1)$ and $A \rightarrow B \in \mathbf{E}(\mathcal{M}_2)$.*

Then the PMG $\mathbb{M}_{i+1}$ also satisfies the five properties.

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 an MAG with an arrowhead and an MAG with a tail here that are consistent to $\mathcal{P}$ and BK regarding $V_1, \ldots, V_k$.*

Till now, we have proved the completeness of the k-step algorithm based on Algorithm 1 to orient a PAG with local BK. Finally, we present Theorem 2 to show the completeness of the orientation rules, by proving that the orientation rules orient the same marks as the complete k-step algorithm.



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

Fig. 2. Fig. 2(a) depicts a PAG $\mathcal{P}$, with $BK(V_1)$ in the form of $V_1 \leftarrow\!\!* V_2, V_1 \leftarrow\!\!* V_5, V_1 -\!\!* V_4$ and $BK(V_2)$ in the form of $V_2 \leftarrow\!\!* V_1, V_2 -\!\!* V_3, V_2 -\!\!* V_5$. Fig. 2(b)/Fig. 2(c) depicts the PMG obtained from $\mathcal{P}/\mathbb{M}_1$ by incorporating $BK(V_1)/BK(V_2)$, where the circle component is denoted by shaded area and the edges oriented by the orientation rules are denoted by red dashed lines. Fig. 2(d) depicts the obtained graph from $\mathcal{P}$ by incorporating the tiered BK partitioning the whole variables into two subsets T_1 and T_2, denoted by shaded area, and with an order where T_1 precedes T_2.

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

Example 2. We give an example to illustrate the k-step algorithm based on Algorithm 1 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 Algorithm 1 and then obtaining $\mathbb{M}_2$ from $\mathbb{M}_1$ with $BK(V_2)$ by Algorithm 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 Theorem 1. Note if we do not consider $\mathcal{R}'_4$, the edge colored red in Fig. 2(b) cannot be oriented.

Discussion Finally, we present a detailed discussion about the difference between local and tiered BK proposed by Andrews et al. [48]. BK is tiered if the variables can be partitioned into two or more mutually exclusive and exhaustive subsets among which there is a known causal order. Local BK and tiered BK focus on totally different aspects of graphs. Roughly speaking, local BK introduces the *fully* structural information of some *specific variables*, while tiered BK introduces the information about the rough causal order of the *whole variables*. Fig. 2(d) shows an example of tiered BK incorporated to the PAG in Fig. 2(a), which partitions the whole variables $V_1, \cdots, V_5$ into two subsets $T_1 = \{V_1, V_2, V_5\}$ and $T_2 = \{V_3, V_4\}$. The tiered BK implies that for any two vertices $A \in T_1$ and $B \in T_2$, there is $A \to B$ if A is adjacent to B. Andrews et al. [48] proved that FCI algorithm is complete to incorporate tiered BK into a PAG. Thus the edge $V_3 \to V_4$ can be identified additionally and the obtained graph is the most informative. In this example, the BK is not local since it just implies the transformation of a part of circles at V_1. Hence tiered BK is not necessarily local. The converse is not true as well. In a PAG shown in Fig. 2(a), $BK(V_1)$ is local but not tiered.

3.2. Proofs for Section 3.1

3.2.1. Proof of Proposition 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. [49] that Markov equivalent MAGs have the same minimal collider paths. Hence the corresponding path of p in $\mathcal{P}$ is also a collider path. □

Proof of Proposition 1. Suppose there is a discriminating path $\langle K, \ldots, A, B, R\rangle$ 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 $A \to R$, the edge between A and B can only be $A \leftrightarrow B$ due to the ancestral property. Hence, there is a collider path $p : K *\!\!\rightarrow \cdots \leftrightarrow A \leftrightarrow B \leftrightarrow R$. If this collider path is minimal, 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. If p is not a minimal collider path from K to R, there is a subpath p_1 that is a minimal collider path from K to R. Note **(1)** for any non-endpoint V in the subpath from K to B of p, there is $V \to R$; **(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 $\langle K, \ldots, B, R\rangle$. According to Lemma 1, $B \leftarrow\!\!* R$ is identifiable in $\mathcal{P}$, thus $B \leftarrow\!\!* R$ in $\mathbb{M}$, contradiction. We conclude the impossibility of the violation of $\mathcal{R}'_4$. □

3.2.2. Proof of Theorem 1

Since the proof of Theorem 1 is complicated, we just show a proof sketch here. A detailed version is given in Appendix B.

Proof sketch of Theorem 1. For brevity, we denote V_{i+1} by X. **(A)** The closed property follows the third step of Algorithm 1.**(B)** The invariant property holds because all the orientations in Algorithm 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 presented by Lemma 13 that only the first two steps of Algorithm 1 possibly introduce new arrowheads, while the third step will only transform the edges as $A \circ\!\!\rightarrow B$ to $A \rightarrow B$. 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 $\bar{\mathbb{M}}_{i+1}[\mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])]$ and in $\bar{\mathbb{M}}_{i+1}[-\mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])]$ are chordal, respectively. Since there are no circle edges connecting $\mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ and $\mathbf{V}\backslash\mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ (otherwise, it will have been oriented in the first step of Algorithm 1), we conclude the desired result. **(D)** The balanced property of $\mathbb{M}_{i+1}$ is proved based on three facts that (1) in Algorithm 1, if we transform a circle to arrowhead at V, then $V \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$; (2) if there is $A \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ and $A \circ\!\!-\!\!* B$, $B \notin \mathbf{C}$, in $\mathbb{M}_{i+1}$, then $B \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$; (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 $\mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$. **(E)** The completeness property is proved by showing two results: (1) for all the edges in the form of $A \circ\!\!-\!\!\circ B$ and $C \circ\!\!\rightarrow D$ in $\mathbb{M}_{i+1}$, $C \circ\!\!\rightarrow D$ can be transformed to $C \rightarrow D$ and $A \circ\!\!-\!\!\circ B$ 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 $C \circ\!\!\rightarrow D$ can be oriented as $C \leftrightarrow D$ 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 graph obtained from $\mathbb{M}_{i+1}$ by transforming the edges as $C \circ\!\!\rightarrow D$ to $C \rightarrow D$ and the circle component into a DAG without new unshielded colliders is an MAG consistent to $\mathcal{P}$ and local BK regarding $V_1, \ldots, V_{i+1}$. If not, we can always find a graph obtained from $\mathbb{M}_i$ by transforming the edges as $C \circ\!\!\rightarrow D$ to $C \rightarrow D$ and the circle component into a DAG without new unshielded colliders that is not an MAG consistent to $\mathcal{P}$ and local BK regarding $V_1, \ldots, V_i$. By induction, a graph obtained from $\mathcal{P}$ by transforming the edges as $C \circ\!\!\rightarrow D$ to $C \rightarrow D$ and the circle component into a DAG without new unshielded colliders is not an MAG consistent to $\mathcal{P}$, contradiction with Thm. 2 of Zhang [35]. □

3.2.3. Proof of Corollary 1

Proof. Previous studies [34,35] showed that the last four properties in Theorem 1 are fulfilled for 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 as no orientation rules of Zhang [35] can lead to such a structure. Hence $\mathcal{P}$ satisfies the five properties. With the induction step implied by Theorem 1, we directly conclude that $\mathbb{M}_k$ satisfies the five properties, thereby satisfying the invariant and complete property. □

3.2.4. Proof of Theorem 2

Proof. The soundness of $\mathcal{R}_4'$ is shown by Proposition 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. The main part is to prove the completeness.

According to Corollary 1, it suffices to prove that in each step of Algorithm 1, the orientations in Algorithm 1 either follow $BK(X)$ directly, or can be achieved by the orientation rules. The second step of Algorithm 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 $F = V_m$ 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. In the first step, $X \leftarrow\!\!* V$ for $V \in \mathbf{C}$ is represented 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 $X -\!\!* V$ represented by $BK(X)$ and $\mathcal{R}_{11}$. The only remaining part is to prove for $K \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])\backslash\{X\}$ and $T \in \mathbf{C}$, if there is $K \circ\!\!-\!\!* T$ in $\mathbb{M}_i$, $K \leftarrow\!\!* T$ can be oriented by the orientation rules when we incorporate $BK(X)$.

Due to $K \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])\backslash\{X\}$, there is a possible directed path from X to K that does not go through $\mathbf{C}$. According to Lemma 2, 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 $\mathbf{C}$ in $\mathbb{M}_i$. According to $\mathcal{R}_1$ and $\mathcal{R}_{11}$, there is always $X \rightarrow F_1 \rightarrow \cdots \rightarrow F_t$ by the orientation rules after incorporating $BK(X)$. 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 $F_{m-s}, F_{m-s+1}, \ldots, F_{m+l}, T$, $1 \leq s \leq m, 1 \leq l \leq t-m$, 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. Since p is possibly directed, the UC is at either **(i)** F_{m+l} or **(ii)** T (*i.e.*, $*\!\!\rightarrow F_{m+l}($ or $T) \leftarrow\!\!*$). **(i)** If there is a UC at F_{m+l}, $T *\!\!\rightarrow F_{m+l} \leftarrow\!\!* F_{m+l-1}$ is 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 $K \leftarrow\!\!* T$ in $\mathcal{P}$, because there is not an MAG with $K \rightarrow T$ which contains an (almost) directed cycle $F_{m+l} \rightarrow \cdots \rightarrow F_t \rightarrow T *\!\!\rightarrow F_{m+l}$. Hence $K \leftarrow\!\!* T$ is in $\mathbb{M}_i$, contradicting with $K \circ\!\!-\!\!* T$ in $\mathbb{M}_i$. **(ii)** If there is a UC at T. $F_{m-s} *\!\!\rightarrow T \leftarrow\!\!* F_{m+l}$ 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 a possible directed path, $F_{m-s} \rightarrow T$ is identified in $\mathcal{P}$ (otherwise $\mathcal{R}_9$ applies). In this case there is $F_{m-s} \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}]) \cap \mathrm{Pa}(\mathbf{C}, \mathbb{M}_i)$, which contradicts with Lemma 10 in Appendix B. Hence there is always a contradiction if there is some F_m not adjacent to T. The fact that there is not $F_m \rightarrow T$ also directly follows Lemma 10.

Finally, since F_1 is adjacent to T, and $T{*\!\!\rightarrow} X \rightarrow F_1$ is oriented according to $BK(X)$, according to $\mathcal{R}_2$, there is always $T{*\!\!\rightarrow} F_1$ after incorporating the local BK with the orientation rules. Consider $T{*\!\!\rightarrow} F_1 \rightarrow F_2$, there is also $T{*\!\!\rightarrow} F_2$ oriented. We can prove by induction that $T{*\!\!\rightarrow} F_t(=K)$ can be oriented by orientation rules. □

4. Application 1: MAG listing

In this section, based on the theoretical result for the complete causal identification given local BK, we propose a method to list all the MAGs consistent to a given PAG $\mathcal{P}$. Suppose $\mathbf{V}(\mathcal{P}) = \{V_1, V_2, \cdots, V_d\}$. All the proofs for the results in this section are presented in Section 4.2.

4.1. Proposed method

The idea of our method is to transform the circles of each vertex in $\mathcal{P}$ recursively. In each step, we determine all the *valid local transformations* of *one* vertex with circles, where a *local transformation* denotes a kind of transformation of all the circles at this vertex, and a local transformation is said to be *valid* if there exists an MAG consistent to $\mathcal{P}$ that has the non-circle marks in the graph obtained by the local transformation. For any valid local transformation, it is incorporated as a local BK to the partial graph with the complete orientation rules. We recursively execute local transformations of each vertex with circles until all the circles are transformed (to non-circles).

The most crucial part in our method is to determine all the valid local transformation of a vertex. This problem is challenging, because it is unknown under what conditions of the local transformations there exist MAGs consistent to $\mathcal{P}$ that can be obtained by the local transformations, and it is even unclear whether there is such a condition. In fact, it is strongly related to the complete causal identification result in Section 3, especially Algorithm 1 which orients a PMG with local BK. Both local BK and local transformation directly implies and only directly implies all the marks of one vertex. The difference is, when we incorporate local BK in Section 3, Algorithm 1 can always be executed due to the soundness of Algorithm 1 and the correct BK assumption which ensures that there exist MAGs consistent to $\mathcal{P}$ and BK. Here, however, since it is unknown whether a local transformation is valid, it is possible that we generate (almost) directed cycles or new unshielded colliders when we incorporate the local transformation by Algorithm 1, which implies the invalidity of the local transformation. Hence, for a given local transformation, if it is valid, then there should not be (almost) directed cycles or new unshielded colliders generated by Algorithm 1. On the other hand, if for a local transformation we do not generate (almost) directed cycles or new unshielded colliders by Algorithm 1, then the graph obtained by Algorithm 1 fulfills the five properties in Theorem 1 (with some necessary modifications), thus an MAG with the local transformation consistent to $\mathcal{P}$ can be obtained by the similar procedure in Lemma 16.1 in Appendix B. Based on this idea, we build the necessary and sufficient conditions for the existence of MAGs with each local transformation in Theorem 3, which can be determined in $\mathcal{O}(d^3)$. Before showing it, we introduce a graphical characterization, *bridged*, in Definition 2 for the feasibility of Step 2 of Algorithm 1 for the local transformation represented by $\mathbf{C}$. An illustration for introducing bridged is detailed in Example 3.

Definition 2 *(Bridged relative to* $\mathbf{V}'$ *in* H*).* Let H be a partial mixed graph. Denote G a subgraph of H induced by a set of vertices $\mathbf{V}$. Given a set of vertices $\mathbf{V}'$ in H that is disjoint of $\mathbf{V}$, two vertices A and B in the circle component of G are *bridged relative to* $\mathbf{V}'$ if in each minimal circle path $A(=V_0) \circ\!\!-\!\!\circ V_1 \circ\!\!-\!\!\circ \cdots \circ\!\!-\!\!\circ V_n \circ\!\!-\!\!\circ B(=V_{n+1})$ from A to B in G, there exists one vertex $V_s, 0 \leq s \leq n+1$, such that $\mathcal{F}_{V_i} \subseteq \mathcal{F}_{V_{i+1}}, 0 \leq i \leq s-1$ and $\mathcal{F}_{V_{i+1}} \subseteq \mathcal{F}_{V_i}, s \leq i \leq n$, where $\mathcal{F}_i = \{V \in \mathbf{V}' \mid V *\!\!-\!\!\circ V_i \text{ in } H\}$. Evidently, both case $A = B$ and case that A and B are not connected in the circle component are the trivial cases when A and B in G are bridged relative to $\mathbf{V}'$. Further, G is *bridged relative to* $\mathbf{V}'$ *in* H if any two vertices in the circle component of G are bridged relative to $\mathbf{V}'$.

Remark 1. $\mathcal{F}_{V_i} \subseteq \mathcal{F}_{V_{i+1}}$ in Definition 2 can be seen as that vertex V_{i+1} is at a *higher or the same* altitude than V_i. Hence "*bridged*" describes that the path is like a bridge in reality, which goes up then down. Note that it is also valid if the bridge goes towards only one direction.

Example 3. When we try to orient a PMG with a local transformation by Algorithm 1, bridged is introduced as a graphical characterization to describe that no new unshielded colliders will be introduced in the second step when some necessary arrowheads are introduced in the first step. See Fig. 3 for examples. Fig. 3(a) depicts a PAG $\mathcal{P}$. If the local transformation of X is represented by $\mathbf{C} = \{V_1\}$, $V_1 {\circ\!\!\rightarrow} V_2$ is oriented in the first step of Algorithm 1, for otherwise there is a (almost) directed cycle $V_1 {\circ\!\!\rightarrow} X \rightarrow V_2 \rightarrow V_1$. The arrowhead at V_2 on $V_1 {\circ\!\!\rightarrow} V_2$ is introduced in the first step. The second step of Algorithm 1 will orient $V_2 \rightarrow V_3 \rightarrow V_4$ as Fig. 3(b), which does not introduce new unshielded colliders. According to Definition 2, $\mathcal{P}[V_2, V_3, V_4]$ is bridged relative to $\{X, V_1\}$, as for any circle path, such as $V_2 \circ\!\!-\!\!\circ V_3 \circ\!\!-\!\!\circ V_4$, there is $\mathcal{F}_{V_2} = \{X, V_1\}, \mathcal{F}_{V_3} = \mathcal{F}_{V_4} = \{X\}$, which follows that $\mathcal{F}_{V_2} \supset \mathcal{F}_{V_3} = \mathcal{F}_{V_4}$ and thus the circle path is bridged. If we consider the local transformation represented by $\mathbf{C} = \{V_1, V_4\}$, $V_1 {\circ\!\!\rightarrow} V_2$ and $V_3 \leftarrow\!\!\circ V_4$ are introduced in the first step. There is always a new unshielded collider at V_2 or V_3 no matter how we transform $V_2 \circ\!\!-\!\!\circ V_3$ as Fig. 3(c). In this case, $\mathcal{P}[V_2, V_3]$ is not bridged relative to $\{X, V_1, V_4\}$, since V_2 and V_3 are not bridged due to the minimal circle path $V_2 \circ\!\!-\!\!\circ V_3$, where $\mathcal{F}_{V_2} = \{X, V_1\}, \mathcal{F}_{V_3} = \{X, V_4\}$.

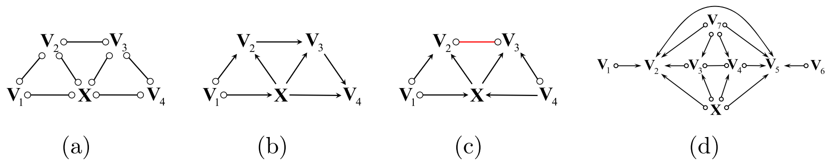


Fig. 3. (a)-(c): graphs considered in Example 3. (d): a graph where the first two conditions of Theorem 3 hold but the third one does not.

Algorithm 2 MagList.

input: A PAG $\mathcal{P}$

$\mathcal{S} = \emptyset$ // Record all the MAGs consistent to $\mathcal{P}$
OrientGraph($\mathcal{P}, \mathcal{S}$)
function OrientGraph($\mathbb{M}, \mathcal{S}$)
  if there are no circles in $\mathbb{M}$ **then**
    $\mathcal{S} \leftarrow \mathcal{S} \cup \{\mathbb{M}\}$
  else
    Select a variable X where there is a circle in $\mathbb{M}$
    $\mathbf{R} = \{V \in \mathbf{V}(\mathbb{M}) \mid X \circ\!\!\rightarrow\!\!* V \text{ in } \mathbb{M}\}$
    for each set $\mathbf{C} \subseteq \mathbf{R}$ **do**
      if the three condition in Theorem 3 are fulfilled **then**
        Update $\mathbb{M}$ with the local transformation represented by $\mathbf{C}$ and apply orientation rules
        OrientGraph($\mathbb{M}, \mathcal{S}$)
      end if
    end for
  end if
end function

output: $\mathcal{S}$

Theorem 3. *Denote $\mathbb{M}$ the obtained graph after some valid local transformations*[5] *from a PAG $\mathcal{P}$ with the orientation rules, and X a variable with circles in $\mathbb{M}$. Given a set $\mathbf{C} \subseteq \{V \mid X \circ\!\!\rightarrow\!\!* V \text{ in } \mathbb{M}\}$, there exists an MAG $\mathcal{M}$ consistent to $\mathbb{M}$ with $X \leftarrow\!\!* V$ for $\forall V \in \mathbf{C}$ and $X \twoheadrightarrow\!\!* V$ for $\forall V \in \{V \mid X \circ\!\!\rightarrow\!\!* V \text{ in } \mathbb{M}\} \backslash \mathbf{C}$ if and only if*

(1) $\mathrm{PossDe}(X, \mathbb{M}[-\mathbf{C}]) \cap \mathrm{Pa}(\mathbf{C}, \mathbb{M}) = \emptyset$;
(2) *the subgraph $\mathbb{M}[\mathbf{C}]$ of $\mathbb{M}$ induced by $\mathbf{C}$ is a complete graph;*
(3) $\mathbb{M}[\mathrm{PossDe}(X, \mathbb{M}[-\mathbf{C}]) \backslash \{X\}]$ *is bridged relative to $\mathbf{C} \cup \{X\}$ in $\mathbb{M}$.*

Remark 2. The third condition in Theorem 3 does not necessarily hold even if the first two conditions are fulfilled. See a PMG $\mathbb{M}$ shown in Fig. 3(d) for an example. When the local transformation is represented by $\mathbf{C} = \{V_2, V_5\}$, the first two conditions are fulfilled. However, in this case $\mathrm{PossDe}(X, \mathbb{M}[-\mathbf{C}]) \backslash \{X\} = \{V_3, V_4\}$, and $\mathbb{M}[V_3, V_4]$ is not bridged relative to $\{V_2, V_5, X\}$ in $\mathbb{M}$ since V_3 and V_4 are not bridged relative to $\{V_2, V_5, X\}$ in $\mathbb{M}$.

Remark 3. The first two conditions of Theorem 3 can be determined in $\mathcal{O}(d^3)$. In implementation, the determination of the third condition of Theorem 3 is equivalent to the determination of whether new unshielded colliders are introduced or an edge $J \circ\!\!-\!\!\circ K$ is oriented as both $J \rightarrow K$ and $J \leftarrow K$ in the second step of Algorithm 1. The equivalence is detailed in the proof of Theorem 3. This process can also be finished in $\mathcal{O}(d^3)$.

With Theorem 3, for a given local transformation of X represented by $\mathbf{C}$, we can determine whether an MAG consistent to $\mathcal{P}$ can be obtained in the follow up transformations after this transformation. By enumerating all the local transformations of X, we can determine all the valid ones. Based on the result, the recursive algorithm to list all MAGs consistent to $\mathcal{P}$ by transforming the circles of each vertex is shown in Algorithm 2. We present Corollary 2 to imply the validity of the method.

Corollary 2. *Algorithm 2 is valid to list all the MAGs consistent to $\mathcal{P}$.*

In the current, it is hard to give a theoretical analysis of the complexity. It is still an open problem how many MAGs are consistent to $\mathcal{P}$, even for the worst case when the PAG is a complete graph. To the best of our knowledge, the related studies are limited in the setting absence of latent variables [36,50–52,46,53,54]. When there are latent variables, the presence of bi-directed edges makes it difficult to topologically order the vertices as DAGs, thus the traditional analysis methods fail. We leave it for future works. Instead, we conduct an intuitive analysis, followed by empirical validation in Section 4.3.

The main advantage of our method is that, we execute a local transformation *if and only if* an MAG consistent to $\mathcal{P}$ can be obtained after some further circles transformation, which saves a large amount of computation on the *invalid MAGs*

[5] The local transformations could be null, in which case $\mathbb{M} = \mathcal{P}$.

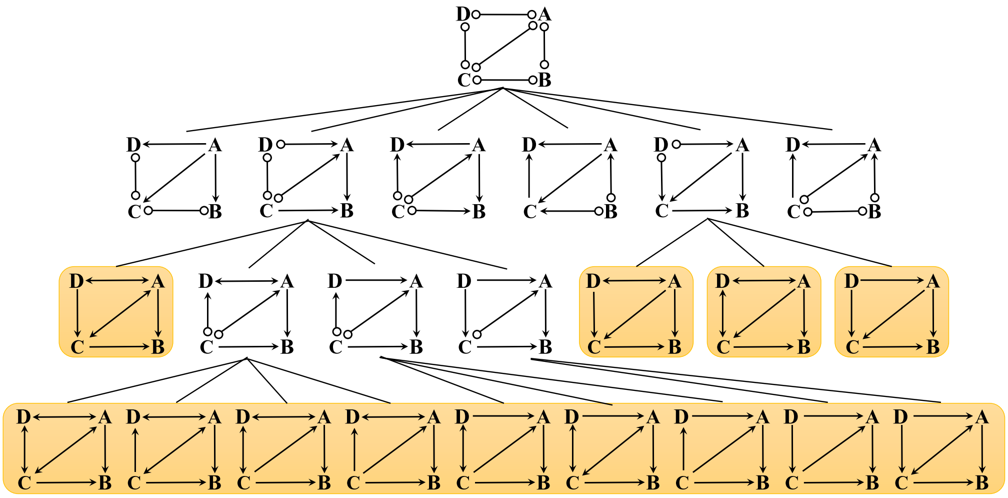


Fig. 4. A realization process of Algorithm 2. The graphs in the second/third/fourth layer are obtained from the previous layer by transforming the circles of $A/D/C$.

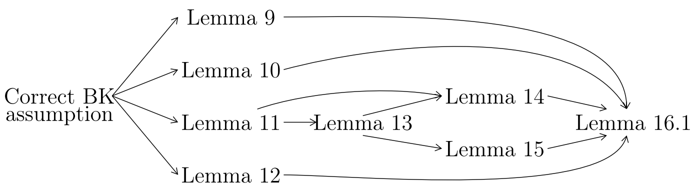


Fig. 5. The proof procedure of Lemma 16.1.

which are not MAGs or are not consistent to $\mathcal{P}$. The space of invalid MAGs grows super-exponentially with respect to the vertices number d, the enumeration of which costs the main computing time. In our method, with an additional $\mathcal{O}(d^3)$ cost for the determination of Theorem 3, we circumvent the computation on invalid MAGs. Roughly speaking, the completeness of the orientation rules and invalid-MAG-free search ensure that the search in our method is *necessary*. In addition, our method separates the MAG space into disjoint sets by transforming local circles into distinct marks. Hence, our method can be executed in parallel; and for each MAG consistent to $\mathcal{P}$, our method only obtain it for only once.

Example 4. A search tree for Algorithm 2 is shown in Fig. 4. The top root node denotes the given PAG $\mathcal{P}$. Each node in the search tree is expanded from its parent in the previous layer by additionally transforming the circles of a selected variable and applying orientation rules. The graph shaded with yellow is a leaf node that depicts a valid MAG. For example, the first four graphs in the third layer are obtained from a common parent node by transforming the circles of variable D. We omit some branches of the search tree (those unshaded but unexpanded) for brevity.

4.2. Proofs for Section 4.1

4.2.1. Proof of Theorem 3

Proof. We first prove the "if" statement. We prove the result by presenting a procedure that always constructs an MAG with the local transformation represented by **C** if the given conditions are satisfied. The generating process totally follows that in the proof of Lemma 16.1 in Appendix B. See Fig. 5 for the proof procedure of Lemma 16.1. The only difference is that in the proof of Lemma 16.1, there is a basic assumption that the BK is correct, *i.e.*, there exists an MAG consistent to $\mathcal{P}$ and BK, which is used in the proof of Lemma 9, Lemma 10, Lemma 11, and Lemma 12. However, here we do not have such an assumption, with the three conditions in Theorem 3 instead. Hence, it suffices to show that Lemma 9, Lemma 10, Lemma 11, and Lemma 12 also hold given the three conditions. Lemma 9 and Lemma 10 directly follow the second and the first conditions in Theorem 3, respectively. Next we prove that Lemma 11 and Lemma 12 hold given the third condition (bridged) without the assumption that the local BK is correct. Note that the PMG $\mathbb{M}$ obtained after some valid local transformations from $\mathcal{P}$ with the proposed orientation rules fulfill the five properties according to Theorem 1, because the valid local transformation ensures that there exists an MAG with the local transformations consistent to $\mathcal{P}$, which is equivalent to local BK assumption in implications. Hence Lemma 3, 7 and 8 also hold for $\mathbb{M}$.

Lemma 11: there is not an edge oriented as both $J \leftarrow K$ and $J \rightarrow K$ in the second step of Algorithm 1 For simplicity, denote $\mathbb{M}[\mathrm{PossDe}(X, \mathbb{M}[-\mathbf{C}])\backslash\{X\}]$ by $\mathbb{M}_1$. According to Definition 2, there is $\mathcal{F}_J \subseteq \mathcal{F}_K$ or $\mathcal{F}_K \subseteq \mathcal{F}_J$. We only present the proof for the case $\mathcal{F}_J = \mathcal{F}_K$. The proof for the case $\mathcal{F}_J \neq \mathcal{F}_K$ is similar by deriving a contradiction through finding a minimal circle path such that the two endpoints are not bridged, thus we leave them for readers.

By Lemma 8, if we orient $J \rightarrow K$ in the second step, there is a minimal circle path $V_0 \circ\!\!-\!\!\circ V_1 \circ\!\!-\!\!\circ \cdots V_{m-1}(= J) \circ\!\!-\!\!\circ V_m(= K)$ where $\mathcal{F}_{V_0} \supset \mathcal{F}_{V_1} = \cdots = \mathcal{F}_{V_m}$. If we also orient $J \leftarrow K$ in the second step, there is another minimal circle path $V_{m-1}(= J) \circ\!\!-\!\!\circ V_m(= K) \circ\!\!-\!\!\circ \cdots \circ\!\!-\!\!\circ V_n, n > m$ in $\mathbb{M}_1$ 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 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}, V_{m-1}, V_m, V_{m+1} are distinct vertices. According to Lemma 3, there cannot be non-circle edge between the variables in the circle path. Also note no circle edges in $\mathbb{M}_1$ are oriented in the first step. Hence the circle component in $\mathbb{M}_1$ after the first step 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 is a circle cycle 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}. Since $V_0, \cdots, V_n \in \mathrm{PossDe}(X, \mathbb{M}[-\mathbf{C}])\backslash\{X\}$, V_0 and V_n are not bridged relative to $\mathbf{C}$, contradicting with the third condition of Theorem 3.

Lemma 12: In the second step of Algorithm 1 when the local transformation of X represented by $\mathbf{C}$ *is introduced, there is not a new unshielded collider generated* Suppose there is a new unshielded collider $A \rightarrow B \leftarrow C$ generated in the second step. According to Lemma 8 there is a minimal path $F_1 \rightarrow \cdots, \rightarrow F_m(= A) \rightarrow B, m \geq 2$ and a minimal path $V_1 \rightarrow \cdots V_n(= C) \rightarrow B, n \geq 2$ such that $\mathcal{F}_{F_1} \supset \mathcal{F}_{F_2} = \cdots = \mathcal{F}_B$ and $\mathcal{F}_{V_1} \supseteq \mathcal{F}_{V_2} = \cdots = \mathcal{F}_B$. A and C are evidently different vertices that are not adjacent. In this case there is a circle path $p : F_1 \circ\!\!-\!\!\circ \cdots \circ\!\!-\!\!\circ F_m(= A) \circ\!\!-\!\!\circ B \circ\!\!-\!\!\circ V_n(= C) \circ\!\!-\!\!\circ \cdots \circ\!\!-\!\!\circ V_1$ in $\mathbb{M}$ such that $\mathcal{F}_{F_1} \supset \mathcal{F}_{F_2} = \cdots = \mathcal{F}_B = \cdots = \mathcal{F}_{V_2} \subset \mathcal{F}_{V_1}$. According to Lemma 3, there are no non-circle edges between the variables in p. In this case, there is always a minimal circle path from F_1 to V_1 such that F_1 and V_1 are not bridged relative to $\mathbf{C} \cup \{X\}$ in $\mathbb{M}$, contradiction.

Then we prove the "only if" statement We prove it by reduction to absurdity. Suppose an MAG $\mathcal{M}$ consistent to $\mathbb{M}$ has the local structure of X represented by $\mathbf{C}$.

If $\mathbb{M}[\mathbf{C}]$ is not complete, there are new unshielded colliders in $\mathcal{M}$ relative to $\mathbb{M}$. It is evident that $\mathcal{M}$ is not consistent to $\mathbb{M}$, contradiction.

If $\mathrm{PossDe}(X, \mathbb{M}[-\mathbf{C}]) \cap \mathrm{Pa}(\mathbf{C}, \mathbb{M}) \neq \emptyset$, suppose $V \rightarrow T$ where $V \in \mathrm{PossDe}(X, \mathbb{M}[-\mathbf{C}])$ and $T \in \mathbf{C}$. By Lemma 4, $V \in \mathrm{De}(X, \mathcal{M})$, thus $T \in \mathrm{De}(X, \mathcal{M})$. According to the definition of $\mathbf{C}$, there is $X \leftrightarrow\!\!* T$, a directed or almost directed cycle forms, contradiction.

If $\mathbb{M}[\mathrm{PossDe}(X, \mathbb{M}[-\mathbf{C}])\backslash\{X\}]$ is not bridged relative to $\mathbf{C} \cup \{X\}$ in $\mathbb{M}$, we will prove the result by showing that either Lemma 11 or 12 is violated for the graph updated by Algorithm 1 with the local transformation represented by $\mathbf{C}$. Note the orientations in Algorithm 1 are sound according to Lemma 7. If Lemma 11 is violated, it is only possible that the set of the MAGs with the local transformation consistent to $\mathbb{M}$ is empty, otherwise the sound orientations suggest totally different directions; and if Lemma 12 is violated, there are always new unshielded colliders generated relative to $\mathbb{M}$ when the local transformation represented by $\mathbf{C}$ is introduced, which also implies that the set of the MAGs with the local transformation consistent to $\mathbb{M}$ is empty.

Suppose two vertices J, K in $\mathbb{M}[\mathrm{PossDe}(X, \mathbb{M}[-\mathbf{C}])\backslash\{X\}]$ are not bridged relative to $\mathbf{C}$ due to the minimal circle path $J(= V_0) \circ\!\!-\!\!\circ V_1 \cdots V_n \circ\!\!-\!\!\circ K(= V_{n+1})$ in $\mathbb{M}[\mathrm{PossDe}(X, \mathbb{M}[-\mathbf{C}])\backslash\{X\}]$. There are two possible cases (they possibly happen simultaneously). One is that there exists $0 \leq s \leq n$ such that $\mathcal{F}_{V_s} \nsubseteq \mathcal{F}_{V_{s+1}}$ and $\mathcal{F}_{V_{s+1}} \nsubseteq \mathcal{F}_{V_s}$. The other is that there exists $1 \leq s \leq n$ such that $\mathcal{F}_{V_s} \subset \mathcal{F}_{V_{s-1}}$ and $\mathcal{F}_{V_s} \subset \mathcal{F}_{V_{s+1}}$.

For the first case, suppose there are two vertices $T_1, T_2 \in \mathbf{C}$ such that $T_1 \in \mathcal{F}_{V_s}\backslash\mathcal{F}_{V_{s+1}}$ and $T_2 \in \mathcal{F}_{V_{s+1}}\backslash\mathcal{F}_{V_s}$. According to Algorithm 1 to update $\mathbb{M}$ with the local transformation represented by $\mathbf{C}$, when $T_1, T_2 \in \mathbf{C}$, there is $V_s \rightarrow V_{s+1}$ due to $T_1 \in \mathcal{F}_{V_s}\backslash\mathcal{F}_{V_{s+1}}$, and there is $V_s \leftarrow V_{s+1}$ due to $T_2 \in \mathcal{F}_{V_{s+1}}\backslash\mathcal{F}_{V_s}$. Lemma 11 is violated.

For the second case, suppose a vertex $T_1 \in \mathcal{F}_{V_{s-1}}\backslash\mathcal{F}_{V_s}$. By Algorithm 1, there is $V_{s-1} \rightarrow V_s$ oriented. And suppose a vertex $T_2 \in \mathcal{F}_{V_{s+1}}\backslash\mathcal{F}_{V_s}$, there is $V_{s+1} \rightarrow V_s$ oriented. Hence there is a new unshielded collider $V_{s-1} \rightarrow V_s \leftarrow V_{s+1}$ generated by Algorithm 1 relative to $\mathbb{M}$, thus Lemma 12 is violated.

Combining the results above, we conclude that there does not exist an MAG consistent to $\mathbb{M}$ with the local structure of X represented by $\mathbf{C}$ when the three conditions are violated. □

4.2.2. Proof of Corollary 2

Proof. Denote the set of MAGs returned by Algorithm 2 and the set of MAGs consistent to $\mathcal{P}$ by $\hat{\mathcal{S}}$ and $\mathcal{S}$, respectively. $\hat{\mathcal{S}} \subseteq \mathcal{S}$ directly follows from Theorem 3, which implies that each MAG $\mathcal{M} \in \hat{\mathcal{S}}$ is consistent to $\mathcal{P}$. It suffices to prove $\mathcal{S} \subseteq \hat{\mathcal{S}}$. Suppose an MAG $\mathcal{M} \in \mathcal{S}$. Without loss of generality, suppose the set of vertices with circles in $\mathcal{P}$ is $\{V_1, \cdots, V_k\}$, and first vertex that is locally transformed in Algorithm 2 is V_1. For brevity, we say a local transformation of a vertex V is *consistent to* $\mathcal{M}$ if the local marks implied by the transformation are identical to those in $\mathcal{M}$. Note Algorithm 2 considers all possible local transformations. For the set $\mathbf{C}^1$ which represents the local transformation of V_1 consistent to $\mathcal{M}$, due to the existence of MAGs ($\mathcal{M}$) consistent to $\mathcal{P}$, the conditions on Line 10 of Algorithm 2 are fulfilled according to Theorem 3. Hence Algorithm 2 will transform the other circles based on the local transformation of V_1 represented by $\mathbf{C}^1$ on Line 12.

Algorithm 3 BRUTEFORCE.

input: A PAG $\mathcal{P}$
1: $\mathcal{S} = \emptyset$ // Record all the MAGs consistent to $\mathcal{P}$
2: Obtain an MAG $\mathcal{M}$ from $\mathcal{P}$ by transforming the circle component into a DAG and the edges $\circ\!\!\rightarrow$ into $\rightarrow$
3: $C_{set} = \{(i, j) \mid$ there is $V_i *\!\!-\!\!\circ V_j$ in $\mathcal{P}\}$ // Record the indexes of all the circles in $\mathcal{P}$
4: **for** each set $\mathbf{C} \subseteq C_{set}$ **do**
5: Obtain a graph G by transforming the circles in $\mathbf{C}$ to arrowheads and others to tails
6: **if** there is an edge with two tails in G **then**
7: continue // It violates the absence of selection bias
8: **end if**
9: **if** there is a directed or almost directed cycle in G **then**
10: continue // It violates the ancestral property
11: **end if**
12: **if** there is an inducing path in G **then**
13: continue // It violates the maximal property
14: **end if**
15: **if** G is Markov equivalent to $\mathcal{M}$ by Thm. 3.7 of Ali et al. [55] **then**
16: $\mathcal{S} \leftarrow \mathcal{S} \cup \{G\}$ // It is consistent to $\mathcal{P}$
17: **end if**
18: **end for**
output: $\mathcal{S}$

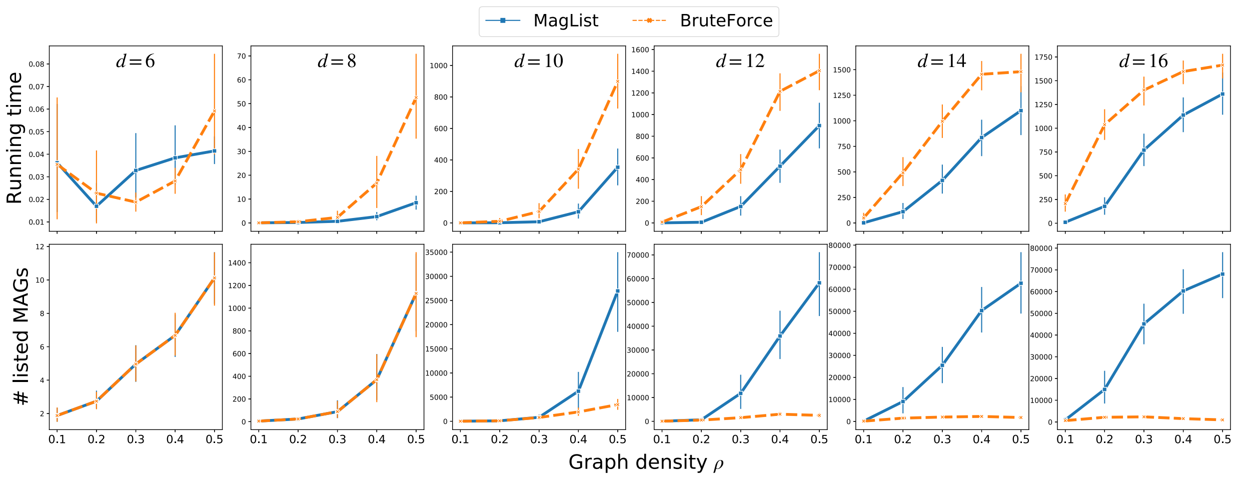


Fig. 6. Results of running time and number of listed MAGs over 100 simulations for each vertice number (including 3 latent ones)/graph density. The vertical line represents the 95% confidence interval generated by bootstrap sampling. It is determined by the 2.5th and 97.5th percentiles of 1000 estimates $\{\hat{\theta}_1, \hat{\theta}_2, \ldots, \hat{\theta}_{1000}\}$, where $\hat{\theta}_i$ is an empirical mean of a new random sample of equal size with replacement from the original sample.

Further, suppose the second vertex locally transformed in Algorithm 2 is V_2. Similar to the proof above, we can prove that for the set $\mathbf{C}^2$ which represents the local transformation of V_2 consistent to $\mathcal{M}$, the conditions on Line 10 of Algorithm 2 are fulfilled and Line 12 is executed for $\mathbf{C}^2$. By induction, we can prove that for the set $\mathbf{C}^i, 1 \le i \le k$ which represents the local transformations of V_i that has the identical local marks of V_i with $\mathcal{M}$, Line 12 is executed. Thus, after the local transformation of $V_1, \cdots, V_k$ represented by $\mathbf{C}^1, \cdots, \mathbf{C}^k$, we can obtain $\mathcal{M}$ (note the algorithm possibly stops in a round $s < k$, since the orientation rules may help reveal all of the circles at $V_{s+1}, \cdots, V_k$ with the local BK regarding $V_1, \cdots, V_s$. The obtained graph is in this case is also $\mathcal{M}$ due to the soundness of the orientation rules). We conclude $\mathcal{S} \subseteq \hat{\mathcal{S}}$. □

4.3. Experiments

In this part, we evaluate the effectiveness and efficiency of the proposed methods to list all the MAGs consistent to a PAG $\mathcal{P}$. We call our method MAGLIST. MAGLIST is compared to the baseline brute force enumeration method, which is called BRUTEFORCE and shown in Algorithm 3. According to Thm. 2 of Zhang [35], an MAG consistent to $\mathcal{P}$ is obtained on Line 2 of Algorithm 3. Next, all the possible transformations of the circles in $\mathcal{P}$ are considered. For any graph G obtained after a transformation, we test whether it is an MAG from Line 6 to 14. If it is, we further evaluate whether it is consistent to $\mathcal{P}$ by testing whether it is Markov equivalent to $\mathcal{M}$ on Line 15. There are many solid methods in the literature for testing Markov equivalence [49,55,56,42].

We generate 100 Erdös-Rényi random DAGs for each setting, where the number of nodes $d \in \{6, 8, 10, 12, 14, 16\}$ and density[6] $\rho \in \{0.1, 0.2, 0.3, 0.4, 0.5\}$. The weight of each edge is drawn from $\mathcal{U}[1, 2]$. We then take three of variables as latent variables and others as observed variables. Based on each DAG, we obtain the truth PAG. Then, we adopt the two methods (MagList, BruteForce) to list all the MAGs consistent to the PAG. Due to the possibility that for some PAGs it is hard to list all the MAGs in limited time, we set the maximum running time for each PAG by 1800 seconds. If the running time exceeds the threshold, the method will immediately output the MAGs that have been found. The number of listed MAGs is shown as Fig. 6. When the number of vertices is not large ($d < 10$), both of the methods can finish within 1800 seconds. In this case MagList and BruteForce output the same set of MAGs. It verifies the effectiveness of our proposed method. Fig. 6 shows that MagList has a significant advantage on efficiency compared to BruteForce. For example, when $d = 10$ and $\rho = 0.5$, the number of MAGs listed by MagList is more than five times that by BruteForce. And the difference is larger as d and ρ grows. Note the number of MAGs listed by BruteForce does not necessarily increase as d or ρ grows. The reason is, as d or ρ grows, the space of graphs becomes larger and there are more invalid graphs which are not MAGs consistent to $\mathcal{P}$. Since the number of searched graphs in 1800 seconds is limited, when there are more invalid MAGs which are not MAGs or are not consistent to $\mathcal{P}$, it is possible that fewer MAGs consistent to $\mathcal{P}$ are listed in the limited time. This problem will not occur for MagList, because the search in MagList is invalid-MAG-free. That also validates the efficiency of MagList.

5. Application 2: active causal discovery framework

With the establishment of the sound and complete orientation rules for causal identification with local BK, we propose an active causal discovery framework in the presence of latent variables in this section, with the target of learning the MAG with as fewer interventions as possible. Suppose we have the observational data of $\{V_1, V_2, \cdots, V_d\}$.

5.1. The learning framework

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 $X \in \{V_1, \dots, V_d\}$ to intervene and collect a few interventional data. In Stage 3, we learn causal relations with the interventional data. For each edge $X \circ\!\!\rightarrow\!* V_i$, 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 $X \leftarrow\!* V_i$ learned if they are equal, and $X -\!* V_i$ otherwise. Hence, the knowledge taken by the interventional data is local, and we can further update the graph with the orientation rules. We repeat the second and third stages until we identify an MAG. 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 $V_1, V_2, \dots, V_i$, and will select a variable from $\{V_{i+1}, \dots, V_d\}$ to intervene. We adapt the maximum entropy criterion used in DAG discovery [23]. 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 combination of marks at X), M is the number of different local structures, l_j is the number of MAGs consistent to $\mathbb{M}_i$ which has the j-th local structure of X, and L is the total number of MAGs consistent to $\mathbb{M}_i$. Intuitively, 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.

When the number of vertices is not large, we can execute Algorithm 2 to list all the MAGs consistent to $\mathbb{M}_i$,[7] and then count the number of MAGs with each local structure. When the number is large, however, it is hard to list all the MAGs. Even in causal sufficiency setting, implementing such operation (generally called *counting maximally oriented partial DAGs*) is #P-complete [53]. 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 [57], to uniformly sample from the space of MAGs. Here, we introduce an important result of Zhang and Spirtes [58], Tian [59] for MAGs transformation in Proposition 2, which supports the feasibility of the MH algorithm in sampling MAGs.

Proposition 2 *(Zhang and Spirtes [58], Tian [59]). Let $\mathcal{M}$ be an arbitrary MAG, and $A \to B$ 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*

[6] Density denotes the probability of including an edge between any two nodes.

[7] Despite Algorithm 2 proposed for listing all MAGs consistent to $\mathcal{P}$, it can be directly applied in listing all the MAGs consistent to $\mathbb{M}$ which is obtained from $\mathcal{P}$ by incorporating some local BK.

Algorithm 4 Intervention variable selection based on maximum entropy criterion with MH algorithm.

input: A PMG $\mathbb{M}_i$ oriented based on $\mathcal{P}$ and BK regarding $V_1, \ldots, V_i$
1: 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
2: **for** $t = 1, 2, \ldots, L$ **do**
3: Sample an MAG $\mathcal{M}'$ from $S(\mathcal{M}_{t-1})$ $\rho = \min(1, \frac{|S(\mathcal{M}_{t-1})|}{|S(\mathcal{M}')|})$
4: Sample u from uniform distribution $\mathcal{U}[0, 1]$
5: **if** $u \le \rho$ **then**
6: $\mathcal{M}_t = \mathcal{M}'$
7: **else**
8: $\mathcal{M}_t = \mathcal{M}_{t-1}$
9: **end if**
10: **end for**
11: $s \leftarrow 0$, $X \leftarrow \emptyset$
12: **for** $V_j = V_{i+1}, \ldots, V_d$ **do**
13: Denote $\mathbf{V}(V_j) = \{V \in \mathbf{V}(\mathbb{M}_i) \mid V_j \circ\!\!-\!\!* V \text{ in } \mathbb{M}_i\}$
14: For each possible local structure $\mathcal{L}_k$ of V_j, $1 \le k \le 2^{|\mathbf{V}(V_j)|}$, we count the number $\mathcal{N}_k$ of the appearance of $\mathcal{L}_k$ in the L MAGs
15: $s' = -\sum_{k=1}^{2^{|\mathbf{V}(V_j)|}} \frac{\mathcal{N}_k}{L} \log \frac{\mathcal{N}_k}{L}$
16: **if** $s \le s'$ **then**
17: $X \leftarrow V_j$, $s \leftarrow s'$
18: **end if**
19: **end for**
output: The selected intervention variable X

(1) *there is no directed path from A to B other than $A \to B$ in $\mathcal{M}$;*
(2) *for any $C \to A$ in $\mathcal{M}$, $C \to B$ is also in $\mathcal{M}$; and for any $D \leftrightarrow A$ in $\mathcal{M}$, either $D \to B$ 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 $\mathcal{M}$.*

The algorithm begins from an MAG $\mathcal{M}_0$ consistent to $\mathbb{M}_i$, which can be obtained by transforming all the edges $A \circ\!\!\rightarrow B$ to $A \to B$ and the circle component into a DAG without unshielded colliders according to Lemma 16.1. For any MAG $\mathcal{M}$ consistent to $\mathbb{M}_i$, we say a mark change is *legitimate* if it satisfies the three conditions in Proposition 2 and it is a circle in $\mathbb{M}_i$. We obtain a new MAG $\mathcal{M}_1$ by a legitimate mark change. Then we decide to accept the candidate MAG or not. Given an MAG $\mathcal{M}$, let $S(\mathcal{M})$ denote the set of MAGs that can be obtained from $\mathcal{M}$ by a legitimate mark change according to Proposition 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

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

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 [60]. Here the last problem is whether any two MAGs consistent to $\mathbb{M}_i$ can be transformed to each other in limited steps. It has been proved by Zhang and Spirtes [58] that any two MAGs consistent to $\mathcal{P}$ can be transformed to each other in limited steps. We generalize it to the case for the MAGs consistent to $\mathbb{M}_i$ in Proposition 3. Hence, MH algorithm is valid to sample MAGs uniformly from the space of MAGs consistent to $\mathbb{M}_i$.

Proposition 3 *(generalization of Theorem 3 of Zhang and Spirtes [58] from $\mathcal{P}$ to $\mathbb{M}$). Denote $\mathbb{M}$ the obtained graph by incorporating local BK in a PAG $\mathcal{P}$ with the orientation rules. Two MAGs $\mathcal{M}$ and $\mathcal{M}'$ are consistent to $\mathbb{M}$ if and only if there exists a sequence of single mark changes in $\mathcal{M}$ such that*

(1) *after each mark change, the resulting graph is also an MAG consistent to $\mathbb{M}$;*
(2) *after all the mark changes, the resulting graph is $\mathcal{M}'$.*

Remark 4. The proof directly follows that of Thm. 3 of Zhang and Spirtes [58]. The only difference is, to generalize the result that any two MAGs consistent to $\mathcal{P}$ can be transformed to each other in limited steps to the cases for two MAGs consistent to $\mathbb{M}$, we say a mark in an MAG $\mathcal{M}$ consistent to $\mathbb{M}$ is invariant if it is present in all the MAGs consistent to $\mathbb{M}$ instead of all the MAGs consistent to $\mathcal{P}$. Then the proof directly follows Zhang and Spirtes [58] because we have proved in Theorem 1 that all the properties (chordal, balanced, complete) of $\mathcal{P}$ used in their proof hold for $\mathbb{M}$ as well.

We propose Algorithm 4 to select the intervention variable X based on MH algorithm. From Line 2-Line 10, we execute MH algorithm to sample L MAGs consistent to $\mathbb{M}_i$. Finally, we estimate the entropy in (1) and select X on Line 11-Line 19.

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

Stage	Stage 1		Stage 2	Stage 3		Whole process	
Strategy-p	# correct PAG	# wrong PAG	# int.	# correct int.	# wrong int.	Norm. SHD	F1
Random-0.10	4.78 ± 3.11	0.40 ± 0.84	2.83 ± 1.21	3.92 ± 2.33	0.11 ± 0.55	0.02 ± 0.04	0.86 ± 0.28
MCMC-0.10			2.82 ± 1.13	4.01 ± 2.38	0.02 ± 0.14	0.02 ± 0.04	0.86 ± 0.28
Random-0.15	7.21 ± 3.85	0.41 ± 0.92	3.32 ± 1.19	5.21 ± 2.65	0.06 ± 0.31	0.02 ± 0.04	0.91 ± 0.18
MCMC-0.15			3.21 ± 1.01	5.22 ± 2.63	0.05 ± 0.30	0.02 ± 0.04	0.92 ± 0.16
Random-0.20	9.26 ± 3.94	0.63 ± 1.23	3.57 ± 1.17	6.28 ± 2.53	0.17 ± 0.51	0.04 ± 0.07	0.92 ± 0.16
MCMC-0.20			3.45 ± 1.13	6.38 ± 2.73	0.07 ± 0.36	0.03 ± 0.06	0.92 ± 0.16
Random-0.25	11.9 ± 4.03	1.58 ± 2.75	3.43 ± 1.36	6.94 ± 3.36	0.17 ± 0.51	0.08 ± 0.13	0.89 ± 0.18
MCMC-0.25			3.20 ± 1.17	7.01 ± 3.43	0.10 ± 0.41	0.08 ± 0.14	0.89 ± 0.18
Random-0.30	12.6 ± 4.05	2.69 ± 3.14	3.59 ± 1.26	6.94 ± 3.28	0.40 ± 0.93	0.15 ± 0.15	0.82 ± 0.19
MCMC-0.30			3.50 ± 1.28	6.97 ± 3.34	0.37 ± 0.80	0.15 ± 0.15	0.82 ± 0.19

5.2. Experiments

In this part, we conduct a simulation of the three-stage active learning framework. We generate 100 Erdös-Rényi random DAGs for each setting, where the number of variables $d = \{6, 8, 10, 12, 14, 16\}$ 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 Algorithm 4, we collect $L = 1000$ sampled MAGs. For each intervention variable X, we collect 200 samples under $do(X = 2)$, and learn the circles at X by a two-sample test with a significance level of 0.05.

We compare the maximum entropy criterion (MaxEnt) with a baseline random criterion where we randomly select one variable with circles to intervene in each round. We evaluate the three stages respectively and show the results[8] for only $d = 10$ in Table 1. More results are shown in Appendix C. 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, which 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.. The effectiveness of MaxEnt is verified by noting that the number of interventions with MaxEnt is fewer than that with random criterion. And we evaluate the performance of Stage 3 by # correct int./# wrong int., which denotes the number of edges that 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), 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 d or 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 framework, the PAG identification in the first stage is the bottleneck of having a good performance.

However, we note that although MaxEnt can reduce the number of interventions relative to random strategy, the reduction is inconspicuous (4.5% on average), which is less than the reduction taken by MaxEnt relative to random strategy in causal sufficiency setting (CS) [23]. The effectiveness of MaxEnt on MAG identification is weaken in causal insufficiency setting (CIS). We argue that it is due to the intrinsic hardness posed by the latent variables: the learned marks are mainly directly from BK, and the rules reveal fewer marks in CIS setting. For example, for $A \circ\!\!-\!\!\circ X$, when the intervention on X does not result in a change on A, *only* $A \circ\!\!\rightarrow X$ can be learned and another intervention is necessary to determine the circle at A. In the following, we conduct a further study to verify our view.

We consider all the possible aspects that could be the reason for the weaken effectiveness. There are three possible ones: 1. PAG learning. Learning PAG is harder than learning CPDAG which latent variables are not involved. 2. The MH sampling method: it is possible that the sampled MAGs are not representative enough to describe the uniform distribution of the MAGs consistent to a given PMG. 3. The basic assumption of MaxEnt does not hold under CIS. This is not quite intuitive. When we adopt MaxEnt, we uniformly sample MAGs from the space of MAGs. There is a potential assumption that each graph is with the equal possibility to be the true causal graph. It is valid when we generate directed cyclic graphs. However, it is not the case when we generate MAGs, where we first obtain a set of DAGs and then obtain MAGs by randomly selecting latent vertices. The core reason is on the non-bijective mapping from DAGs to MAGs. For example, consider a DAG

[8] The experimental results are slightly different from that of [40]. We re-conduct the experiments in this paper, because the MAG sampling method is *improved* in Algorithm 4. In the preliminary version, *many* sampled MAGs will be discarded, while through Proposition 3 *all* the sampled MAGs (Line 2-9) of Algorithm 4 can be used in the following steps.

Table 2
The ratio of reduced intervention times by MaxEnt relative to random strategy and the ratio of marks learned by rules under CS and CIS over 100 simulations with varying d and $p = 0.2$ in the format of mean ± std.

d	%diff-CIS	%diff-CS	%rule-CIS	%rule-CS
6	3.48 ± 2.18%	15.5± 5.09%	16.0 ± 2.07%	57.8± 8.49%
8	6.63 ± 3.78%	19.9± 3.78%	21.0 ± 2.26%	65.6± 5.94%
10	7.64 ± 1.60%	21.4± 4.21%	22.1 ± 0.87%	67.3± 3.21%
12	8.16 ± 1.66%	24.5± 3.68%	20.6 ± 1.99%	70.3± 2.67%
14	7.43 ± 1.52%	24.6± 5.06%	20.4 ± 0.74%	70.7± 1.87%
16	6.45 ± 1.87%	24.2± 2.93%	19.7 ± 1.34%	71.0± 2.19%

of A, B, C with only a directed edge $B \to C$, and another DAG of A, B, C with $C \to A \to B \leftarrow C$. When A is latent, both of them generates an MAG $B \to C$. The non-bijective mapping makes the distribution of MAGs non-uniform, thereby the basic assumption of MaxEnt violated.[9]

In light of the three aspects, we conduct a study to compare the intervention number reduction of MaxEnt relative to random strategy under CS and CIS setting by removing the possible influence of these three aspects. For CS, we generate DAGs with $d - 3$ nodes to ensure the identical number of observed variables under CS and CIS. We learn PAG/CPDAG with the true covariance matrix, which guarantees the correctness of Stage 1. For MaxEnt, we use Algorithm 2 to list all the MAGs instead of MH sampling. And to ensure the equal possibility of each MAG, we randomly select an MAG $\mathcal{M}'$ from the listed MAGs consistent to PAG $\mathcal{P}$ as the true one instead of the original MAG $\mathcal{M}$. The two points above ensure the correctness of the entropy estimation. When we intervene on X, we directly take the local marks of X in $\mathcal{M}'$ as the learned BK, which guarantees that the BK is correct. Hence, the whole process is ideal.

We estimate the ratio %diff-CIS/%diff-CS of reduced intervention times by MaxEnt relative to random strategy under CIS/CS. %diff-CIS is calculated by $(\#Int_{random} - \#Int_{MaxEnt})/\#(Int_{MaxEnt})$, where $\#Int_{random}$ and $\#Int_{MaxEnt}$ denote the total number of interventions by random and MaxEnt in 100 simulations under CIS. %diff-CS is calculated similarly under CS. We repeat the experiments for 10 times and estimate the mean and standard error (std) accordingly. The results are shown in the second/third column of Table 2 for the case $p = 0.2$. See Appendix C for additional results. It demonstrates that MaxEnt has quite different contributions to the reduction of intervention numbers in the two settings. Note %diff-CIS (%diff-CS) is a ratio value related to d and ρ. Although $\#\ Int_{random}$ and $\#\ Int_{MaxEnt}$ increase with d and ρ, the *ratio* does not necessarily follow a monotonic trend. According to the experimental results, when d and ρ are not too small or large, %diff-CIS and %diff-CS are more likely to be large. Further, we divide the learned marks by interventions into two parts: those oriented directly by BK and those learned by the orientation rules. We show the ratio of marks learned by rules to the total learned marks for CIS and CS in the forth/fifth column of Table 2. The mean and std are calculated similar to %diff-CIS. It implies that for CIS, most learned marks are directly from BK, while for CS most learned marks are from applying orientation rules. Hence, a larger number of interventions is needed in learning an MAG in contrast to learning a DAG, which leads to the weakened effectiveness of MaxEnt under CIS.

6. Conclusion

In this paper, we propose sound and complete orientation rules that resolve the causal identification problem given local BK in the presence of latent variables. Based on the results, we present two applications. Firstly, for MAG listing, the new approach significantly improves the efficiency. Secondly, for causal discovery, we propose the first active learning framework in the presence of latent variables. In the future, it is worthy to investigate the causal identifiability given general background knowledge.

Beyond causal identification, there are two directions that might be interesting. A recent advancement is the introduction of a novel learning paradigm called *abductive learning*, which bridges logical reasoning and machine learning [61,62]. The causal relations, as a form of logical formula, have the potential to collaborate effectively with machine learning. In addition, the studies on causality have greatly influenced decision-making methods [12,63–65,46,66]. Recently, Zhou [67] emphasized the importance of correlation for prediction and causation for scientific discovery, while recognizing the need for an intermediate relation for decision-making, referred to as *rehearsation*. Exploring the potential of decision-making without relying on causal identification could also be a valuable direction for future research.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

[9] In practice, even if under CS, we can never assert that the DAGs consistent to the CPDAG is uniform. It is impossible for us to know the distribution of DAGs in advance.

Data availability

Data will be made available on request.

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Appendix A. Orientation rules 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 $A \ast\!\!\rightarrow B \circ\!\!-\!\!\ast R$, and A and R are not adjacent, then orient the triple as $A \ast\!\!\rightarrow B \rightarrow R$.
$\mathcal{R}_2$: If $A \rightarrow B \ast\!\!\rightarrow R$ or $A \ast\!\!\rightarrow B \rightarrow R$, and $A \ast\!\!-\!\!\circ R$, then orient $A \ast\!\!-\!\!\circ R$ as $A \ast\!\!\rightarrow R$.
$\mathcal{R}_3$: If $A \ast\!\!\rightarrow B \leftarrow\!\!\ast R$, $A \ast\!\!-\!\!\circ D \circ\!\!-\!\!\ast R$, A and R are not adjacent, and $D \ast\!\!-\!\!\circ B$, then orient $D \ast\!\!-\!\!\circ B$ as $D \ast\!\!\rightarrow B$.
$\mathcal{R}_4$: If $\langle K, \ldots, A, B, R\rangle$ is a discriminating path between K and R for B, and $B \circ\!\!-\!\!\ast R$; then if $B \in \mathrm{Sepset}(K, R)$, orient $B \circ\!\!-\!\!\ast R$ 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 $p = \langle A, B, D, \ldots, R\rangle$ 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 $A \rightarrow R$.

Appendix B. Detailed proof of Theorem 1

We first provide some facts, which are used to prove Theorem 1.

Lemma 2. *Consider $\mathbb{M}_i$ in Theorem 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. Suppose the possible directed path $p = \langle V_0(= A), V_1, \ldots, V_m(= B)\rangle$. If p is minimal, the result trivially holds. If not, we can always find a subpath $\langle V_i, V_{i+1}, \ldots, V_j\rangle$, $j - i \geq 2$ such that any non-consecutive vertices are not adjacent except for an edge between V_i and V_j. We will show the impossibility of $V_i \leftarrow\!\!\ast V_j$ in $\mathbb{M}_i$. Suppose $V_i \leftarrow\!\!\ast V_j$ in $\mathbb{M}_i$. Note there is a circle/tail at V_i on the edge between V_i and V_{i+1} due to the possible directed path p. If $j - i = 2$, there is always an edge $V_{i+1} \leftarrow\!\!\ast V_{i+2}(= V_j)$ due to the balanced/closed property of $\mathbb{M}_i$, contradicting the possible directed path p. If $j - i > 2$, due to the non-adjacency of the V_j and V_{i+1}, there is either $V_i \rightarrow V_{i+1} \rightarrow \ldots V_j$ or $V_i \leftarrow\!\!\ast V_{i+1}$ identified in $\mathcal{P}$. The latter case is impossible due to the possible directed path p. For the former case, there is an almost directed or directed cycles, contradiction. Hence, the edge between V_i and V_j is either $V_i \rightarrow V_j$ or $V_i \circ\!\!-\!\!\ast V_j$, we thus find a shorter possible directed path $\langle V_0, V_1, \ldots, V_i, V_j, V_{j+1}, \ldots, V_m\rangle$ in $\mathbb{M}_i$. Repeat this process until obtaining a possible directed path such 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 Theorem 1 that satisfies the five properties. If there is $A \ast\!\!\rightarrow B$ in $\mathbb{M}_i$, then there is an edge as $A \ast\!\!\rightarrow V$ for any V in a connected circle component with B in $\mathbb{M}_i$, and A and B are not connected in a circle component.*

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

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

Proof. We first prove the "only if" statement. If $V \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$, there is a minimal possible directed path $p = \langle X, F_1, \ldots, F_m(= V)\rangle$ by Lemma 2. Due to $F_1 \notin \mathbf{C}$, there is $X \rightarrow V_1$ in $\mathcal{M}$. Hence p 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 $\mathcal{M}$, which is identified in $\mathcal{P}$ and $\mathbb{M}_i$, contradicting with that p is a minimal possible directed path from X to F_m in $\mathbb{M}_i[-\mathbf{C}]$.

We then prove the "if" statement. According to the ancestral property, there must be a minimal directed path $X \rightarrow F_1 \cdots \rightarrow F_{m-1}, F_m(=V)$ in $\mathcal{M}$, where X is not 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 $F_1 \in \mathbf{C}$ due to $F_2, F_3, \ldots, F_m \notin \mathbf{C}$ as they are not adjacent to X. In this case $X \leftarrow\!\!* F_1$ should be represented by $\mathbf{C}$, which contradicts $X \rightarrow F_1$ in $\mathcal{M}$. $\square$

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

Proof. It follows from the third step of Algorithm 1. $\square$

Lemma 6. *Suppose $\mathbb{M}_s, 0 \le s \le i$ in Theorem 1 satisfy the five properties, there must exist an MAG consistent to $\mathbb{M}_i$.*

Proof. It follows from the complete property of $\mathbb{M}_i$. $\square$

Lemma 7. *The PMG $\mathbb{M}_{i+1}$ in Theorem 1 satisfies the invariant property.*

Proof. Denote the graph obtained from $\mathbb{M}_i$ and the local BK represented by $\mathbf{C}$ after the first two steps of Algorithm 1 by $\bar{\mathbb{M}}_{i+1}$. Note in the third step we only update $\bar{\mathbb{M}}_{i+1}$ with the orientation rules. It is easy to prove the orientation rules are sound to orient $\bar{\mathbb{M}}_{i+1}$ referring to Proposition 1 and the results of Ali et al. [68], Zhang [35] as new unshielded colliders, or directed or almost directed cycles will be introduced otherwise, we do not present the details here. It suffices to show that the non-circle marks introduced in the first two steps are invariant in all the MAGs consistent to $\mathbb{M}_i$ and the local BK of X represented by $\mathbf{C}$. For brevity, we call the MAGs consistent to $\mathbb{M}_i$ and $\mathbf{C}$ for short in the following.

Consider $\forall K \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ and $\forall T \in \mathbf{C}$. According to Lemma 4, there is $K \in \text{De}(X, \mathcal{M})$. Considering $T {*\!\!\rightarrow} X \rightarrow \cdots \rightarrow K$, the edge between K and T can only be as $K \leftarrow\!\!* T$ in any MAG $\mathcal{M}$ due to the ancestral property if $K \neq X$. If $K = X$, the orientation $X \leftarrow\!\!* T$ in $\mathcal{M}$ just follows the local BK of X represented by $\mathbf{C}$. The proof completes.

Next we prove that the oriented edges in the second step are invariant in any MAG $\mathcal{M}$ consistent to $\mathbb{M}_i$ and $\mathbf{C}$. Suppose the first edge oriented in the second step which is not invariant is $V_l \rightarrow V_j$. 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 possible cases. 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 $V_j \rightarrow T$, otherwise there must be a directed or almost directed cycles $X \rightarrow \cdots \rightarrow V_j \rightarrow T {*\!\!\rightarrow} X$ 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 as there is always a contradiction if adjacent. Thus $V_j {*\!\!\rightarrow} V_l \leftarrow\!\!* T$ is a new unshielded collider introduced in the second step. **(B)** If there is $V_m \rightarrow V_l \circ\!\!-\!\!\circ V_j$ where $V_m \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}]) \backslash \{X\}$ is not adjacent to V_j, a new unshielded collider $V_m \rightarrow V_l \leftarrow\!\!* V_j$ introduced in the second step. Hence in the MAG $\mathcal{M}$ consistent to $\mathcal{P}$, there are always new unshielded colliders relative to $\mathcal{P}$ introduced, contradiction. $\square$

Lemma 8. *Consider $\mathbb{M}_i$ in Theorem 1 that satisfies the five properties. Denote $\mathcal{F}_{V_l} = \{V \in \mathbf{C} \cup \{X\} \mid V *\!\!-\!\!\circ V_l \text{ in } \mathbb{M}_i\}$ for $\forall V_l \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}]) \backslash \{X\}$. For an edge $J \circ\!\!-\!\!\circ K$ in $\mathbb{M}_i[\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}]) \backslash \{X\}]$, if it is oriented as $J \rightarrow K$ in the second step of Algorithm 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 $V_m \circ\!\!-\!\!\circ \ldots \circ\!\!-\!\!\circ V_1(=J) \circ\!\!-\!\!\circ V_0(=K), m \ge 1$ 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 $J \rightarrow K$ 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 $L \rightarrow J$. Note $L \rightarrow J$ can only be oriented in the second step as well, as it cannot be oriented in the first step when only the edges containing vertices in $\{\mathbf{C}, X\}$ are transformed, and it cannot appear in $\mathbb{M}_i$ otherwise either $J \rightarrow K$ or $J \leftarrow\!\!* K$ is identified in $\mathbb{M}_i$ due to the complete property of $\mathbb{M}_i$.

If $\mathcal{F}_{V_0} \subset \mathcal{F}_{V_1}$, there is a desired path where $m = 1$. If $\mathcal{F}_{V_0} = \mathcal{F}_{V_1}$, we could find $V_2 \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}]) \backslash \{X\}$ that is not adjacent to V_0 and there is $V_2 \rightarrow V_1$ oriented in the second step. Similarly, we conclude either $\mathcal{F}_{V_1} \subset \mathcal{F}_{V_2}$, in which case there is a desired path where $m = 2$; or $\mathcal{F}_{V_1} = \mathcal{F}_{V_2}$, in which case there is $V_3 \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}]) \backslash \{X\}$ that is not adjacent to V_1 and there is $V_3 \rightarrow V_2$ oriented in the second step. Repeat the process and we can always find an uncovered path $V_m \circ\!\!-\!\!\circ \ldots \circ\!\!-\!\!\circ V_1(=J) \circ\!\!-\!\!\circ V_0(=K), m \ge 1$ in $\mathbb{M}_i[\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}]) \backslash \{X\}]$ where $\mathcal{F}_{V_0} = \cdots = \mathcal{F}_{V_{m-1}} \subset \mathcal{F}_{V_m}$. Finally, it suffices to prove that the path is minimal. If not, there exists a sub-structure $V_k \circ\!\!-\!\!\circ V_{k+1} \circ\!\!-\!\!\circ \cdots \circ\!\!-\!\!\circ V_j, j > k + 2$ where any two non-consecutive vertices are not adjacent except for an edge between V_k and V_j. Since only the edges containing vertices in $\{\mathbf{C}, X\}$ are transformed in the first step, if there is a non-circle edge between V_k and V_j before the second step, the edge is non-circle in $\mathbb{M}_i$, in which case V_k and V_j cannot be in a circle component according to Lemma 3, contradicting with the circle path comprised of $V_k, V_{k+1}, \ldots, V_j$. Hence there is $V_k \circ\!\!-\!\!\circ V_j$ in $\mathbb{M}_i$, in which case the chordal property of $\mathbb{M}_i$ is not fulfilled due to $V_k \circ\!\!-\!\!\circ V_{k+1} \circ\!\!-\!\!\circ \cdots \circ\!\!-\!\!\circ V_j \circ\!\!-\!\!\circ V_k$. Thus the path can only be minimal. $\square$

Lemma 9. *Consider $\mathbb{M}_{i+1}$ in Theorem 1. The subgraph $\mathbb{M}_{i+1}[\mathbf{C}]$ is a complete graph.*

Proof. If it is not a complete graph, new unshielded colliders are introduced by the local BK of X represented by $\mathbf{C}$ when obtaining $\mathbb{M}_{i+1}$ by Algorithm 1. Hence there does not exist an MAG consistent to $\mathbb{M}_{i+1}$. According to Lemma 7 and the basic assumption that BK is correct, there is not an MAG consistent to $\mathbb{M}_i$, contradicting with Lemma 6. □

Lemma 10. *Suppose $\mathbb{M}_s, 0 \le s \le i$ in Theorem 1 satisfy the five properties. And the local BK of X is represented by $\mathbf{C}$. 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 $V \to T$ where $V \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ and $T \in \mathbf{C}$ in $\mathbb{M}_i$. According to Lemma 4, for any MAG oriented from $\mathbb{M}_i$ with the local BK of X represented by $\mathbf{C}$, there is a directed or almost directed cycle $X \to \cdots V \to T {*\!\!\to} X$, contradiction. Hence there is not an MAG consistent to $\mathbb{M}_i$ and local BK. Due to the assumption that BK is correct, there cannot be an MAG consistent to $\mathbb{M}_i$, contradicting with Lemma 6. □

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

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 7 implies that the arrowhead added in Algorithm 1 is invariant in all the MAGs consistent to $\mathbb{M}_i$ and local BK of X represented 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 $A {*\!\!\to} J$ and $B {*\!\!\to} K$ 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 7, there is not an MAG consistent to $\mathbb{M}_i$, which contradicts with Lemma 6. 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 $J \to K$ oriented in the second step, it implies there is $L \to J$ oriented in the second step where L is not adjacent to K. In this case, no matter we orient $J \to K$ 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 $J \to K$ and $J \leftarrow K$ in the second step.

By Lemma 8, if we orient $J \to K$ 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 Algorithm 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 7, 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 inconsistent to $\mathcal{P}$. Given the fact that the local BK represented by $\mathbf{C}$ is correct, there does not exist an MAG consistent to $\mathbb{M}_i$, contradicting with Lemma 6. □

Lemma 12. *Suppose $\mathbb{M}_s, 0 \le s \le i$ in Theorem 1 satisfy the five properties. If there exists an MAG consistent to $\mathbb{M}_{i+1}$, then there is not a new unshielded collider introduced in Algorithm 1.*

Proof. If there are new unshielded colliders introduced in Algorithm 1, due to the invariant property of $\mathbb{M}_{i+1}$ in Lemma 7, there are additional unshielded colliders relative to $\mathcal{P}$ in any MAG consistent to $\mathbb{M}_{i+1}$. Due to the assumption that the local BK is correct, there cannot be MAGs consistent to $\mathbb{M}_i$, contradicting with Lemma 6. □

Lemma 13. *Consider $\mathbb{M}_i$ in Theorem 1 that satisfies the five properties. In the third step of Algorithm 1 to obtain $\mathbb{M}_{i+1}$ based on $\mathbb{M}_i$ and the local BK of X represented 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: $A \circ\!\!-\!\!\circ B$ edges transformed to the edges with arrowheads; $A \leftarrow\!\!\circ B$ edges transformed to $A \leftrightarrow B$; $A \leftarrow\!\!\circ B$ edges transformed to $A \leftarrow B$ ($A \circ\!\!\to B$ 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. Denote the graph obtained from $\mathbb{M}_i$ and BK regarding V_{i+1} after the first two steps of Algorithm 1 by $\bar{\mathbb{M}}_{i+1}$. The proof idea is, suppose in the third step we orient $A \leftarrow\!\circ R$ edges to $A \leftrightarrow R$ 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 directed or bi-directed edges in the third step. If we prove that this edge can be neither an edge $A \leftarrow\!\circ R$ transformed to $A \leftrightarrow B$ nor a circle edge, we have a contradiction. Hence we can conclude that there are no $A \leftarrow\!\circ R$ edges transformed to $A \leftrightarrow R$ or circle edges transformed to directed or bi-directed edges in the third step.

If we transform some edges $A \leftarrow\!\circ R$ to $A \leftrightarrow R$ or transform some circle edges in the third step, the first such edge is not as $A \leftarrow\!\circ R$ and transformed to $A \leftrightarrow R$. Note in the edge aforementioned an arrowhead is introduced. Recall the orientation rules. $\mathcal{R}_3$ is triggered in only the process of obtaining $\mathcal{P}$. $\mathcal{R}'_4$ does not transform an edge $A \leftarrow\!\circ R$ to bi-directed. $\mathcal{R}_8 - \mathcal{R}_{10}$ introduces only 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 $A \leftrightarrow R$. 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 Algorithm 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)** $A \rightarrow B \leftrightarrow R \circ\!\!\rightarrow A$ or **(ii)** $A \leftrightarrow B \rightarrow R \circ\!\!\rightarrow A$. We then prove two results: (**1**) the bi-directed edges in **(i)** or **(ii)** cannot appear in $\mathbb{M}_i$; (**2**) the bi-directed edges cannot be introduced in the first two steps of Algorithm 1 to obtain $\mathbb{M}_{i+1}$ based on the local BK of X represented by $\mathbf{C}$.

(**1**) For **(i)**, suppose there is $B \leftrightarrow R$ in $\mathbb{M}_i$. Since after the first two steps of Algorithm 1 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 $A \rightarrow B$ as case **(i)**. For **(ii)**, suppose there is $A \leftrightarrow B$ in $\mathbb{M}_i$. Since after the first two steps there is $B \rightarrow R$, there must be $B \rightarrow R$ or $B \circ\!\!-\!\!\ast R$ in $\mathbb{M}_i$. For the former case, $A \ast\!\!\rightarrow R$ is in $\mathbb{M}_i$ since $\mathbb{M}_i$ is closed under $\mathcal{R}_2$. For the latter case, $A \ast\!\!\rightarrow R$ is 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.

(**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 Algorithm 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 $A \rightarrow B$ in case **(i)**. For the latter case, since $B \leftarrow\!\circ R$ is transformed to $B \leftrightarrow R$ by the first two steps of Algorithm 1, there is $R \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ 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 Algorithm 1, contradicting with $R \circ\!\!\rightarrow A$ in case **(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 $A \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$, hence $A \leftarrow\!\ast B$ is oriented in the first step, contradicting with $A \rightarrow B$ in case **(i)**. The contradiction for **(ii)** is similar, we do not present the details.

Combining the results in (**1**) and (**2**), the first edge cannot be transformed from $A \leftarrow\!\circ R$ to $A \leftrightarrow R$ by $\mathcal{R}_2$ as well. Hence the first edge mentioned above is not an edge transformed from $A \leftarrow\!\circ R$ to $A \leftrightarrow R$ as no orientation rules can achieve it.

If we transform some edges $A \leftarrow\!\circ R$ to $A \leftrightarrow R$ or transform some circle edges in the third step, the first such edge is not a circle edge. Recall the orientation rules. The result is evident for $\mathcal{R}_8 - \mathcal{R}_{10}$ since the transformed edge is $A \circ\!\!\rightarrow R$. $\mathcal{R}_3$ 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 Algorithm 1. We first consider $\mathcal{R}_1$. Suppose there is $A \ast\!\!\rightarrow B \circ\!\!-\!\!\circ R$ where A and R are not adjacent after the first two steps of Algorithm 1. Since $\mathbb{M}_i$ satisfies the complete property, the arrowhead at B on $A \ast\!\!\rightarrow B$ can only be oriented in the first two steps, otherwise the arrowhead is in $\mathbb{M}_i$ and thus there is either $B \rightarrow R$ or $B \leftarrow\!\ast R$ in $\mathbb{M}_i$. Note the fact that in the first two steps of Algorithm 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 Algorithm 1. Hence there is $R \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$. The edge $A \ast\!\!\rightarrow B$ is oriented in either the first or second step. If $A \ast\!\!\rightarrow B$ is oriented in the first step, $B \rightarrow R$ should be oriented in the second step since $A \in \mathcal{F}_B \backslash \mathcal{F}_R$; if $A \ast\!\!\rightarrow B$ is oriented in the second step, $B \rightarrow R$ is also oriented in the second step, in both of cases there is not $B \circ\!\!-\!\!\circ R$ after the first two steps. Hence $\mathcal{R}_1$ cannot be triggered.

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

(i) For the first case, there is $B \ast\!\!\rightarrow R$ and $A \circ\!\!-\!\!\circ R$ in $\mathbb{M}_i$. According to the balanced property of $\mathbb{M}_i$, there is $A \leftarrow\!\ast B$ in $\mathbb{M}_i$. 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 balanced 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 $B \circ\!\!-\!\!\ast R$ in $\mathbb{M}_i$, there is $B \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$, thus there is $A \ast\!\!\rightarrow R$ 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 Algorithm 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 $A \ast\!\!\rightarrow R$ 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 $A \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$. 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 $A \ast\!\!\rightarrow B$ and $B \rightarrow R$ or $B \circ\!\!-\!\!\ast R$ 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 $A \ast\!\!\rightarrow R$ in $\mathbb{M}_i$, thus there is $A \ast\!\!\rightarrow R$ in $\bar{\mathbb{M}}_{i+1}$, contradiction. If $A \ast\!\!\rightarrow B \circ\!\!-\!\!\ast R$ in $\mathbb{M}_i$, according to the balanced property of $\mathbb{M}_i$, there is also $A \ast\!\!\rightarrow R$ in $\mathbb{M}_i$, thus there is $A \ast\!\!\rightarrow R$ 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 $A \ast\!\!\rightarrow B \leftarrow\!\ast R$ or $A \leftarrow\!\ast B \ast\!\!\rightarrow R$ in $\mathbb{M}_i$. We just show the contradiction for the first case, and the proof for the other 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 the first two steps of Algorithm 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 $A \to B$ 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 PossDe$(X, \mathcal{P}[-\mathbf{C}])$ is oriented in only the second step of Algorithm 1, where we transform circle edges to directed edges, hence there is $A \to B \to R$ in $\bar{\mathbb{M}}_{i+1}$. Then we will prove the impossibility of $A \to B \to R \circ\!\!-\!\!\circ A$ in $\bar{\mathbb{M}}_{i+1}$. According to Lemma 8 and Lemma 11, if $A \to B \to R$ 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 $A \to R$ oriented by the second step of Algorithm 1, contradiction. If there is $\mathcal{F}_A = \mathcal{F}_B = \mathcal{F}_R$, we will prove its impossibility. According to Algorithm 1, there is another vertex $C \in$ PossDe$(X, \mathbb{M}_i[-\mathbf{C}])$ such that $C \to A$ is oriented in the second step of Algorithm 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 $A \to R$ will be oriented to $A \to R$ in the second step of Algorithm 1. Due to Lemma 7, in each MAG $\mathcal{M}$ consistent to $\mathbb{M}_i$ and $\mathbf{C}$, there is $C \to A \to B \to R$, hence there can only be $C \to R$ in $\mathcal{M}$. In this case there is a new unshielded collider $C \to R \leftarrow B$ in $\mathcal{M}$ relative to $\mathbb{M}_i$, which implies that $\mathcal{M}$ cannot be consistent to $\mathbb{M}_i$, contradiction.

With **(i)** and **(ii)**, it is concluded that $\mathcal{R}_2$ is not triggered in the third step of Algorithm 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 there is always a contradiction if new arrowheads are introduced in the third step. Hence, in the third step of Algorithm 1, only the transformation as $A \leftarrow\!\!\circ R$ to $A \leftarrow R$ is possibly triggered by the orientation rules. $\square$

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

Proof. Denote the graph obtained from $\mathbb{M}_i$ and the local BK represented by $\mathbf{C}$ after the first two steps of Algorithm 1 by $\bar{\mathbb{M}}_{i+1}$. According to Lemma 13, no circle edges are oriented in the third step of Algorithm 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 in the form 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 $V_1 \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ and $V_1 \circ\!\!-\!\!\circ V_2$, contradiction. Hence $V_2 \in \mathbf{C}$. In the first step of Algorithm 1, $V_1 \circ\!\!-\!\!\circ V_2$ is transformed to $V_1 \leftarrow\!\!\circ V_2$. Hence after the first step there is not a circle edge connecting $\bar{\mathbb{M}}_{i+1}[\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])]$ and $\bar{\mathbb{M}}_{i+1}[-\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])]$. And there are not circle edges between X and 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 use $\bar{\mathbb{M}}^1_{i+1}$ to denote $\bar{\mathbb{M}}_{i+1}[\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}]) \backslash \{X\}]$.

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 of Algorithm 1 in the process of obtaining $\bar{\mathbb{M}}_{i+1}$ from $\mathbb{M}_i$; **(iii)** Lemma 11.

Suppose the circle component in $\bar{\mathbb{M}}^1_{i+1}$ is not chordal, there is $V_0 \circ\!\!-\!\!\circ V_1 \circ\!\!-\!\!\circ \cdots \circ\!\!-\!\!\circ V_n \circ\!\!-\!\!\circ V_0, n \geq 3$, where there is not a circle edge between every two unconsecutive vertices. There must exist non-circle 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 $\mathbb{M}_i$. Hence, 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, $V_k \to V_m$ is without loss of generality.). According to Lemma 3, $V_k \to V_m$ 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 sub-structure can only be three. Hence it holds $m = k + 2$ and there is $V_k \circ\!\!-\!\!\circ V_{k+1} \circ\!\!-\!\!\circ V_{k+2} \leftarrow V_k$ 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 $V_k \to V_{k+2}$ is oriented in the second step, there is another vertex $F_1 \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}]) \backslash \{X\}$ such that there is $F_1 \to V_k$ oriented in the second step 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, in light of $F_1 \to V_k$, there is $\mathcal{F}_{V_k} \subseteq \mathcal{F}_{F_1}$ according to Algorithm 1 and 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, 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 conclude that in any uncovered directed path $F_t \to \cdots \to F_1 \to V_k \to V_{k+2}$, 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 8. Hence, there cannot be a sub-structure as $V_k \circ\!\!-\!\!\circ V_{k+1} \circ\!\!-\!\!\circ V_{k+2} \leftarrow V_k$ in $\bar{\mathbb{M}}^1_{i+1}$. $\square$

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

Proof. If there is $V_i \ast\!\!\rightarrow V_j \circ\!\!-\!\!\ast V_k$, 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 $V_i \ast\!\!\rightarrow V_j$ is oriented in Algorithm 1. According to Lemma 13, 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 $V_j \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$. In this case if $V_k \in \mathbf{C}$, there is $V_j \leftarrow\!\!\ast V_k$ oriented in the first step, contradiction. Then we consider the case $V_k \notin \mathbf{C}$. If **(i)** 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 $V_j \rightarrow V_k$ is oriented in the second step, contradiction. If **(ii)** $V_j \circ\!\!\rightarrow V_k$ in $\mathbb{M}_i$, it will be oriented as $V_j \rightarrow V_k$ by $\mathcal{R}_1$ in the third step, contradiction. So V_i is adjacent to V_k.

Next we consider the case that V_i is adjacent to V_k. If there is $V_i \ast\!\!\rightarrow V_j \circ\!\!-\!\!\ast V_k$ in $\mathbb{M}_i$, there is $V_i \ast\!\!\rightarrow V_k$ due to the balanced property of $\mathbb{M}_i$, hence $V_i \ast\!\!\rightarrow V_k$ is in $\mathbb{M}_{i+1}$. It then suffices to consider there is $V_i \ast\!\!-\!\!\circ V_j \circ\!\!-\!\!\ast V_k$ in $\mathbb{M}_i$ while $V_i \ast\!\!\rightarrow V_j \circ\!\!-\!\!\ast V_k$ in $\mathbb{M}_{i+1}$. Note in Algorithm 1, arrowheads 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, $V_k \notin \mathbf{C}$, for otherwise there is $V_j \leftarrow\!\!\ast V_k$ in $\mathbb{M}_{i+1}$, contradiction. Combining $V_j \circ\!\!-\!\!\ast V_k$ 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 $V_i \notin \mathbf{C}$, there is $V_i \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ due to $V_i \ast\!\!-\!\!\circ V_j$ 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 $V_i \circ\!\!-\!\!\circ V_j \ast\!\!\rightarrow V_k \leftarrow\!\!\ast V_i$, 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 $V_i \rightarrow V_j \ast\!\!\rightarrow V_k \leftarrow\!\!\ast V_i$ 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 $V_j \circ\!\!-\!\!\ast V_k$ in $\mathbb{M}_{i+1}$. So balanced property holds in $\mathbb{M}_{i+1}$ for the first case. For the latter case, $V_i \rightarrow V_j \circ\!\!-\!\!\circ V_k$ is oriented in the second step. According to the proof of Lemma 14, 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 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 $V_i \rightarrow V_k$ is 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 13 that there are no circle edges oriented in the third step, impossibility.

(ii). If $V_i \in \mathbf{C}$, there is $V_i \ast\!\!\rightarrow V_j$ and $V_i \ast\!\!\rightarrow V_k$ after the first step of Algorithm 1. It is then easy to prove that the balanced property is fulfilled, we do not give the details.

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

Lemma 16. *The PMG $\mathbb{M}_{i+1}$ in Theorem 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 16.1, 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 $\mathbb{M}_{i+1}$, it can be both $A \rightarrow B$ and $A \leftarrow B$ in the MAGs consistent to $\mathcal{P}$ and local BK regarding $V_1, \cdots, V_{i+1}$ according to Lemma 5 of Meek [47]; and for the edge $C \circ\!\!\rightarrow D$ in $\mathbb{M}_{i+1}$, it is $C \rightarrow D$. In Lemma 16.2, we show for the edge $A \circ\!\!\rightarrow B$ in $\mathbb{M}_{i+1}$, it can be $A \leftrightarrow B$. Here the most difficult part is to prove Lemma 16.1, *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 16.2 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 of Lemma 16.2 is too lengthy and completely follows that of Theorem 3 of Zhang [35], we just show the proof sketch.

Lemma 16.1. *Consider $\mathbb{M}_{i+1}$ in Theorem 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. At first, we introduce some notations. We use $\mathcal{M}(\mathbb{M}_j), 0 \le j \le i+1$ to denote the set of graphs that can be obtained from $\mathbb{M}_j$ by transforming all edges $\circ\!\!\rightarrow$ to $\rightarrow$ and orient the circle component into a DAG without unshielded colliders. Our proof is by induction: given the closed, invariant, chordal, and balanced property of $\mathbb{M}_{i+1}$, we will prove that if there is a graph $\mathcal{H}_{i+1} \in \mathcal{M}(\mathbb{M}_{i+1})$ such that $\mathcal{H}_{i+1}$ is not an MAG consistent to $\mathcal{P}$ and local BK regarding $V_1, \cdots, V_{i+1}$, then there is a graph $\mathcal{H}_i \in \mathcal{M}(\mathbb{M}_i)$such that $\mathcal{H}_i$ is not an MAG consistent to $\mathcal{P}$ and local BK regarding $V_1, \cdots, V_i$. By induction, we conclude there is not a graph $\mathcal{H}_0 \in \mathcal{M}(\mathcal{P})$ consistent to $\mathcal{P}$, which contradicts with Theorem 2 of Zhang [35].

In the following there are mainly two parts. The first part is that we construct an auxiliary graph $\mathcal{H}_i$ *based on* $\mathcal{H}_{i+1}$, and we show that $\mathcal{H}_i \in \mathcal{M}(\mathbb{M}_i)$. The second part is we show that if $\mathcal{H}_i$ is an MAG consistent to $\mathcal{P}$ and local BK regarding $V_1, \cdots, V_i$, then $\mathcal{H}_{i+1}$ is an MAG consistent to $\mathcal{P}$ and local BK regarding $V_1, \cdots, V_{i+1}$.

(A) Auxiliary graph $\mathcal{H}_i \in \mathcal{M}(\mathbb{M}_i)$. We construct an auxiliary graph $\mathcal{H}_i$ based on $\mathcal{H}_{i+1}$ by transforming *only and all* the bi-directed edges $K \leftrightarrow T$ to $K \rightarrow T$ which are $K \leftrightarrow T$ in $\mathbb{M}_{i+1}$ but $K \circ\!\!\rightarrow T$ in $\mathbb{M}_i$. Recall Algorithm 1 that obtains $\mathbb{M}_{i+1}$ from $\mathbb{M}_i$. There is $K \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ and $T \in \mathbf{C}$. We want to prove $\mathcal{H}_i \in \mathcal{M}(\mathbb{M}_i)$. Given the fact that the orientation of the circle component in $\mathcal{H}_i$ totally follows that in $\mathcal{H}_{i+1}$, it suffices to show that there are no (almost) directed cycles or unshielded colliders introduced in $\mathcal{H}_{i+1}$ relative to $\mathbb{M}_i$. We show the process of obtaining $\mathcal{H}_{i+1}$ from $\mathbb{M}_i$ as follows.

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

(Step 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_i and V_j such that V_i ∘–∘ V_j, orient it as $V_i \to V_j$ 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 $V_k \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])\backslash\{X\}$ not adjacent to V_j such that $V_k \to V_i$ ∘–∘ V_j, where $\mathcal{F}_{V_l} = \{V \in \mathbf{C} \cup \{X\} \mid V$ ∗–∘ V_l 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 $\mathbb{M}_{i+1}[\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])\backslash\{X\}]$, orient it into a DAG without new unshielded colliders;
(Step 5) for the circle component in subgraph $\mathbb{M}_{i+1}[-\text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])]$, orient it into a DAG without new unshielded colliders;
(Step 6) transform edges ∘→ to →.

Note Step 1 - Step 3 are Algorithm 1. And in Step 4 - Step 6 we transform the edges ∘→ to → and transform the circle component in $\mathbb{M}_{i+1}$ into a DAG without unshielded colliders. The feasibility of transforming the circle component into a DAG without unshielded colliders is due to the fact that the circle component is chordal and every chordal graph has a perfect elimination order, through which we can orient the chordal circle component into a DAG without unshielded colliders. When proving $\mathcal{H}_i \in \mathcal{M}(\mathbb{M}_i)$, 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 $\mathcal{H}_i$ totally follows those in $\mathcal{H}_{i+1}$, which are oriented by either Step 2 or Step 4. There are no new unshielded colliders or directed or almost directed cycles oriented in CC_1 according to the three following facts. **(1).** There are no new unshielded colliders or directed or almost directed cycles in CC_1 oriented by Step 2 according to Lemma 12. **(2).** There are no unshielded colliders or directed or almost directed cycles in 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 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 $\mathcal{H}_{i+1}$. Although when X∘→ T in $\mathbb{M}_i$ where $T \in \mathbf{C}$, there is $X \leftrightarrow T$ in $\mathcal{H}_{i+1}$ while $X \to T$, such edge is not in the circle component CC_2 because it is as X∘→ 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∗→ X ←∗B in edges of CC_2 in Step 2 due to Lemma 9. **(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 $V \to X$.

Then we consider the circle edge in the circle component which connects $K \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])\backslash\{X\}$ 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 $T \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])\backslash\{X\}$ due to $K \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])\backslash\{X\}$ and K ∘–∘ T. Hence in $\mathcal{H}_{i+1}$ the circle edge is oriented as $K \leftarrow T$ in Step 1 and 6. According to the relation between $\mathcal{H}_{i+1}$ and $\mathcal{H}_i$, there is $K \leftarrow T$ in $\mathcal{H}_i$. Hence, for each circle edge K ∘–∘ 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 $\mathcal{H}_i$ and $T \in \mathbf{C} \cup \{X\}$. Hence in $\mathcal{H}_i$ there is not 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 $\mathcal{H}_i$ 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 also appears in $\mathbb{M}_{i+1}$, which contradicts with Lemma 12.

Hence, we prove that $\mathcal{H}_i \in \mathcal{M}(\mathbb{M}_i)$.

(B) If $\mathcal{H}_i$ is an MAG consistent to $\mathcal{P}$ and local BK regarding $V_1, \cdots, V_i$, then $\mathcal{H}_{i+1}$ is an MAG consistent to $\mathcal{P}$ and local BK regarding $V_1, \cdots, V_{i+1}$. Suppose $\mathcal{H}_i$ is an MAG consistent to $\mathcal{P}$ and local BK regarding $V_1, \cdots, V_i$. Since $\mathcal{H}_{i+1}$ has the non-circle marks in $\mathbb{M}_{i+1}$, and $\mathcal{H}_i$ belongs to the MEC represented by $\mathcal{P}$, it suffices to prove that $\mathcal{H}_{i+1}$ is an MAG Markov equivalent to $\mathcal{H}_i$ according to Lemma 1 of Zhang and Spirtes [58].

Note that the only difference between $\mathcal{H}_{i+1}$ and $\mathcal{H}_i$ is that for $\forall K \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ and $\forall T \in \mathbf{C}$ such that K∘→ T in $\mathbb{M}_i$, there is $K \to T$ in $\mathcal{H}_i$ but $K \leftrightarrow T$ in $\mathcal{H}_{i+1}$. Denote the set of different edges in $\mathcal{H}_i^0(=\mathcal{H}_i)$ by $Edge(\mathcal{H}_i^0) = \{K \to T \text{ in } \mathcal{H}_i \mid K \in \text{PossDe}(X, \mathbb{M}_i[-\mathbf{C}]), T \in \mathbf{C}, K$∘→ T in $\mathbb{M}_i\}$. We could obtain $\mathcal{H}_{i+1}$ from $\mathcal{H}_i$ by transforming these edges to bi-directed edges. We transform one edge one time. At first, we select the edge $K \to T$ in $Edge(\mathcal{H}_i^0)$ 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 $V_1 \to V_2$ in $Edge(\mathcal{H}_i^0)$; 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 $K \to V_2$ in $Edge(\mathcal{H}_i^0)$. Then we obtain $Edge(\mathcal{H}_i^1)$ by deleting $K \to T$ from $Edge(\mathcal{H}_i^0)$. By such operation, we obtain a new graph $\mathcal{H}_i^1$ and $Edge(\mathcal{H}_i^1)$. Repeat the process above and we could obtain a series of graphs $\mathcal{H}_i^0(=\mathcal{H}_i), \mathcal{H}_i^1, \cdots, \mathcal{H}_i^m, \mathcal{H}_i^{m+1}(=\mathcal{H}_i)$. We prove the desired result by induction. Given $\mathcal{H}_i$ is an MAG consistent to $\mathcal{P}$, we will show that for any $\mathcal{H}_i^j$ and $\mathcal{H}_i^{j+1}$, where $0 \le j \le m$, if $\mathcal{H}_i^j$ is an MAG, then $\mathcal{H}_i^{j+1}$ is an MAG Markov equivalent to $\mathcal{H}_i^j$. Suppose the edge transformed in $\mathcal{H}_i^j$ is $K \to T$. According to Lemma 1 of Zhang and Spirtes [58], given $\mathcal{H}_i^j$ is an MAG, it suffices to show that (1) there is no directed path from K to T in $\mathcal{H}_i^j$ other than $K \to T$; (2) for any $A \to K$ in $\mathcal{H}_i^j$, $A \to T$ is also in $\mathcal{H}_i^j$; and for any $B \leftrightarrow K$ in $\mathcal{H}_i^j$, either $B \to T$ or $B \leftrightarrow T$ is in $\mathcal{H}_i^j$; (3) there is no discriminating path for K on which T is the endpoint adjacent to K in $\mathcal{H}_i^j$.

(1) For the sake of contradiction, suppose there is a directed path from K to T in $\mathcal{H}_i^j$ other that $K \rightarrow T$, 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 whole process, the directed path is also in $\mathcal{H}_i^0$. We first prove that there must be a vertex $F_n, 1 \le n \le m$ 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 $\mathcal{H}_{i+1}$, there is $F_m \leftarrow T$ in $\mathcal{H}_{i+1}$. Since we never reverse an edge in the process from $\mathcal{H}_i$ to $\mathcal{H}_{i+1}$, there cannot be an edge $F_m \rightarrow T$ in $\mathcal{H}_i^j$. **(iii.)** If there is $F_m \circ\!\!\rightarrow T$ in $\mathbb{M}_i$, there is $F_m \rightarrow T$ in $\mathcal{H}_i^0$ and $\mathcal{H}_i^j$. According to the edge selection criterion, when there is both $F_m \rightarrow T$ and $K \rightarrow T$ in $\mathcal{H}_i^j$, we 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 $\mathcal{H}_i^j$. Hence we conclude there is a vertex $F_n, 1 \le n \le m$ such that $F_n \in \mathbf{C}$.

Without loss of generality, we suppose $F_n \in \mathbf{C}$ and $F_l \notin \mathbf{C}, \forall 1 \le l \le n-1$. We first prove there is not a vertex $F_l, 1 \le l \le n-1$ adjacent to T. If there is, since $F_l \rightarrow \cdots \rightarrow F_m \rightarrow T$ in $\mathcal{H}_i$, there is $F_l \rightarrow T$ in $\mathcal{H}_i$ 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 $\mathcal{H}_i$, 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 $\forall 1 \le l \le n-1$. **(i.)** If $n \ge 2$, **(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 $\mathcal{R}_9$ 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 $\mathcal{H}_i$, 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 $\mathcal{H}_i^j$, contradiction. **(ii.)** If $n = 1$, there is $K \rightarrow T' \rightarrow T$ in $\mathcal{H}_{i+1}$, 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 $\mathcal{H}_i^j$; if there is $K \circ\!\!\rightarrow T'$ in $\mathbb{M}_i$, there is thus both $K \rightarrow T'$ and $K \rightarrow T$ in $\mathcal{H}_i$, $K \circ\!\!\rightarrow T'$ is transformed to bi-directed ahead of $K \rightarrow T$ due to $T' \rightarrow T$, thereby there is not an edge $K \rightarrow T'$ in $\mathcal{H}_i^j$. Hence there cannot be a sub-structure $K \rightarrow T' \rightarrow T$ in $\mathcal{H}_i^j$, contradiction. Hence, there is always a contradiction if there is a directed path from K to T in $\mathcal{H}_i^j$.

(2) In this part, we prove that if there is an edge $A \rightarrow K$ in $\mathcal{H}_i^j$, there is $A \rightarrow T$ in $\mathcal{H}_i^j$; if there is $B \leftrightarrow K$ in $\mathcal{H}_i^j$, either $B \rightarrow T$ or $B \leftrightarrow T$ is in $\mathcal{H}_i^j$. 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 A such that $A \rightarrow K$ or $A \leftrightarrow K$ in $\mathcal{H}_i^j$, A is adjacent to T. According to the ancestral property of $\mathcal{H}_i^j$, we get the desired result due to $K \rightarrow T$ in $\mathcal{H}_i^j$.

We discuss the possible cases of the edge between A and K in $\mathbb{M}_i$. If there is $A *\!\!\rightarrow K \circ\!\!\rightarrow T$ in $\mathbb{M}_i$, due to 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 $A \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ due to $K \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$. Suppose T is not adjacent to A for contradiction. In this case, we orient $K \rightarrow A$ in the second step due to $T \in \mathcal{F}_K \backslash \mathcal{F}_A$, there is thus $K \rightarrow A$ in $\mathcal{H}_i^0$. Considering we never reverse a directed edge in the whole procedure, there is not $A \rightarrow K$ in $\mathcal{H}_i^j$. And since only the directed edge connecting a vertex in $\mathbf{C}$ and a vertex in $\mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ is possibly converted to a bi-directed edge in the process from $\mathcal{H}_i^0$ to $\mathcal{H}_i^j$, $A \leftarrow K$ cannot be transformed to $A \leftrightarrow K$ due to $A, K \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$, so that $A \leftrightarrow K$ is not in $\mathcal{H}_i^j$. Hence when $A \circ\!\!-\!\!\circ K$ in $\mathbb{M}_i$ and $A \notin \mathbf{C}$, there is not an edge $A \rightarrow K$ or $A \leftrightarrow K$ in $\mathcal{H}_i^j$. 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 $\mathcal{H}_i$. Since we never reverse a directed edge in the whole process, and only the directed edge connecting a vertex in $\mathbf{C}$ and a vertex in $\mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ is possibly converted to a bi-directed edge in the process from $\mathcal{H}_i$ to $\mathcal{H}_{i+1}$, we only need to consider there is $A \leftrightarrow K$ in $\mathcal{H}_i^j$, where $A \in \mathbf{C}$. In this case, A is adjacent to T according to 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 $A \rightarrow K$ or $A \leftrightarrow K$ in $\mathcal{H}_i^j$. We thus have considered all the possible cases and conclude that if there is $A \rightarrow K$ in $\mathcal{H}_i^j$, there is $A \rightarrow T$ in $\mathcal{H}_i^j$; if there is $A \leftrightarrow K$ in $\mathcal{H}_i^j$, either $A \rightarrow T$ or $A \leftrightarrow T$ is in $\mathcal{H}_i^j$ 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 $\mathcal{H}_i^j$. The proof refers to that of (T3) of Theorem 3 by Zhang [35], with modifications due to the additional background knowledge.

Suppose a path $p = (V_0, V_1, \cdots, V_n = K, T)$ in $\mathcal{H}_i^j$ which is a discriminating path for K. Without loss of generality, suppose p is the shortest path. According to the construction of $\mathrm{Edge}(\mathcal{H}_i^j)$, 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 $i \ge 1$ (there is local BK) it will be oriented as $K \rightarrow T$ by $\mathcal{R}_4'$ or if $i = 0$ (there is not local BK) it will be oriented as $K \rightarrow T$ 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 $\mathcal{H}_i^j$, 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 $\mathcal{H}_i^j$, contradiction. It follows that every edge on the subpath from V_1 to K is bi-directed in $\mathcal{H}_i^j$.

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 $\mathbb{M}_i$ due to the 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 $\mathcal{H}_i^j$ and $\mathcal{H}_i^j$ is an MAG Markov equivalent to $\mathcal{H}_i$ 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 $\mathcal{H}_i^j$, 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 $\mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$, and we never orient an edge connecting two vertices from $\mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ as bi-directed, hence $V_0 {*\!\!\rightarrow} V_1$ and $V_1 \leftrightarrow V_2$ cannot be oriented at the same time in the process of obtaining $\mathcal{H}_{i+1}$ from $\mathcal{H}_i$.

(ii). Suppose $V_0 \leftarrow\!\circ V_1$. Due to the fact that a bi-directed edge is oriented in $\mathcal{H}_i^j$ compared to $\mathbb{M}_i$ only if the edge connects a vertex in $\mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ and a vertex in $\mathbf{C}$, and the fact that an arrowhead is added only at the vertex in $\mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$, there is $V_0 \in \mathbf{C}$ and $V_1 \in \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$. 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 that there is $V_0 {*\!\!\rightarrow} V_1$ in $\mathbb{M}_i$. The remaining part is to prove by induction that for every $1 \le i \le n-1$, 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 $V_1 \notin \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$ due to $\mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}]) \cap \mathrm{Pa}(\mathbf{C}, \mathbb{M}_i) = \emptyset$ as Lemma 10. Hence, there cannot be an edge $V_1 \to V_2$ in $\mathbb{M}_i$ since the edge cannot be oriented as $V_1 \leftrightarrow V_2$ in $\mathcal{H}_i^j$. If there is not a collider at V_1 in $\mathbb{M}_i$, there is $V_1 {\circ\!\!\rightarrow} V_2$. It is impossible because we never transform it to bi-directed in the process from $\mathbb{M}_i$ to $\mathcal{H}_i^0$ as $V_1 \notin \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$. Hence the collider is identifiable in $\mathbb{M}_i$. Similarly, we could prove $V_2 \to T$ in $\mathbb{M}_i$. Then we prove there is $V_2 \leftarrow\!* V_3$ in $\mathbb{M}_i$. If the edge is a circle edge, then there must be $V_1 \circ\!\!-\!\!\circ V_3$ according to the balance property, in which case there is a shorter discriminating path, contradiction. Then we consider the edge is $V_2 {*\!\!\rightarrow} V_3$. Due to $T \in \mathbf{C}$ and $\mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}]) \cap \mathrm{Pa}(\mathbf{C}, \mathbb{M}_i) = \emptyset$, $V_2 \notin \mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$. Hence $V_2 {*\!\!\rightarrow} V_3$ in $\mathbb{M}_i$ can never be transformed to bi-directed since arrowhead is added at only the vertex in $\mathrm{PossDe}(X, \mathbb{M}_i[-\mathbf{C}])$. Thus $V_1 \leftrightarrow V_2 \leftarrow\!* V_3$ is identifiable in $\mathbb{M}_i$. 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 $i \ge 1$ 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 $K {\circ\!\!\rightarrow} T$ in $\mathbb{M}_i$.

Hence, we conclude that $\mathcal{H}_{i+1}$ is an MAG Markov equivalent to $\mathcal{H}_i$. It is evident that $\mathcal{H}_{i+1}$ has the non-circle marks in $\mathbb{M}_{i+1}$. Since $\mathcal{H}_i$ belongs to the MEC represented by $\mathcal{P}$, $\mathcal{H}_{i+1}$ also belongs to the MEC. We conclude that $\mathcal{H}_{i+1}$ 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, (**A**) $\mathcal{H}_i \in \mathcal{M}(\mathbb{M}_i)$ (**B**), if a graph $\mathcal{H}_{i+1} \in \mathcal{M}(\mathbb{M}_{i+1})$ is not an MAG consistent to $\mathcal{P}$ and the local BK regarding $V_1, \cdots, V_{i+1}$, then a graph $\mathcal{H}_i \in \mathcal{M}(\mathbb{M}_i)$ is not an MAG consistent to $\mathcal{P}$ and the local BK regarding $V_1, \cdots, V_i$. By induction, we conclude that if a graph $\mathcal{H}_{i+1} \in \mathcal{M}(\mathbb{M}_{i+1})$ is not an MAG consistent to $\mathcal{P}$ and the local BK regarding $V_1, \cdots, V_{i+1}$, there is an MAG $\mathcal{H}_0 \in \mathcal{M}(\mathcal{P})$ that is not an MAG consistent to $\mathcal{P}$, which contradicts with Theorem 2 of Zhang [35]. □

Lemma 16.2. *Suppose there is $A {\circ\!\!\rightarrow} B$ in the PMG $\mathbb{M}_{i+1}$ in Theorem 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 15. 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 16.1, 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 $\mathcal{H}_{i+1}$ with $A \leftrightarrow B$ by the same procedure of Theorem 3 of Zhang [35] and prove $\mathcal{H}_{i+1}$ 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 16.1, $\mathcal{H}_0$ is an MAG in the MEC represented by $\mathcal{P}$. Hence $\mathcal{H}_{i+1}$ 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 $V_1, \cdots, V_{i+1}$. □

Proof of Theorem 1. The closed, invariant, chordal, balanced, complete properties of $\mathbb{M}_{i+1}$ are proved by Lemma 5, 7, 14, 15, 16. □

Appendix C. Additional experimental results in Section 5.2

We show the experimental results for the respective three stages of the active learning framework in Tables C.3/C.4/C.5/C.6/C.7 for $d = 6/8/12/14/16$ (see Table 1 in the main paper for $d = 10$). And we show the ratio of reduced intervention times by MaxEnt relative to random strategy and the ration of marks learned by rules to the total learned marks under CIS/CS in Table C.8.

Table C.3
Number of correctly/wrongly learned marks in PAG, Number of interventions, number of correctly/ wrongly learned marks by interventions, normalized SHD, and F1 score over 100 simulations with $d = 6$ and varying p in the format of mean ± std.

Stage	Stage 1		Stage 2	Stage 3		Whole process	
strategy-p	# correct PAG	# wrong PAG	# int.	# correct int.	# wrong int.	Norm. SHD	F1 score
Random-0.10 MCMC-0.10	0.78 ± 1.30	0.10 ± 0.30	0.73 ± 0.93 0.65 ± 0.86	0.73 ± 1.22 0.72 ± 1.22	0.01 ± 0.10 0.02 ± 0.20	0.04 ± 0.10 0.04 ± 0.10	0.89 ± 0.31 0.89 ± 0.31
Random-0.15 MCMC-0.15	1.35 ± 1.38	0.06 ± 0.40	1.11 ± 0.96 0.98 ± 0.86	1.22 ± 1.35 1.25 ± 1.34	0.09 ± 0.40 0.06 ± 0.31	0.05 ± 0.13 0.05 ± 0.13	0.87 ± 0.33 0.89 ± 0.32
Random-0.20 MCMC-0.20	1.51 ± 1.53	0.05 ± 0.39	1.14 ± 0.97 1.00 ± 0.86	1.33 ± 1.44 1.32 ± 1.39	0.10 ± 0.41 0.11 ± 0.53	0.05 ± 0.13 0.05 ± 0.15	0.88 ± 0.32 0.89 ± 0.30
Random-0.25 MCMC-0.25	1.93 ± 1.59	0.09 ± 0.38	1.41 ± 0.88 1.33 ± 0.83	1.71 ± 1.47 1.67 ± 1.38	0.06 ± 0.31 0.10 ± 0.50	0.05 ± 0.13 0.06 ± 0.16	0.88 ± 0.32 0.88 ± 0.32
Random-0.30 MCMC-0.30	2.64 ± 1.79	0.05 ± 0.39	1.60 ± 0.84 1.55 ± 0.82	2.24 ± 1.68 2.25 ± 1.62	0.08 ± 0.54 0.07 ± 0.33	0.04 ± 0.15 0.05 ± 0.13	0.91 ± 0.27 0.92 ± 0.25

Table C.4
Number of correctly/wrongly learned marks in PAG, Number of interventions, number of correctly/ wrongly learned marks by interventions, normalized SHD, and F1 score over 100 simulations with $d = 8$ and varying p in the format of mean ± std.

Stage	Stage 1		Stage 2	Stage 3		Whole process	
strategy-p	# correct PAG	# wrong PAG	# int.	# correct int.	# wrong int.	Norm. SHD	F1 score
Random-0.10 MCMC-0.10	2.43 ± 2.26	0.32 ± 0.72	1.73 ± 1.27 1.63 ± 1.10	2.15 ± 2.01 2.17 ± 2.01	0.05 ± 0.30 0.03 ± 0.22	0.04 ± 0.07 0.04 ± 0.07	0.84 ± 0.33 0.85 ± 0.32
Random-0.15 MCMC-0.15	3.72 ± 2.61	0.25 ± 0.56	2.17 ± 1.07 2.09 ± 1.06	3.12 ± 1.98 3.09 ± 1.92	0.04 ± 0.24 0.07 ± 0.41	0.03 ± 0.06 0.03 ± 0.06	0.89 ± 0.26 0.88 ± 0.26
Random-0.20 MCMC-0.20	5.12 ± 3.18	0.32 ± 1.16	2.16 ± 1.03 2.21 ± 1.01	3.61 ± 2.16 3.67 ± 2.17	0.14 ± 0.55 0.08 ± 0.39	0.05 ± 0.12 0.04 ± 0.12	0.91 ± 0.21 0.93 ± 0.19
Random-0.25 MCMC-0.25	6.17 ± 3.42	0.44 ± 1.31	2.56 ± 1.17 2.52 ± 1.02	4.62 ± 2.75 4.57 ± 2.70	0.15 ± 0.56 0.20 ± 0.62	0.06 ± 0.14 0.06 ± 0.13	0.90 ± 0.23 0.91 ± 0.20
Random-0.30 MCMC-0.30	7.91 ± 3.84	0.38 ± 0.95	2.97 ± 1.18 2.85 ± 1.09	5.57 ± 3.09 5.43 ± 2.96	0.20 ± 0.51 0.34 ± 0.79	0.06 ± 0.10 0.07 ± 0.10	0.93 ± 0.13 0.92 ± 0.12

Table C.5
Number of correctly/wrongly learned marks in PAG, Number of interventions, number of correctly/ wrongly learned marks by interventions, normalized SHD, and F1 score over 100 simulations with $d = 12$ and varying p in the format of mean ± std.

Stage	Stage 1		Stage 2	Stage 3		Whole process	
Strategy-p	# correct PAG	# wrong PAG	# int.	# correct int.	# wrong int.	Norm. SHD	F1
Random-0.10 MCMC-0.10	7.93 ± 3.78	0.48 ± 1.02	3.84 ± 1.34 3.67 ± 1.24	5.95 ± 2.37 5.95 ± 2.39	0.09 ± 0.40 0.09 ± 0.38	0.02 ± 0.03 0.02 ± 0.03	0.92 ± 0.14 0.92 ± 0.14
Random-0.15 MCMC-0.15	11.0 ± 3.66	0.87 ± 1.68	4.49 ± 1.33 4.07 ± 1.09	7.12 ± 2.59 7.20 ± 2.68	0.17 ± 0.65 0.09 ± 0.43	0.03 ± 0.05 0.03 ± 0.05	0.92 ± 0.11 0.92 ± 0.11

References

[1] J. Tian, J. Pearl, A general identification condition for causal effects, in: Proceedings of the 18th AAAI Conference on Artificial Intelligence, 2002, pp. 567–573.
[2] I. Shpitser, J. Pearl, Identification of joint interventional distributions in recursive semi-Markovian causal models, in: Proceedings of the 21st AAAI Conference on Artificial Intelligence, 2006, pp. 1219–1226.
[3] S. Lee, E. Bareinboim, Causal effect identifiability under partial-observability, in: Proceedings of the 37th International Conference on Machine Learning, 2020, pp. 5692–5701.

Table C.5 (*continued*)

Stage	Stage 1		Stage 2	Stage 3		Whole process	
Strategy-p	# correct PAG	# wrong PAG	# int.	# correct int.	# wrong int.	Norm. SHD	F1
Random-0.20 MCMC-0.20	14.5 ± 4.11	2.06 ± 2.77	4.69 ± 1.22 4.40 ± 1.14	9.04 ± 2.96 9.03 ± 3.03	0.27 ± 0.58 0.28 ± 0.64	0.06 ± 0.08 0.06 ± 0.08	0.88 ± 0.13 0.88 ± 0.14
Random-0.25 MCMC-0.25	14.3 ± 3.74	5.46 ± 5.19	4.10 ± 1.47 3.98 ± 1.58	7.84 ± 3.36 7.89 ± 3.40	0.41 ± 0.85 0.36 ± 0.67	0.16 ± 0.15 0.16 ± 0.15	0.75 ± 0.21 0.75 ± 0.21
Random-0.30 MCMC-0.30	14.3 ± 4.32	8.00 ± 6.21	4.13 ± 1.55 4.09 ± 1.56	7.43 ± 3.49 7.49 ± 3.51	0.65 ± 1.04 0.59 ± 0.95	0.24 ± 0.18 0.24 ± 0.18	0.65 ± 0.24 0.65 ± 0.24

Table C.6
Number of correctly/wrongly learned marks in PAG, Number of interventions, number of correctly/ wrongly learned marks by interventions, normalized SHD, and F1 score over 100 simulations with $d = 14$ and varying p in the format of mean ± std.

Stage	Stage 1		Stage 2	Stage 3		Whole process	
Strategy-p	# correct PAG	# wrong PAG	# int.	# correct int.	# wrong int.	Norm. SHD	F1
Random-0.10 MCMC-0.10	12.1 ± 4.91	0.67 ± 1.12	5.20 ± 1.41 4.71 ± 1.42	8.27 ± 2.90 8.25 ± 2.92	0.17 ± 0.55 0.19 ± 0.56	0.02 ± 0.02 0.02 ± 0.02	0.91 ± 0.13 0.91 ± 0.13
Random-0.15 MCMC-0.15	16.8 ± 4.49	1.90 ± 3.10	5.45 ± 1.75 4.93 ± 1.38	10.4 ± 3.70 10.5 ± 3.71	0.28 ± 0.75 0.20 ± 0.55	0.04 ± 0.06 0.04 ± 0.06	0.90 ± 0.14 0.90 ± 0.13
Random-0.20 MCMC-0.20	16.6 ± 5.56	6.50 ± 5.85	5.18 ± 1.68 5.09 ± 1.61	10.3 ± 4.16 10.4 ± 4.29	0.44 ± 0.88 0.43 ± 0.82	0.13 ± 0.11 0.13 ± 0.11	0.74 ± 0.21 0.74 ± 0.21
Random-0.25 MCMC-0.25	14.3 ± 5.73	11.6 ± 8.18	5.27 ± 1.52 5.20 ± 1.55	9.86 ± 3.98 9.83 ± 4.04	0.84 ± 1.14 0.87 ± 1.14	0.23 ± 0.16 0.23 ± 0.16	0.59 ± 0.25 0.59 ± 0.25
Random-0.30 MCMC-0.30	12.6 ± 5.77	16.8 ± 9.07	5.31 ± 1.63 5.37 ± 1.53	8.82 ± 3.84 8.88 ± 3.76	1.30 ± 1.54 1.24 ± 1.35	0.33 ± 0.17 0.33 ± 0.17	0.45 ± 0.23 0.45 ± 0.23

Table C.7
Number of correctly/wrongly learned marks in PAG, Number of interventions, number of correctly/ wrongly learned marks by interventions, normalized SHD, and F1 score over 100 simulations with $d = 16$ and varying p in the format of mean ± std.

Stage	Stage 1		Stage 2	Stage 3		Whole process	
Strategy-p	# correct PAG	# wrong PAG	# int.	# correct int.	# wrong int.	Norm. SHD	F1
Random-0.10 MCMC-0.10	16.0 ± 5.48	1.19 ± 1.90	10.4 ± 3.41 10.5 ± 3.49	0.27 ± 0.78 0.25 ± 0.63	6.12 ± 1.65 5.58 ± 1.55	0.02 ± 0.03 0.02 ± 0.03	0.92 ± 0.10 0.92 ± 0.10
Random-0.15 MCMC-0.15	20.3 ± 5.51	4.10 ± 4.47	12.2 ± 3.63 12.2 ± 3.66	0.45 ± 1.02 0.48 ± 1.06	6.18 ± 1.51 5.85 ± 1.54	0.06 ± 0.06 0.06 ± 0.06	0.83 ± 0.15 0.83 ± 0.16
Random-0.20 MCMC-0.20	18.0 ± 5.99	10.2 ± 8.72	12.8 ± 3.90 12.8 ± 3.88	0.91 ± 1.33 0.95 ± 1.29	6.78 ± 1.67 6.20 ± 1.69	0.14 ± 0.12 0.14 ± 0.12	0.67 ± 0.23 0.67 ± 0.23
Random-0.25 MCMC-0.25	11.8 ± 6.72	21.3 ± 10.3	9.81 ± 3.82 10.1 ± 3.67	1.49 ± 1.42 1.18 ± 1.17	6.19 ± 1.72 6.08 ± 1.86	0.29 ± 0.14 0.29 ± 0.14	0.40 ± 0.22 0.41 ± 0.22
Random-0.30 MCMC-0.30	8.17 ± 4.93	29.6 ± 9.81	7.69 ± 2.96 7.71 ± 2.96	2.17 ± 1.68 2.15 ± 1.56	6.14 ± 1.73 6.27 ± 1.66	0.41 ± 0.13 0.41 ± 0.13	0.24 ± 0.15 0.23 ± 0.14

Table C.8
The ratio of reduced intervention times by MaxEnt relative to random strategy and the ratio of marks learned by orientation rules under CS and CIS over 100 simulations with varying d and p in the format of mean ± std.

d	p	#diff-CIS	#diff-CS	%rule-CIS	%rule-CS
6	0.10 0.15 0.20 0.25 0.30	2.62 ± 1.58% 2.53 ± 2.11% 3.48 ± 2.18% 3.97 ± 1.37% 3.64 ± 2.22%	8.11± 4.33% 13.3± 4.90% 15.5± 5.09% 16.4± 5.75% 18.0± 6.06%	14.9 ± 1.78% 15.0 ± 3.21% 16.0 ± 2.07% 15.8 ± 1.97% 16.7 ± 2.07%	52.6± 12.2% 54.8± 11.1% 57.8± 8.49% 58.3± 7.08% 59.9± 7.52%
8	0.10 0.15 0.20 0.25 0.30	4.02 ± 2.80% 6.48 ± 2.27% 6.63 ± 3.78% 6.26 ± 1.59% 5.79 ± 1.61%	14.0± 4.64% 16.9± 3.98% 19.9± 3.78% 22.0± 3.62% 23.2± 5.13%	18.5 ± 2.58% 21.0 ± 1.92% 21.0 ± 2.26% 21.2 ± 1.11% 21.6 ± 1.42%	59.4± 5.41% 62.1± 4.88% 65.6± 5.94% 66.8± 4.77% 67.1± 3.81%

(*continued on next page*)

Table C.8 (*continued*)

d	p	#diff-CIS	#diff-CS	%rule-CIS	%rule-CS
10	0.10	5.13 ± 1.79%	14.2± 2.17%	19.8 ± 1.65%	61.6± 3.28%
	0.15	6.21 ± 2.93%	17.0± 4.05%	21.1 ± 1.76%	65.2± 3.61%
	0.20	7.64 ± 1.60%	21.4± 4.21%	22.1 ± 0.87%	67.3± 3.21%
	0.25	6.73 ± 1.73%	23.4± 3.10%	21.2 ± 1.61%	68.9± 2.59%
	0.30	6.14 ± 1.92%	22.1± 4.14%	21.4 ± 1.08%	69.3± 2.27%
12	0.10	6.77 ± 1.29%	16.4± 1.41%	21.0 ± 1.64%	66.2± 2.01%
	0.15	8.15 ± 1.50%	18.9± 3.82%	21.5 ± 1.06%	66.7± 2.69%
	0.20	8.16 ± 1.66%	24.5± 3.68%	20.6 ± 1.99%	70.3± 2.67%
	0.25	6.96 ± 1.69%	24.2± 2.71%	20.2 ± 1.24%	71.0± 2.26%
	0.30	6.52 ± 1.19%	24.7± 6.66%	21.4 ± 1.66%	72.2± 3.06%
14	0.10	6.45 ± 1.72%	19.7± 3.60%	20.7 ± 1.34%	66.3± 2.40%
	0.15	6.72 ± 2.02%	22.2± 6.54%	20.8 ± 1.12%	69.6± 4.44%
	0.20	7.43 ± 1.52%	24.6± 5.06%	20.4 ± 0.74%	70.7± 1.87%
	0.25	5.90 ± 1.84%	24.7± 4.94%	19.5 ± 1.04%	71.9± 2.64%
	0.30	5.28 ± 0.65%	25.0± 4.11%	19.7 ± 0.70%	73.0± 1.54%
16	0.10	7.79 ± 1.93%	18.3± 4.16%	22.4 ± 1.55%	66.9± 2.30%
	0.15	6.82 ± 1.43%	24.5± 2.92%	20.6 ± 1.35%	71.2± 1.65%
	0.20	6.45 ± 1.87%	24.2± 2.93%	19.7 ± 1.34%	71.0± 2.19%
	0.25	6.16 ± 1.16%	23.0± 3.16%	19.1 ± 1.47%	72.4± 2.01%
	0.30	4.86 ± 1.50%	24.3± 2.01%	19.2 ± 1.48%	73.3± 1.63%

[4] T. Qin, T.-Z. Wang, Z.-H. Zhou, Budgeted heterogeneous treatment effect estimation, in: Proceedings of the 38th International Conference on Machine Learning, 2021, pp. 8693–8702.
[5] J. von Kügelgen, A.-H. Karimi, U. Bhatt, I. Valera, A. Weller, B. Schölkopf, On the fairness of causal algorithmic recourse, arXiv preprint, arXiv:2010.06529, 2020.
[6] N. Kilbertus, M. Rojas-Carulla, G. Parascandolo, M. Hardt, D. Janzing, B. Schölkopf, Avoiding discrimination through causal reasoning, in: Advances in Neural Information Processing Systems, 2017, pp. 656–666.
[7] W. Cheng, K. Zhang, H. Chen, G. Jiang, Z. Chen, W. Wang, Ranking causal anomalies via temporal and dynamical analysis on vanishing correlations, in: Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, 2016, pp. 805–814.
[8] W. Yang, K. Zhang, S.C. Hoi, Causality-based multivariate time series anomaly detection, arXiv preprint, arXiv:2206.15033, 2022.
[9] Z.-H. Zhou, Open-environment machine learning, Nat. Sci. Rev. 9 (2022) nwac123.
[10] M. Arjovsky, L. Bottou, I. Gulrajani, D. Lopez-Paz, Invariant risk minimization, arXiv preprint, arXiv:1907.02893, 2019.
[11] B. Schölkopf, F. Locatello, S. Bauer, N.R. Ke, N. Kalchbrenner, A. Goyal, Y. Bengio, Towards causal representation learning, arXiv preprint, arXiv:2102.11107, 2021.
[12] J. Pearl, Causality, Cambridge University Press, 2009.
[13] P. Spirtes, C. Glymour, R. Scheines, Causation, Prediction, and Search, MIT Press, 2000.
[14] D.M. Chickering, Optimal structure identification with greedy search, J. Mach. Learn. Res. 3 (2002) 507–554.
[15] S. Magliacane, T. Claassen, J.M. Mooij, Ancestral causal inference, in: Advances in Neural Information Processing Systems, 2016, pp. 4466–4474.
[16] B. Huang, K. Zhang, Y. Lin, B. Schölkopf, C. Glymour, Generalized score functions for causal discovery, in: Proceedings of the 24th ACM International Conference on Knowledge Discovery and Data Mining, 2018, pp. 1551–1560.
[17] D.I. Bernstein, B. Saeed, C. Squires, C. Uhler, Ordering-based causal structure learning in the presence of latent variables, in: Proceedings of the 23rd International Conference on Artificial Intelligence and Statistics, 2020, pp. 4098–4108.
[18] J. Peters, J.M. Mooij, D. Janzing, B. Schölkopf, Causal discovery with continuous additive noise models, J. Mach. Learn. Res. 15 (2014) 2009–2053.
[19] R. Cai, J. Qiao, K. Zhang, Z. Zhang, Z. Hao, Causal discovery from discrete data using hidden compact representation, in: Advances in Neural Information Processing Systems, 2018, pp. 2666–2674.
[20] I. Ng, S. Lachapelle, N.R. Ke, S. Lacoste-Julien, K. Zhang, On the convergence of continuous constrained optimization for structure learning, in: Proceedings of the 25th International Conference on Artificial Intelligence and Statistics, 2022, pp. 8176–8198.
[21] J. Peters, P. Bühlmann, N. Meinshausen, Causal inference by using invariant prediction: identification and confidence intervals, J. R. Stat. Soc., Ser. B, Stat. Methodol. 78 (2016) 947–1012.
[22] B. Huang, K. Zhang, J. Zhang, J.D. Ramsey, R. Sanchez-Romero, C. Glymour, B. Schölkopf, Causal discovery from heterogeneous/nonstationary data, J. Mach. Learn. Res. 21 (2020) 89.
[23] Y. He, Z. Geng, Active learning of causal networks with intervention experiments and optimal designs, J. Mach. Learn. Res. 9 (2008) 2523–2547.
[24] A. Hauser, P. Bühlmann, Characterization and greedy learning of interventional Markov equivalence classes of directed acyclic graphs, J. Mach. Learn. Res. 13 (2012) 2409–2464.
[25] K. Shanmugam, M. Kocaoglu, A.G. Dimakis, S. Vishwanath, Learning causal graphs with small interventions, in: Advances in Neural Information Processing System, 2015, pp. 3195–3203.
[26] S. Triantafillou, I. Tsamardinos, Constraint-based causal discovery from multiple interventions over overlapping variable sets, J. Mach. Learn. Res. 16 (2015) 2147–2205.
[27] Y. Wang, L. Solus, K. Yang, C. Uhler, Permutation-based causal inference algorithms with interventions, in: Advances in Neural Information Processing Systems, 2017, pp. 5824–5833.
[28] J. Gamella, C. Heinze-Deml, Active invariant causal prediction: experiment selection through stability, in: Advances in Neural Information Processing Systems, 2020, pp. 15464–15475.
[29] A. Jaber, M. Kocaoglu, K. Shanmugam, E. Bareinboim, Causal discovery from soft interventions with unknown targets: characterization and learning, in: Advances in Neural Information Processing Systems, 2020, pp. 9551–9561.
[30] T.-Z. Wang, Z.-H. Zhou, Actively identifying causal effects with latent variables given only response variable observable, in: Advances in Neural Information Processing Systems, 2021, pp. 15007–15018.
[31] K. Yu, L. Liu, J. Li, Learning Markov blankets from multiple interventional data sets, IEEE Trans. Neural Netw. Learn. Syst. 31 (2019) 2005–2019.
[32] X. Shen, S. Ma, P. Vemuri, S. Gyorgy, W.M. W, A. Paul, P. Ronald, J.C. R, S.A. J, J. William, et al., Challenges and opportunities with causal discovery algorithms: application to Alzheimer's pathophysiology, Sci. Rep. 10 (2020) 2975.

[33] T. Richardson, P. Spirtes, et al., Ancestral graph Markov models, Ann. Stat. 30 (2002) 962–1030.
[34] R.A. Ali, T. Richardson, P. Spirtes, J. Zhang, Orientation rules for constructing Markov equivalence classes of maximal ancestral graphs, Technical Report, 2005.
[35] J. Zhang, On the completeness of orientation rules for causal discovery in the presence of latent confounders and selection bias, Artif. Intell. 172 (2008) 1873–1896.
[36] F. Eberhardt, Causation and intervention, Unpublished doctoral dissertation, Carnegie Mellon University, 2007.
[37] D. Malinsky, P. Spirtes, Estimating causal effects with ancestral graph Markov models, in: Proceedings of the 8th International Conference on Probabilistic Graphical Models, 2016, pp. 299–309.
[38] D. Malinsky, P. Spirtes, Estimating bounds on causal effects in high-dimensional and possibly confounded systems, Int. J. Approx. Reason. 88 (2017) 371–384.
[39] D. Cheng, J. Li, L. Liu, K. Yu, T.D. Le, J. Liu, Toward unique and unbiased causal effect estimation from data with hidden variables, IEEE Trans. Neural Netw. Learn. Syst. 10 (2022) 1–13.
[40] T.-Z. Wang, T. Qin, Z.-H. Zhou, Sound and complete causal identification with latent variables given local background knowledge, in: Advances in Neural Information Processing Systems, 2022, pp. 10325–10338.
[41] E. Perkovic, J. Textor, M. Kalisch, M.H. Maathuis, Complete graphical characterization and construction of adjustment sets in Markov equivalence classes of ancestral graphs, J. Mach. Learn. Res. 18 (2017) 1–62.
[42] M. Wienöbst, M. Bannach, M. Liskiewicz, A new constructive criterion for Markov equivalence of mags, in: Proceedings of the 38th Conference on Uncertainty in Artificial Intelligence, 2022, pp. 2107–2116.
[43] D. Cheng, J. Li, L. Liu, K. Yu, T.D. Lee, J. Liu, Discovering ancestral instrumental variables for causal inference from observational data, arXiv preprint, arXiv:2206.01931, 2022.
[44] M. Kalisch, M. Mächler, D. Colombo, M.H. Maathuis, P. Bühlmann, Causal inference using graphical models with the R package pcalg, J. Stat. Softw. 47 (2012) 1–26.
[45] A. Hauser, P. Bühlmann, Two optimal strategies for active learning of causal models from interventional data, Int. J. Approx. Reason. 55 (2014) 926–939.
[46] T.-Z. Wang, X.-Z. Wu, S.-J. Huang, Z.-H. Zhou, Cost-effectively identifying causal effects when only response variable is observable, in: Proceedings of the 37th International Conference on Machine Learning, 2020, pp. 10060–10069.
[47] C. Meek, Causal inference and causal explanation with background knowledge, in: Proceedings of the 11st Annual Conference on Uncertainty in Artificial Intelligence, 1995, pp. 403–410.
[48] B. Andrews, P. Spirtes, G.F. Cooper, On the completeness of causal discovery in the presence of latent confounding with tiered background knowledge, in: Proceedings of the 23rd International Conference on Artificial Intelligence and Statistics, 2020, pp. 4002–4011.
[49] H. Zhao, Z. Zheng, B. Liu, On the Markov equivalence of maximal ancestral graphs, Sci. China Ser. A, Math. 48 (2005) 548–562.
[50] Y. He, J. Jia, B. Yu, Counting and exploring sizes of Markov equivalence classes of directed acyclic graphs, J. Mach. Learn. Res. 16 (2015) 2589–2609.
[51] A. Ghassami, S. Salehkaleybar, N. Kiyavash, K. Zhang, Counting and sampling from Markov equivalent dags using clique trees, in: Proceedings of the 33rd AAAI Conference on Artificial Intelligence, 2019, pp. 3664–3671.
[52] T. Talvitie, M. Koivisto, Counting and sampling Markov equivalent directed acyclic graphs, in: Proceedings of the 33rd AAAI Conference on Artificial Intelligence, 2019, pp. 7984–7991.
[53] M. Wienöbst, M. Bannach, M. Liskiewicz, Polynomial-time algorithms for counting and sampling Markov equivalent dags, in: Proceedings of the 35th AAAI Conference on Artificial Intelligence, 2021, pp. 12198–12206.
[54] R. Ganian, T. Hamm, T. Talvitie, An efficient algorithm for counting Markov equivalent dags, Artif. Intell. 304 (2022) 103648.
[55] R.A. Ali, T.S. Richardson, P. Spirtes, et al., Markov equivalence for ancestral graphs, Ann. Stat. 37 (2009) 2808–2837.
[56] Z. Hu, R. Evans, Faster algorithms for Markov equivalence, in: Proceedings of the 36th Conference on Uncertainty in Artificial Intelligence, 2020, pp. 739–748.
[57] S. Chib, E. Greenberg, Understanding the Metropolis-Hastings algorithm, Am. Stat. 49 (1995) 327–335.
[58] J. Zhang, P. Spirtes, A transformational characterization of Markov equivalence for directed acyclic graphs with latent variables, in: Proceedings of the 21st Conference in Uncertainty in Artificial Intelligence, 2005, pp. 667–674.
[59] J. Tian, Generating Markov equivalent maximal ancestral graphs by single edge replacement, in: Proceedings of the 21st Conference in Uncertainty in Artificial Intelligence, 2005, pp. 591–598.
[60] L. Tierney, Markov chains for exploring posterior distributions, Ann. Stat. (1994) 1701–1728.
[61] Z.-H. Zhou, Abductive learning: towards bridging machine learning and logical reasoning, Sci. China Inf. Sci. 62 (2019) 76101.
[62] Z.-H. Zhou, Y.-X. Huang, Abductive learning, in: P. Hitzler, M.K. Sarker (Eds.), Neuro-Symbolic Artificial Intelligence: The State of the Art, IOS Press, Amsterdam, 2022, pp. 353–369.
[63] E. Bareinboim, A. Forney, J. Pearl, Bandits with unobserved confounders: a causal approach, in: Advances in Neural Information Processing Systems, 2015, pp. 1342–1350.
[64] S. Lee, E. Bareinboim, Structural causal bandits: where to intervene?, in: Advances in Neural Information Processing Systems, 2018, pp. 2573–2583.
[65] J. Zhang, Designing optimal dynamic treatment regimes: a causal reinforcement learning approach, in: Proceedings of the 37th International Conference on Machine Learning, 2020, pp. 11012–11022.
[66] S. Lee, E. Bareinboim, Characterizing optimal mixed policies: where to intervene and what to observe, in: Advances in Neural Information Processing Systems, 2020, pp. 8565–8576.
[67] Z.-H. Zhou, Rehearsal: learning from prediction to decision, Front. Comput. Sci. 16 (4) (2022) 164352.
[68] A.R. Ali, T.S. Richardson, P. Spirtes, J. Zhang, Towards characterizing Markov equivalence classes for directed acyclic graphs with latent variables, in: Proceedings of the 21st Conference in Uncertainty in Artificial Intelligence, 2005, pp. 10–17.