# Actively Identifying Causal Effects with Latent Variables Given Only Response Variable Observable

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## Abstract

In many real tasks, it is generally desired to study the causal effect on a specific target (response variable) only, with no need to identify the thorough causal effects involving all variables. In this paper, we attempt to identify such effects by a few active interventions where only the response variable is observable. This task is challenging because the causal graph is unknown and even there may exist latent confounders. To learn the necessary structure for identifying the effects, we provide the graphical characterization that allows us to efficiently estimate all possible causal effects in a partially mixed ancestral graph (PMAG) by generalized back-door criterion. The characterization guides learning a local structure with the interventional data. Theoretical analysis and empirical studies validate the effectiveness and efficiency of our proposed approach.

## 1 Introduction

Identifying causal effects is one prominent task throughout empirical sciences. In many real problems, we are generally desired to study the causal effect on a specific target only, i.e. *response variable*, with no need to identify the thorough causal effects involving all variables. For example, a business person wants to maximize profit. The person has many intervention methods such as lowering price, increasing advertisement investment, improving quality, and so on. A valid approach to guide the decisions is to estimate the causal effect of each variable on the response variable. We call it *target effect identification* in this paper. After identifying all of these causal effects, the person could see which intervention could lead to the most desired response (profit).

To achieve target effect identification, an ideal method is to intervene on each decision variable with different attainable values and collect the interventional data of the response variable. However, when there are many decision variables and many attainable values for each variable, it will take enormous number of interventions, which is economically unfeasible. Considering that there is usually a large amount of observational data in reality, we hope to exploit mainly the observational data to achieve it.

The main obstacle here is that the causal graph of all involved variables is not available, which makes causal effect identification intractable. Hence, we learn the structure at first. As shown by Verma and Pearl [1], only a Markov equivalence class could be learned with observational data without further assumptions, where there are possibly unidentified causal relations resulting in unidentified causal effects. To reveal these effects, we *further* learn the causal relations in the Markov equivalence class by introducing a small amount of *active* hard interventions, i.e., we force some variable to a known value [2, 3, 4]. In practice, generally one can only observe part of variables under interventions rather than all of those, e.g., a business person can observe his profit, but does not know other companies' profit. To make the method applicable in a broader scenario, we consider an extreme situation that only the response variable is observable, which could be trivially extended to any settings with

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part of variables observed. In addition, there are usually latent confounders in practical problems. For instance, economic level influences both price and advertising cost, but it is hard to evaluate accurately and thus a latent confounder. In summary, in this paper we learn the causal knowledge where there are latent confounders and only the response variable is observable under interventions.

This problem is very challenging, because the fact that only the response variable is observable disables the approaches designed for situations where all variables are observable [2, 5, 6], while the existence of latent confounders disables the typical solutions [7]. To get a brief understanding of the challenges taken by latent confounders in techniques, consider a graph learned with observational data by traditional causal discovery methods [8]: If there is no latent confounder, the definite adjacent edges of intervened variable $X$ lead to a definite interventional distribution of the response variable $Y$ by back-door criterion [9], which makes it possible to learn the edges of $X$ by the interventional data of $Y$; when latent confounders exist, however, the mapping no longer holds. Besides, a *partial mixed ancestral graph (PMAG)* is commonly used to describe the relation between variables in this condition. The back-door criterion may fail in this case since there possibly exist latent confounders influencing the two variables of some directed edges. Hence, we also need to identify whether such latent confounders exist behind the directed edges, in addition to just learning the causal edges.

To overcome the difficulties above, we provide a graphical characterization that allows us to efficiently find all possible causal effects of the intervened variable on the response variable in a partial mixed ancestral graph. Guided by the characterization, we learn a local structure and identify the presence of latent confounders behind some directed edges by each intervention, which leads to identifying some causal effects on the response variable. After a few active interventions on different variables, our method **ACIC**, short for **AC**tive target effect **I**dentification with latent **C**onfounding, could achieve target effect identification. Due to space limit, we present related work and all the proofs in Appendix.

## 2 Preliminary

We guide readers to Appendix A.1 for the notions including *causal graph* ($G = (\mathbf{V}, \mathbf{E})$), *mixed graph*, *mark*, *arrowhead*, *tail*, *circle*($\circ$), *partial mixed graph*, *parent*, *child*, *spouse*, *possible directed path*, *(possible) ancestor*, $\mathrm{PossAn}(X, G)$, $\mathrm{An}(X, G)$, *(possible) descendant*, $\mathrm{PossDe}(X, G)$, $\mathrm{De}(X, G)$, *adjacent*, $\mathrm{Adj}(X, G)$, *almost directed cycle*, *collider path*, *minimal path*, *ancestral graph*, *m-separation (m-connecting or active)*, *maximum ancestral graph (MAG, $\mathcal{M}$)*, *discriminating path*, *Markov equivalent*, *Markov equivalence class (MEC)*, *partial ancestral graph (PAG)*, *visible*, $\mathcal{M}_{\underline{X}}$, $\mathcal{P}_{\underline{X}}$, *causal effect* ($P(Y|do(X))$), and the common assumptions including *positivity* and *no selection bias*. $*$ is a wildcard that denotes any of the marks. For a partial mixed graph, we say it is a *partial mixed ancestral graph (PMAG)* if there is no directed or almost directed cycle, and denote it by $\mathcal{P}$. Note *both MAG and PAG are special cases of PMAG*, thus $\mathcal{P}$ could also denote PAG. The relation between PMAG and PAG is similar to that between partial directed acyclic graph (PDAG) and completed partial directed acyclic graph (CPDAG) when there is no latent confounder [10]. MAG $\mathcal{M}$ is *consistent to PMAG* $\mathcal{P}$ if it belongs to the MEC represented by $\mathcal{P}$ (detailed in Appendix A.1).

For a directed edge $V_i \to V_j$ in a graph, we say the edge is *pure* if the two variables are not influenced by common *latent confounders*, denoted by $V_i \xrightarrow{p} V_j$. We use a *purity matrix* to characterize the purity of each edge in a PMAG $G$, in which 1 is in $(i, j)$ entry *only if* the directed edge $V_i \to V_j$ in $G$ is pure, and 0 otherwise. Note that 0 *does not* imply that the edge is impure. It is also possible that we are unaware of whether it is pure or the edge is not directed. In the literature, a graphical characterization to imply that there are no latent confounders behind a directed edge in an MAG or PAG is proposed by Zhang [11], where they call it by *visibility*. Visibility is sufficient but not necessary for purity, which is detailed in Appendix A.2. Thus, given a PMAG, we initialize the purity matrix by setting $(i, j)$ entry to 1 if $V_i \to V_j$ is visible and 0 otherwise. For an MAG $\mathcal{M}$, $\mathcal{M}_{\underset{\sim}{X}}$ denotes the graph by removing the directed edges out of $X$ in $\mathcal{M}$ that are labeled to be pure in purity matrix. For a PMAG $\mathcal{P}$, see Appendix A.4 for the definition of $\mathcal{P}_{\underset{\sim}{X}}$.

Since the graph is continuously learned by interventions in this paper, the graph in the process is a PMAG. Hence we present Prop. 1 to guide causal effect identification in a PMAG with the consideration of purity matrix rather than only in a PAG or MAG. It is based on the generalized back-door criterion (GBC) and the graphical condition for the causal effect identifiability by GBC in MAG or PAG proposed by Maathuis et al. [12]. Before that, we introduce D-SEP$(X, Y, G)$ in Def. 1.

**Definition 1** (D-SEP$(X, Y, G)$ [12]). Let $X$ and $Y$ be two distinct vertices in a mixed graph $G$. We say that $V \in$ D-SEP$(X, Y, G)$ if $V \neq X$, and there is a collider path between $X$ and $V$ in $G$, such that every vertex on this path (including $V$) is an ancestor of $X$ or $Y$ in $G$.

**Proposition 1.** *Let $G$ be a PMAG and $W$ be a purity matrix of $G$. Suppose $X \in \mathrm{An}(Y, G)$ and $Y$ are two distinct vertices in $G$. There exists a generalized back-door set relative to $(X, Y)$ and $(G, W)$ if and only if* D-SEP$(X, Y, G_{\underset{\sim}{X}}) \cap \mathrm{PossDe}(X, G) = \emptyset$*. Moreover, if the set exists,* D-SEP$(X, Y, G_{\underset{\sim}{X}})$ *is such a set. Denote* D-SEP$(X, Y, G_{\underset{\sim}{X}})$ *by $\mathbf{D}$, the causal effect is*

$$P(Y|do(X = x)) = \int_{\mathbf{D}} P(\mathbf{D})P(Y|\mathbf{D}, X = x)\, \mathrm{d}\mathbf{D}. \tag{1}$$

There are two possible unidentifiable cases for $P(Y|do(X))$ by GBC in Prop. 1. One is that there are many possible causal effects due to the missing of exact structure information, but we do not know which is correct. In this case, we could address it by learning the structure with interventional data. The other unidentifiable case is that the causal effect is unidentifiable by GBC *even if we know the MAG and the purity of each edge*. We return “Fail” for such $X$ because GBC is not sufficient for identifying the causal effect in this case, and we say *GBC fails* ( to identify $P(Y|do(X))$).

# 3 The Proposed Approach

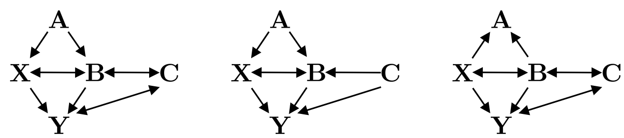
In this paper, we assume faithfulness, positivity, and no selection bias. Denote the decision variables by $X_1, \cdots, X_p$ and the response variable by $Y$. Given the observational data of these variables, our goal is to achieve target effect identification by generalized back-door criterion, i.e., we aim to identify $P(Y|do(X_i))$ by GBC for each variable $X_i, i = 1, 2, \cdots, p$ if GBC does not fail. With the observational data, we can learn a PAG $\mathcal{P}$ that the true MAG is consistent to by FCI algorithm [8]. And we initialize a purity matrix by setting $(i, j)$ entry to $1$ if the directed edge between the two variables is visible in $\mathcal{P}$ and $0$ otherwise. The causal effects of some variables on $Y$ are possibly unidentifiable in $\mathcal{P}$ by Prop. 1. To identify these effects, we further introduce *active* interventions and observe $Y$ under those. Beginning from $\mathcal{P}$, in each round our method selects one variable $X$ from $X_i, i = 1, \cdots, p$ to intervene and exploits the interventional data of $Y$ to learn the structure, including learning an updated PMAG by revealing circles and updating the purity matrix. The process repeats until identifying all effects $P(Y|do(X_i)), i = 1, 2, \cdots, p$ (identifying failing of GBC is also included). Since it is recursive, we just present the method to learn the structure by interventional data in one round. The criterion to select the intervention variable in each round is given at the end.

## 3.1 Two direct methods

A naive method to learn the structure by interventional data is enumerating each MAG $\mathcal{M}$ consistent to the PMAG $\mathcal{P}$. For each $\mathcal{M}$, $P(Y|do(X))$ can be estimated with observational data by (1) and we judge whether the estimated causal effect is consistent with the interventional data. By such judgment, we could rule out the MAGs with inconsistent causal effects. Yet, this method is usually impractical since it takes a huge computation complexity mainly from two parts. One part is the exhaustive search in the space of MAGs. As is known to all, the space of MAGs is extremely large. For each searched MAG, we also need to judge whether it is consistent to $\mathcal{P}$[1]. The other costly part is looking for D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}})$ according to Def. 1 to estimate causal effects by (1) for each MAG.

A cleverer approach instead of enumerating is to directly learn a local structure by interventional data, inspired by ACI proposed by Wang et al. [7]. ACI tackles a similar task but assumes no latent confounders. The core of this approach is to find an equivalent condition that *could be obtained based on a local structure* for causal effect. In this way, there is a bijection between the condition and $P(Y|do(X))$, by which we could learn a local structure with the interventional data of $Y$. Specifically, ACI is comprised of three steps: (a) propose Minimal Parental back-door admissible Set (MPS), a variable set that could be obtained by only the orientation of adjacent edges of $X$, as the equivalent condition for $P(Y|do(X))$; (b) find all possible MPSs in the partial graph to be learned; (c) identify which MPS is correct by interventional data and learn the adjacent edges of $X$ implied by the MPS.

[1]For such judgment, we could first obtain an MAG based on $\mathcal{P}$ by the procedure of Theorem 2 by Zhang [13], as a representative of $\mathcal{P}$. Then we judge whether the searched MAG is Markov equivalent to this MAG by the necessary and sufficient condition for Markov equivalence by Ali et al. [14], Hu and Evans [15].



(a) (b) (c)

Figure 1: Suppose $X \to Y$ is pure. The adjacent edges of $X$ are the same in (a) and (b), but the causal effects are different due to the different marks at $C$. In addition, although D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}})$ are different in (a) and (c), the causal effects of $X$ on $Y$ are the same by (1), since $A \perp Y \mid X, B$.

However, ACI fails if there are latent confounders. In this situation the adjacent edges of $X$ is not sufficient for identifying causal effects. According to Prop. 1, even though there are the same adjacent edges of $X$ in two MAGs, the causal effects of $X$ on $Y$ are possibly different if they have different D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}})$. See Fig. 1(a) and Fig. 1(b) for example. The method of Malinsky and Spirtes [16] is possibly useful here, which estimates all possible causal effects in $\mathcal{P}$ by enumerating the structures in a relatively local region, but the two parts of computational costs above are still large.

Referring to the framework of ACI, we propose the three steps for our setting in the next three sections. Firstly, we propose MCS, as an *equivalent condition for* $P(Y|do(X))$ in MAG by GBC in Sec. 3.2. Secondly, we present how to *find all MCSs in* $\mathcal{P}$ *by graphical characterization* in Sec. 3.3. It is the main challenge here in contrast to ACI. ACI achieves it by considering all possible orientations of adjacent edges of $X$ due to the fact that their proposed MPS merely depends on these edges. In our setting, however, it is unclear which edges MCS depends on. And obviously, enumerating all edges is not efficient. Hence we propose a graphical characterization to guide it. Lastly, we give the method to *learn marks and purity matrix by interventional data* in Sec. 3.4 with all MCSs found before.

### 3.2 The equivalent condition for causal effects

By Prop. 1, D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}})$ can be as the adjustment set to identify $P(Y|do(X))$ when GBC does not fail. Thus, we construct the equivalent condition for $P(Y|do(X))$ based on D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}})$. Note that D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}})$ cannot be used directly since the causal effects are possibly equal in the MAGs with different D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}})$. See Fig. 1 for an example. The D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}})$ in (a) and (c) are $\{A, B\}$ and $\{B\}$, respectively, but $P(Y|do(X))$ are equal. The reason is $A \perp Y|X, B$ in the two MAGs. When calculating (1), the results are equal after integration on the generalized back-door set. To formalize this situation, we introduce *Minimal Conditional Set (MCS) regarding* D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}})$ *in* $\mathcal{M}$. The algorithm to find MCS and the related properties are in Appendix B.

**Definition 2** (Minimal conditional set regarding D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}})$ (MCS))**.** Let $\mathcal{M}$ be an MAG. $X$, $Y$, and $\mathbf{D}$ denote the intervened variable, response variable, and the set D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}})$ in $\mathcal{M}$, respectively. $\overline{\mathbf{D}}$ is a subset of $\mathbf{D}$. $\overline{\mathbf{D}}$ is a minimal conditional set regarding $\mathbf{D}$ in $\mathcal{M}$ if

(1) $(Y \perp \mathbf{D} \backslash \overline{\mathbf{D}} \, | \overline{\mathbf{D}} \cup \{X\})_{\mathcal{M}}$,

(2) $(Y \not\perp \mathbf{D} \backslash \overline{\mathbf{D}}' | \overline{\mathbf{D}}' \cup \{X\})_{\mathcal{M}}$, for any $\overline{\mathbf{D}}' \subset \overline{\mathbf{D}}$.

We call it MCS regarding D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}})$ or MCS for short. Note that MCS is essentially a set of variables. For all MAGs $\mathcal{M}$ satisfying the conditions of Prop. 1 with the same $\overline{\mathbf{D}}$, where $\overline{\mathbf{D}}$ denotes the MCS regarding D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}})$ in respective $\mathcal{M}$, they have the same causal effect as

$$P(Y|do(X = x)) = \int_{\overline{\mathbf{D}}} P(\overline{\mathbf{D}}) P(Y|\overline{\mathbf{D}}, X = x) \, \mathrm{d}\overline{\mathbf{D}}. \tag{2}$$

Since structure inference with interventional data is involved, we make an additional assumption as Assumption 1 to match interventional data to causal graph, playing as the role of faithfulness given only observational data or some intervention-related assumptions[17, 7, 6, 18]. The purpose is to avoid that different causal effects in general (e.g. the causal effects $P(Y|do(X))$ in Fig. 1(a) and Fig. 1(b) ) *happen to* be equal given some *specific* observational distributions. Under the assumption, there is a bijection between MCS and $P(Y|do(X))$ through (2). Finding all possible causal effects could be converted to finding all possible MCSs. In the next section, we present how to find all possible MCSs in a PMAG by our proposed graphical characterization.

**Assumption 1.** *For two Markov equivalent MAGs $\mathcal{M}^1$ and $\mathcal{M}^2$ with the same observational distribution, if there are different minimal conditional sets regarding* D-SEP$(X, Y, \mathcal{M}^1_{\underset{\sim}{X}})$ *and* D-SEP$(X, Y, \mathcal{M}^2_{\underset{\sim}{X}})$ *in the respective graphs, then $P\big(Y|do(X = x)\big)$ are different in the two MAGs.*

### 3.3 Finding all MCSs in $\mathcal{P}$ by graphical characterization

At the beginning, we provide an outline of finding possible MCSs regarding D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}})$ in all $\mathcal{M}$ consistent to $\mathcal{P}$ if GBC does not fail to identify $P(Y|do(X))$ in $\mathcal{M}$. The justification for the restriction on $\mathcal{M}$ is that if $\mathcal{M}$ is the true MAG and GBC fails to identify $P(Y|do(X))$ in $\mathcal{M}$, there is no MCS matched to the interventional data. We thus cannot identify an MCS by the intervention. In this case it is unnecessary to find MCS in such $\mathcal{M}$. Hence, we consider the MAG $\mathcal{M}$ that satisfies D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}}) \cap$ De$(X, \mathcal{M}) = \emptyset$, according to Prop. 1. There are three main parts to achieve it. The first part is to enumerate all mark combinations of $X$. The true MAG is with one mark combination among them. As mentioned earlier, the marks of $X$ are not sufficient for identifying $P(Y|do(X))$. In another word, MCSs could be different in the MAGs with the same marks at $X$. Hence, in the second part we propose the graphical condition to indicate when there are different MCSs in the MAGs with the same marks at $X$. And this graphical condition can be obtained in a partial graph. Based on that, we present the algorithm to find all possible MCSs in $\mathcal{P}$ in the third part.

We first enumerate all possible mark combinations of $X$. To denote the PMAGs with deterministic marks at $X$, we introduce *local MAG of $X$ based on $\mathcal{P}$* in Def. 3. For a local MAG $M$ and an MAG $\mathcal{M}$ consistent to $M$, we then present a sufficient and necessary condition for $V \in$ D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}})$ in Thm. 2, which plays a vital role for the following result involving MCS regarding D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}})$.

**Definition 3** (Local MAG of $X$ based on $\mathcal{P}$)**.** Given a PMAG $\mathcal{P}$ and a variable $X$, a PMAG $M$ is a *local MAG of $X$ based on $\mathcal{P}$* if (1) $M$ is with definite marks (arrowheads or tails) at $X$; (2) $M$ is obtained from $\mathcal{P}$ by marking some circles without generating new unshielded colliders or directed or almost directed cycles. We call it *local MAG* for short if there is no ambiguity and denote it by $M$, which is different from calligraphic $\mathcal{M}$ that denotes MAG.

**Theorem 2.** Let $M$ be a local MAG of $X$ and $\mathcal{M}$ be an MAG consistent to $M$. Suppose $V$ ($V \neq X, Y$) is a variable in $\mathcal{M}$. If D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}}) \cap$ De$(X, \mathcal{M}) = \emptyset$, then $V \in$ D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}})$ holds if and only if there is at least one collider path from $X$ to $V$ starting by an arrowhead at $X$ in $M$ such that each variable except for $X$ on the path is an ancestor of $X$ or $Y$ in $\mathcal{M}$.

The advantage of considering local MAG of $X$ rather than $\mathcal{P}$ with circles at $X$ is that based on local MAG we could obtain a set of variables, PD-SEP$(X, Y, M)$, as Def. 4. This set implies some variables in D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}})$ and has a good property that if PD-SEP$(X, Y, M) \backslash$D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}}) \neq \emptyset$, there must be at least one variable $V \in$ PD-SEP$(X, Y, M)$ which is not an ancestor of $X$ or $Y$ in $\mathcal{M}$, as shown by the combination of Thm. 2 and Def. 4. This property is utilized to prove the main result.

**Definition 4** (PD-SEP$(X, Y, M)$)**.** Let $M$ be a local MAG of $X$ and $\mathcal{M}$ be an MAG consistent to $M$. Variable $V \in$ PD-SEP$(X, Y, M)$ if and only if $V \in$ PossAn$(Y, M) \backslash$De$(X, \mathcal{M})$[2] and there exists a collider path between $X$ and $V$ in $M$, where each non-endpoint variable is an ancestor of $X$ or $Y$ in $M$ but not a descendant of $X$ in $\mathcal{M}$.

*Remark.* In the literature, there is a well-defined notion Possible-D-SEP$(X, Y)$ [8, 19], which is introduced with the similar intention that indicates some variables possibly belonging to D-SEP$(X, Y, \mathcal{M})$. Since ours is pretty different in both required conditions and the restriction on ancestral relations, we use a new name PD-SEP$(X, Y, M)$ to distinguish them.

With the knowledge above, we present our main result in Thm. 3. Perhaps surprisingly, it implies that given a local MAG $M$, although there are possibly different D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}})$ in distinct MAG $\mathcal{M}$

[2]Note all the descendants of $X$ in $\mathcal{M}$ consistent to $M$ are knowable in $M$, which is detailed by Lemma 19 in Appendix C.1. Hence PD-SEP$(X, Y, M)$ can be obtained based on $M$ without the further knowledge about $\mathcal{M}$.

**Algorithm 1** Find all possible MCSs in $\mathcal{P}$

**input:** Intervention variable $X$, PAG $\mathcal{P}$

1: $L \leftarrow \emptyset$ // It is to record each local MAG $M^j$ and corresponding MCS$^j$
2: **for** each local MAG $M^j$ of $X$ based on $\mathcal{P}$ by merely marking the marks at $X$ **do**
3:     **if** there is critical variable set $\mathbf{C}^j$ for $(X, Y)$ in $M^j$ **then**
4:         CRITICAL($M^j, \mathbf{C}^j, \mathbf{S}^j$) // $\mathbf{S}^j$ ($\mathbf{S}^{j_k}$ below) is the set $\mathbf{S}$ defined in Def. 5 in $M^j$ ($M^{j_k}$)
5:     **else**
6:         $L = L \cup (M^j, \text{MCS}^j)$
7:     **end if**
8: **end for**
9: **function** CRITICAL($M^j, \mathbf{C}^j, \mathbf{S}^j$)
10:     **for** each element $\mathbf{C}^{j_k}$ in the power set of $\mathbf{C}^j$ **do**
11:         Obtain a new local MAG $M^{j_k}$ by orienting $F \rightarrow S$ for $\forall F \in \mathbf{C}^{j_k}, \forall S \in \mathbf{S}^j$ and marking the critical marks of $F \in \mathbf{C}^j \backslash \mathbf{C}^{j_k}$ as arrowheads
12:         **if** there is critical variable set $\mathbf{C}^j$ for $(X, Y)$ in $M^{j_k}$ **then**
13:             CRITICAL($M^{j_k}, \mathbf{C}^{j_k}, \mathbf{S}^{j_k}$)
14:         **else**
15:             $L = L \cup (M^{j_k}, \text{MCS}^{j_k})$
16:         **end if**
17:     **end for**
18: **end function**

**output:** $L$

consistent to $M$, the MCSs regarding them are the same if there are no *critical variables for* $(X, Y)$ in $M$. We define critical variables for $(X, Y)$ in Def. 5, and show an example in Fig. 2, where $F_t$ is a critical variable and the circles colored by red are critical marks.

**Definition 5** (Critical variable for $(X, Y)$)**.** In a local MAG $M$ with a path $X \leftrightarrow F_1 \leftrightarrow \cdots \leftrightarrow F_{t-1} \leftrightarrow F_t$ or $X \leftrightarrow F_1 \leftrightarrow \cdots \leftrightarrow F_{t-1} \leftarrow\!\circ F_t$, $t \geq 1$, where $F_1, \cdots, F_{t-1} \in$ PD-SEP$(X, Y, M)$, $F_t$ is called a *critical variable* for $(X, Y)$ if there is a non-empty variable set $\mathbf{S}$ relative to $F_t$ defined as follows: $S \in \mathbf{S}$ if and only if in $M$ (1) $S$ is a child of $X, F_1, \cdots, F_{t-1}$, (2) there is $F_t \circ\!\!-\!\!* S$, (3) $S$ is at one minimal possible directed path from $F_t$ to $Y$, and no variable on the path belongs to PD-SEP$(X, Y, M)$. Each circle at $F_t$ on the edge with $F_{t-1}$ or $S \in \mathbf{S}$ is called a *critical mark* of $F_t$.

**Theorem 3.** Let $M$ be a local MAG of $X$ based on a PMAG $\mathcal{P}$. Then condition (1) below is sufficient for condition (2):

(1) there is no critical variable for $(X, Y)$ in $M$.

(2) for any an MAG $\mathcal{M}$ consistent to $M$ such that $(a)$ D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}}) \cap$ De$(X, \mathcal{M}) = \emptyset$, $(b)$ $X \in$ An$(Y, \mathcal{M})$, it holds that $\mathbf{A}_{\mathcal{M}} = \mathbf{A}'_{\mathcal{M}}$, where $\mathbf{A}_{\mathcal{M}}$ denotes the MCS regarding D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}})$ in $\mathcal{M}$ and $\mathbf{A}'_{\mathcal{M}}$ denotes the MCS regarding PD-SEP$(X, Y, M)$ in $\mathcal{M}$;

*Remark.* It is noteworthy that all the MAGs consistent to $M$ are Markov equivalent. Hence the MCSs regarding PD-SEP$(X, Y, M)$ in these MAGs are the same, namely, $\mathbf{A}'_{\mathcal{M}}$ is invariant for different $\mathcal{M}$. If there is no critical variable as condition (1), then for any MAG $\mathcal{M}$ consistent to $M$, $\mathbf{A}_{\mathcal{M}} = \mathbf{A}'_{\mathcal{M}}$ holds according to Thm. 3. We thus conclude $\mathbf{A}_{\mathcal{M}}$ is invariant for different $\mathcal{M}$ consistent to $M$, i.e., different D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}})$ in distinct $\mathcal{M}$ consistent to $M$ share the same MCS regarding them.

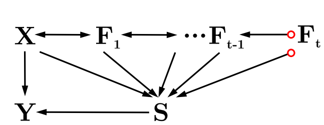



Figure 2: An illustration for critical variable $F_t$ and critical marks (red).

Def. 5 and Thm. 3 form a graphical characterization that allows us to obtain all possible MCSs in all MAGs consistent to a local MAG $M$. We propose Alg. 1 to find all MCSs in $\mathcal{P}$ based on it. Given a PMAG $\mathcal{P}$, it is easy to find local MAGs $M$ based on $\mathcal{P}$ by differently marking the circles at $X$ without generating new unshielded colliders and directed or almost directed cycles (Line 2). For each $M$, if there is no critical variable in $M$, the MCS regarding D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}})$ is unique, and it equals to the MCS regarding PD-SEP$(X, Y, M)$ (Line 6). When there is a non-empty critical variable set $\mathbf{C}$, the MCSs in the MAGs consistent to $M$ could be different. The reason is that the variable in $\mathbf{C}$ could be the ancestor of $X$ or $Y$ in some MAGs but the non-ancestor in other MAGs, due to the unidentified critical marks. Conditioning on the non-ancestor variables above makes some generalized back-door paths from $X$ to $Y$ active, thus these variables cannot appear in MCS. Hence, we further discuss the critical marks. For any subset $\mathbf{C}_k$ of the critical variable set $\mathbf{C}$, there could possibly be some MAG $\mathcal{M}$ consistent to $M$ where $\mathbf{C}_k \subseteq \text{D-SEP}(X, Y, \mathcal{M}_{\underset{\sim}{X}})$ and $(\mathbf{C} \backslash \mathbf{C}_k) \cap \text{D-SEP}(X, Y, \mathcal{M}_{\underset{\sim}{X}}) = \emptyset$. We use a new local MAG to represent the common parts of these MAGs (Line 10,11). And in the new one, we further consider whether critical variable exists (Line 12). The soundness of Alg. 1 is shown in Lemma 4, i.e. no matter what the true MAG $\mathcal{M}$ is, the MCS regarding $\text{D-SEP}(X, Y, \mathcal{M}_{\underset{\sim}{X}})$ in $\mathcal{M}$ could be returned as long as $\text{D-SEP}(X, Y, \mathcal{M}_{\underset{\sim}{X}}) \cap \text{De}(X, \mathcal{M}) = \emptyset$.

**Lemma 4.** *Let $\mathcal{P}$ be a PMAG of MAG $\mathcal{M}$. If $X \in \text{An}(Y, \mathcal{M})$ and $\text{D-SEP}(X, Y, \mathcal{M}_{\underset{\sim}{X}}) \cap \text{De}(X, \mathcal{M}) = \emptyset$, then the MCS regarding $\text{D-SEP}(X, Y, \mathcal{M}_{\underset{\sim}{X}})$ in $\mathcal{M}$ and the corresponding local MAG are contained in the output of Algorithm 1.*

### 3.4 Learning marks and purity matrix by interventional data

In this section we propose how to learn marks and purity matrix by the interventional data of $Y$. After intervening on $X$, there are three possible situations implied by the interventional data of $Y$.

(1) $X$ has no causal effect on $Y$, i.e., $P(Y|do(X)) = P(Y)$,

(2) $X$ has causal effect on $Y$ and it can be identified by GBC, i.e., there exists a generalized back-door set $\mathbf{D}$ such that $P(Y|do(X)) = \int P(\mathbf{D})P(Y|X, \mathbf{D})\,\mathrm{d}\mathbf{D}$,

(3) $X$ has causal effect on $Y$ but GBC fails to identify it.

For situation $(1)$, it is trivial to learn the marks by the interventional data according to Prop. 5.

**Proposition 5.** *If $P(Y|do(X)) = P(Y)$, the marks at $X$ are arrowheads in all the minimal possible directed paths from $X$ to $Y$ in a partially mixed ancestral graph.*

If $P(Y|do(X))$ is not equal to $P(Y)$, it implies that the interventional data accords with situation $(2)$ or situation $(3)$ but is uncertain to us. Hence, we need to find all possible MCSs based on $\mathcal{P}$, then judge whether one of the estimated causal effects with the observational data by (2) is consistent to the interventional data. If so, we can see that the causal effect of $X$ on $Y$ can be identified by GBC in the true MAG. Specifically, we first obtain a group of pairs $(M^j, \text{MCS}^j)$ by Alg. 1, where $M^j$ is a local MAG and $\text{MCS}^j$ is the corresponding MCS. Let $\hat{P}_{M^j}\big(Y|do(X = x)\big)$ and $\hat{P}\big(Y|do(X = x)\big)$ denote the estimated causal effect in each $M^j$ by $\text{MCS}^j$ and that under real intervention respectively. *Disc*$(P, Q)$ is the distribution discrepancy between $P$ and $Q$. If there are $m$ intervention samples $\big((do(X = x_1), Y_1), \cdots, \big(do(X = x_s), Y_s\big), \cdots, \big(do(X = x_m), Y_m\big)\big)$, we take $\text{MCS}^\star$ by

$$\text{MCS}^\star = \underset{\text{MCS}^j}{\arg\min} \sum_{s=1}^{m} \textit{Disc}\Big(\hat{P}_{\text{MCS}^j}\big(Y|do(X = x_s)\big), \hat{P}\big(Y|do(X = x_s)\big)\Big). \tag{3}$$

Any distance metric can be used here. Since the attention is not on calculation, we take the expectation difference as the metric for convenience, i.e., $\text{MCS}^\star = \arg\min_{\text{MCS}^j} \sum_{s=1}^{m} |\hat{\mathbb{E}}_{\text{MCS}^j}\big(Y|do(X = x_s)\big) - Y_s|$. If the distance between the estimated causal effect by $\text{MCS}^\star$ and interventional data is larger than a given threshold, we think that GBC fails to identify such causal effect. We thus mark such $X$ as "FAIL" and orient some edges by Prop. 6. Otherwise, if there is only one local MAG $M^*$ corresponding to $\text{MCS}^\star$, we orient $\mathcal{P}$ by $M^*$. If there are more than one local MAG corresponding to $\text{MCS}^\star$, we orient $\mathcal{P}$ by the common marks of the local MAGs with $\text{MCS}^\star$. Besides, when GBC does not fail to identify the causal effect, all the edges out of $X$ in the minimal directed paths from $X$ to $Y$ in the PMAG are learned to be pure. Thus we could update the purity matrix accordingly.

**Proposition 6.** *In situation $(3)$, let $\mathbf{T}$ denote all variables adjacent to $X$ in the minimal possible directed paths from $X$ to $Y$. For $T \in \mathbf{T}$, if for $\forall V \in \mathbf{T} \backslash T$, it holds either $T \notin \text{Adj}(V, \mathcal{P})$ or there is a variable $S \notin \text{Adj}(V, \mathcal{P})$ such that there is a collider path $X \circ\!\!\rightarrow T \leftrightarrow \cdots \leftarrow\!\!* S$ and every vertex except $S$ on the path is a parent of $V$, then $X \rightarrow T$.*

After the learning process above, we can further update the PMAG according to the property of MAG. Zhang [13] proposed ten complete rules with only observational data. However, how to orient PMAG

**Algorithm 2** ACIC (ACtive target effect Identification with latent Confounding)

**input:** PAG $\mathcal{P}$ by FCI algorithm;
1: Initialize $\mathcal{I}_1 = \{V | V \in \mathbf{V}(\mathcal{P}), V \in \text{PossAn}(Y, \mathcal{P})$ and $P(Y|do(V))$ is unidentifiable by Prop. 1 in $\mathcal{P}\}$ // Record the variables whose causal effects on $Y$ are unidentifiable by Prop. 1
2: Initialize $\mathcal{I}_2 = \emptyset$ // Record the variables whose causal effects are failed to be identified by GBC
3: **while** $\mathcal{I}_1 \backslash \mathcal{I}_2 \neq \emptyset$ **do**
4:     Select a variable $X$ with the maximum number of circles from $\mathcal{I}_1 \backslash \mathcal{I}_2$ to intervene
5:     **if** $P(Y|do(X))$ equals to $P(Y)$ **then**
6:         Update $\mathcal{P}$ by Prop. 5
7:     **else**
8:         Find all possible MCSs in $\mathcal{P}$ by Alg. 1 and select MCS$^*$ by Eq. 3
9:         **if** $\frac{1}{m} \sum_{s=1}^{m} |\hat{\mathbb{E}}_{\text{MCS}^*} \big(Y|do(X = x_s)\big) - Y_s| \leq \tau$ **then** // $\tau$ is a pre-set threshold
10:             **if** there is only local MAG $M^*$ with MCS$^*$ **then**
11:                 Update $\mathcal{P}$ to $M^*$, and label all the edges out of $X$ in the minimal directed paths from $X$ to $Y$ pure
12:             **else** there is more than one local MAG $M_1^*, M_2^*, \cdots, M_k^*$
13:                 Update $\mathcal{P}$ with the common marks in $M_1^*, M_2^*, \cdots, M_k^*$, and label all the edges out of $X$ in the minimal directed paths from $X$ to $Y$ pure
14:             **end if**
15:             Update $\mathcal{P}$ further based on the 11 rules for orienting PAGs with background knowledge, and update the purity matrix if some directed edges are newly identified to be visible
16:         **else** // In this case GBC fails to identify $P(Y|do(X))$
17:             Update $\mathcal{P}$ by Prop. 6
18:             $\mathcal{I}_2 = \mathcal{I}_2 \cup \{X\}$
19:         **end if**
20:     **end if**
21:     Update $\mathcal{I}_1$ by Prop. 1 with the updated PMAG $\mathcal{P}$ and the updated purity matrix
22: **end while**
**output:** The estimated causal effect of each variable on $Y$.

completely with the learned knowledge by interventional data is still an open problem. We add an additional rule referring to the known results for CPDAG [20]. But regretfully, whether the eleven rules are complete is unknown. In the updated graph, some directed edges are newly identified to be visible, thus they are identified to be pure. Hence we could also update the purity matrix accordingly.

> Rule 11: If $a \circ\!\!\rightarrow b \rightarrow c$, $a, b, c \in \text{Adj}(d)$, $a \notin \text{Adj}(c)$, and $a, d, c$ do not form an unshielded collider, then $d \rightarrow c$.

**Proposition 7.** *Rule 11 is sound.*

Combining all the parts above, we present the whole process in Alg. 2. In a PMAG obtained by FCI or learned after interventions, we judge which variables are possible ancestors of $Y$ by Prop 8. If there are variables with unidentified causal effects on $Y$ (Line 1) among them and we are not sure whether GBC fails to identify the effects (Line 3), we select one variable from them to intervene (Line 4) and learn structure by the interventional data (Line 5 - Line 20). Since intervention is expensive in reality, we hope achieving target effect identification with fewer intervention times. Hence, among the variables mentioned above, we greedily intervene on the one with the maximum number of circles. A running example is given in Appendix F to illustrate the detailed procedure of the proposed method.

**Proposition 8.** *In a PMAG $\mathcal{P}$, if there is no minimal possible directed path from $X$ to $Y$, then $X$ cannot be ancestor of $Y$ in any MAG consistent to $\mathcal{P}$. And it holds that $X \notin \text{PossAn}(Y, \mathcal{P})$.*

## 4 Theoretical Results

In this section, we first prove the identifiability of causal effects[3]. Then we provide an analysis about the computation complexity of estimating all possible causal effects of each variable $X$ on $Y$.

[3] Note when we intervene, we have the information of $P(Y|do(X = x)$. However, we aim to identify $P(Y|do(X))$ when we say causal effect identification.

**Theorem 9.** Given the observational distribution of the observed variables, if there exists a valid generalized back-door set for $(X, Y)$ in the true MAG with the knowledge of the purity of each directed edge, then we can identify this set by only additional data of $Y$ under intervention on $X$.

Thm. 9 implies causal effect identifiability of each $X$ on $Y$ by interventions. In practice, when we intervene on $X$, in addition to identifying $P(Y|do(X))$, our method could learn some marks and the purity of some edges, which lead to the causal effect identification of *other variables* on $Y$. Hence we usually make target effect identification by far fewer intervention times than the variable number.

Estimating all possible causal effects takes the main computational cost. The process of estimating possible effects in a PMAG comprises finding all MCSs in Sec. 3.3 and using (2). We analyze the complexity of Sec. 3.3. Since the complexity is strongly related to the graph, it is hard to analyze for a general graph due to the randomness of the skeleton. We consider a special case - the complete graph, which is often considered as the most difficult graph to learn, because it has the most edges and we can learn no marks by only observational data as a result of no conditional independent relationship between the variables. To ensure that the interventional data accords with situation (2) or (3) when finding all MCSs in the PMAG is necessary, we set $Y$ as the descendant of all of $X_1, \cdots, X_p$. Due to space limit, we present a brief analysis here, while a detailed version is provided in Appendix E.2.

**Proposition 10.** *Let $\mathcal{M}$ be a complete MAG with $p+1$ variables $X_1, \cdots, X_p, Y$, where the causal order of the variables except $Y$ is completely random and $Y$ is at the last. Denote the graph obtained by FCI with observational data by $\mathcal{P}$ and intervention variable by $X_i$. And let $M$ be a local MAG of $X_i$ with $p-1-k$ tails and $k$ arrowheads at $X_i$. The computational complexity of finding all possible causal effects $P(Y|do(X_i))$ in all the MAGs consistent to $M$ is $O(2^k)$. Further, the computational complexity of finding all causal effects $P(Y|do(X_i))$ in all the MAGs consistent to $\mathcal{P}$ is $O(3^p)$.*

Let $\mathbf{S}$ denote the set of variable that has an edge with an arrowhead at $X_i$. Since the graph is complete, for any subset $\mathbf{S}_1$ of $\mathbf{S}$, we could construct an MAG $\mathcal{M}$ based on $M$ such that MCS in $\mathcal{M}$ is $\mathbf{S}_1$, which is detailed in Appendix E.2. Hence there are $2^k$ causal effects of $X_i$ on $Y$ in the MAGs consistent to $M$. Our method thus achieves the minimum complexity in finding possible causal effects in $M$.

However, when estimating causal effects of $X_i$ on $Y$ in $\mathcal{P}$, the complexity of our method is $O(3^p)$, while there are $2^{p-1}$ causal effects in $\mathcal{P}$. The gap is from two aspects. One is the search for critical variables. The other is that the causal effects in MAGs from different local MAGs are possibly equal, while these causal effects are considered separately based on each local MAG. The complexity of the latter part dominates. While if we do not consider the graphical characterization based on critical variable and adopt the local method of Malinsky and Spirtes [16] in estimating causal effects that enumerates MAGs in a subregion, the complexity is exponentially larger than ours, as shown in Table 1.

| | local MAG $M$ | PAG $\mathcal{P}$ |
|---|---|---|
| # Possible causal effects | $2^k$ | $2^{p-1}$ |
| Ours | $O(2^k)$ | $O(3^p)$ |
| Malinsky and Spirtes (2016) | None | $O(3^{p^2})$ |

Table 1: Complexity of estimating all effects.

## 5 Experiments

In this section, we apply our method on synthetic dataset to validate the effectiveness and efficiency of the proposed method. The code is developed based on R package "pcalg" [21].

We generate 100 random causal graphs and evaluate the number of correctly identified causal effects. In each graph, there are $p = 15$ variables and an edge occurs between two variables with probability 0.3. We randomly take 3 variables as latent confounders. And the last observed variable in the causal order is set to the response variable. We generate linear Gaussian data[4] according to the causal graph. Based on these information, we know not only the true MAG, but also whether each edge is pure. Hence we have the ground truth causal effect of each variable on the response variable by GBC. Beginning from the PAG obtained by the true MAG, we record the number of correctly identified causal effects under different intervention times with different methods.

[4] When variables are continuous, the positivity assumption tends to be violated. Here we ignore such risks because the identifiability has been proven and we just want to test whether the proposed method could accurately learn the structure and identify the generalized back-door set.

In our method, we adopt a greedy strategy to select the intervention variable. To verify the feasibility, we design a baseline method *ACIC-simple*, where we randomly select the intervention variable of which the causal effect on $Y$ has not been identified. To distinguish the methods with different strategies, we call our method *ACIC-greedy*. There are two additional baseline methods, *Do* and *ACI* [7]. For Do, it identifies causal relations by judging whether the distribution of observed variable takes a change under intervention, which idea is applied widely in many active causal discovery methods [2, 3]. Since in these methods all the variables could be observed under intervention, we allow Do to select which variable $X_j$ to observe under intervention instead of observing $Y$. The results are shown in Figure 3. The superiority of ACIC-greedy to ACIC-simple implies the greedy strategy to intervene helps saving intervention times. The phenomenon that ACIC-greedy is more efficient than Do verifies that exploiting causal effect elaborately could take us more message about the structure. There are many effects wrongly identified by ACI, which indicates the risk of ignoring latent confounders.

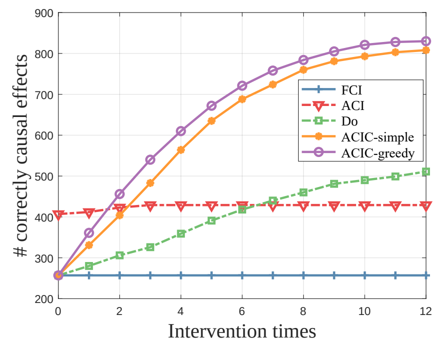



Figure 3: The number of correctly identified causal effects by different methods.

## 6 Conclusion

In this paper, we tackle the problem of identifying the causal effect of each variable on the response variable when the causal graph is unknown and there may exist latent confounders. We present the graphical characterization that allows us to find all possible causal effects in a PMAG. The characterization guides learning structure with the interventional data of only the response variable. Our method can achieve target effect identification effectively and efficiently in both saving intervention times and reducing computational complexity. And they are verified theoretically and empirically.

There are two main aspects to improve the method. One is on how to completely update a PMAG with the learned knowledge by interventional data. The other is on how to reduce the computational complexity further if possible. We look forward to future work that could address these problems.

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# Appendix A Preliminary

In this part, we first show some well-defined notions in Section A.1. The relation between pure and visible is displayed in Section A.2. Then, we review the generalized back-door criterion and some related results such as the necessary and sufficient condition for the existence of a generalized back-door set in Section A.3. Finally, we generalize these results to adapt to partial mixed ancestral graph taking purity into account in Section A.4.

## A.1 Well-defined notions

In Pearl's causality framework, we use a graph $G = (\mathbf{V}(G), \mathbf{E}(G))$ to describe the causal relation between the variables, where $\mathbf{V}(G)$ denotes the variable set and $\mathbf{E}(G)$ denotes the causal relation. A *mixed graph* is a graph containing two kinds of edges: directed edges $\rightarrow$ and bi-directed edges $\leftrightarrow$. The two ends of an edge are called *mark* and have two types *arrowhead* or *tail*. If there are some *circles* ($\circ$) in a graph, the graph is a *partial mixed graph*. The circle implies that the mark could be either arrowhead or tail but they are uncertain to us. $V_i$ is a *parent/child/spouse* of $V_j$ if $V_i \rightarrow V_j$/$V_i \leftarrow V_j$/$V_i \leftrightarrow V_j$. A *possible directed path* from $V_i$ to $V_j$ is a path without arrowheads at the marks near $V_i$ on every edge. $V_i$ is an *(possible) ancestor* of $V_j$ if there is a *(possible) directed path* from $V_i$ to $V_j$ or $V_i = V_j$. The (possible) ancestor set is denoted by $\text{An}(V_j, G)$ ($\text{PossAn}(V_j, G)$). Similar definitions are for *(possible) descendant*, denoted by $\text{De}(V_j, G)$ ($\text{PossDe}(V_j, G)$). If $V_i \in \text{An}(V_j, G)$ and $V_i \leftrightarrow V_j$, it forms an *almost directed cycle*. There is a *collider path* between $V_i$ and $V_j$ if they are adjacent or there is a path between them where all passing nodes are colliders in the path. A path from $V_i$ to $V_j$ is a *minimal path* if there is not a path with order preserving subsequence from $V_i$ to $V_j$.

A mixed graph is an *ancestral graph* if there is no directed or almost directed cycle (since we assume no selection bias, we do not consider undirected edges in this paper). $m$*-separation* ($m$*-connecting* or *active*) is proposed by Richardson et al. [22] to describe the conditional independence (or not) in ancestral graph. An ancestral graph is a *maximal ancestral graph (MAG)* if for any two non-adjacent vertices, there is a set of vertices that m-separates them.

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, $(2)$ every vertice between $X$ and $V$ in 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)* to denote an MEC, where circle occurs if the marks here are not the same in all Markov equivalent MAGs, while tail (arrowhead) occurs if all the marks here are tails (arrowheads).

Given an MAG $\mathcal{M}$ or a PAG $\mathcal{P}$, A directed edge $A \rightarrow B$ is *visible* if there is a vertex $C$ not adjacent to $B$, such that either there is an edge between $C$ and $A$ that is into $A$, or there is a collider path between $C$ and $A$ that is into $A$ and every vertex on the path is a parent of $B$. Otherwise $A \rightarrow B$ is said to be *invisible*. As shown in Zhang [11], Maathuis et al. [12], the intention to introduce "visible" is to imply the situation that there cannot be a latent confounder influencing the two variables of the edge. Let $G$ denote an MAG $\mathcal{M}$ or a PAG $\mathcal{P}$. $G_{\underline{X}}$ is the graph obtaining from $G$ by removing all directed edges out of $X$ that are visible in $G$. *Positivity* requires that any one combination of the values of all the variables is with a positive probability. *Selection bias* says that when we collect the observational data, some latent variables are given, which are influenced by more than one observed variables.

For a partial mixed graph, we say it is a *partial mixed ancestral graph (PMAG)* if there is no directed or almost directed cycle and denote it by $\mathcal{P}$. The relation between PMAG and PAG is like that between partially directed acyclic graph (PDAG) and completed partial directed acyclic graph (CPDAG) when there are no latent confounders [10]. Both MAG and PAG are seen as special cases of PMAG. Next, we define the Markov Equivalent Class of PMAG $\mathcal{P}$. Before that, we present the definition of a triples *with order* and a necessary and sufficient condition about Markov equivalence by Ali et al. [14].

**Definition 6** (with order)**.** Let $\mathfrak{D}_i (i \geq 0)$ be the set of triples of *with order* $i$ in an MAG $\mathcal{M}$, defined recursively as follows:

| | |
|---|---|
| Order 0 | A triple $\langle a, b, c \rangle \in \mathfrak{D}_0$ if $a$ and $C$ are not adjacent |
| Order $i+1$ | A triple $\langle a, b, c \rangle \in \mathfrak{D}_{i+1}$ if<br>(1) for all $j < i+1$, $\langle a, b, c \rangle \notin \mathfrak{D}_j$, and,<br>(2) there is a discriminating path $\langle x, q_1, \cdots, q_p, b, y \rangle$ for $b$ with either $\langle a, b, c \rangle = \langle q_p, b, y \rangle$ or $\langle a, b, c \rangle = \langle y, b, q_p \rangle$ and the $p$ colliders $\langle x, q_1, q_2 \rangle, \cdots, \langle q_{p-1}, q_p, b \rangle \in \bigcup_{j \leq i} \mathfrak{D}_j$. |

The Markov Equivalent Class of PMAG $\mathcal{P}$ is comprised of all the MAGs $\mathcal{M}$ such that if $(1)$ $\mathcal{M}$ and $\mathcal{P}$ have the same adjacencies, $(2)$ all the colliders with order in $\mathcal{M}$ are colliders in $\mathcal{P}$, $(3)$ all the non-circle marks in $\mathcal{P}$ are also in $\mathcal{M}$. In another word, $\mathcal{P}$ could be seen as a partial graph oriented by PAG of $\mathcal{M}$ with all non-circle marks consistent to $\mathcal{M}$.By classical causal discovery method, FCI for example, we could only obtain a PAG. In our method, we need to keep identifying some circles at PAG until achieving target effect identification. We thus introduce $\mathcal{P}$ to denote the continuously updated graph "between" the initial PAG and the truth MAG $\mathcal{M}$.

### A.2 The relation between pure and visible

Here, we illustrate that visibility is sufficient but not necessary for purity. It is trivially concluded by Zhang [11]. By Lemma 10 of Zhang [11], we can see that for each invisible edge $V_i \to V_j$ in an MAG $\mathcal{M}$, there could be a DAG whose MAG is $\mathcal{M}$ as well as $V_i$ and $V_j$ are influenced by a common latent variable. It also evidently holds that there is a DAG whose MAG is $\mathcal{M}$ and the two variables of any an invisible edge are not influenced by common latent variables. Hence invisibility is not sufficient for the existence of latent confounders. That is, visibility is not necessary for purity. Also, By the converse negative proposition of Lemma 9 of Zhang [11], we know if a directed edge is visible, there cannot be latent confounding effects for this edge. It thus holds visibility is sufficient for purity. Hence we see that visibility is sufficient but not necessary for purity.

### A.3 Generalized back-door criterion and the graphical condition for the existence of generalized back-door set proposed by Maathuis et al. [12]

In this part, we first show the definition of back-door paths. Then we present some related concepts, followed by the necessary and sufficient graphical criteria for the existence of a set of variables that satisfies generalized back-door criterion. All of these results are presented by Zhang [11], Maathuis et al. [12].

**Definition** (Back-door path)**.** Let $(X, Y)$ be an ordered pair of vertices in $G$ , where $G$ is a DAG, CPDAG, MAG or PAG. We say that a path between $X$ and $Y$ is a back-door path from $X$ to $Y$ if it does not have a visible edge out of $X$.

**Definition** (Definite noncollider; Zhang [11])**.** A nonendpoint vertex $X_j$ on a path $\langle \cdots, X_i, X_j, X_k, \cdots \rangle$ in a partial mixed graph $G$ is a *definite non-collider* on the path if $(1)$ there is a tail mark at $X_j$, that is $X_i \ast\!\!- X_j$ or $X_j -\!\!\ast X_k$, or $(2)$ $\langle X_i, X_j, X_k\rangle$ is unshielded and has circle marks at $X_j$, that is, $X_i \ast\!\!-\!\!\circ\, X_j \circ\!\!-\!\!\ast\, X_k$ and $X_i$ and $X_k$ are not adjacent in $G$.

**Definition** (Definite status path; Zhang [11], Maathuis et al. [12])**.** A nonendpoint vertex $X$ on a path $p$ in a partial mixed graph is said to be of a definite status if it is either a collider or a definite noncollider on $p$. The path $p$ is said to be of a definite status if all nonendpoint vertices on the path are of a definite status.

**Definition** (Generalized back-door criterion; Maathuis et al. [12])**.** Let $\mathbf{X}$, $\mathbf{Y}$ and $\mathbf{Z}$ be pairwise disjoint sets of vertices in $G$, where $G$ represents a DAG, CPDAG, MAG or PAG. Then $\mathbf{Z}$ satisfies the *generalized back-door criterion* relative to $(\mathbf{X}, \mathbf{Y})$ and $G$ if $(1)$ $\mathbf{Z}$ does not contain possible descendants of $\mathbf{X}$ in $G$; $(2)$ for every $X \in \mathbf{X}$, the set $\mathbf{Z} \cup \mathbf{X}\backslash\{X\}$ blocks every definite status back-door path from $X$ to any member of $\mathbf{Y}$, if any, in $G$. A set $\mathbf{Z}$ that satisfies the generalized back-door criterion relative to $(\mathbf{X}, \mathbf{Y})$ and $G$ is called a *generalized back-door set* relative to $(\mathbf{X}, \mathbf{Y})$ and $G$.

Given a graph $G$, Maathuis et al. [12] proposed the necessary and sufficient graphical criteria for the existence of a set of variables that satisfies generalized back-door criterion with *only observational data*. Before that, the definition of D-SEP$(X, Y, G)$ is presented in Def. 1. Then we show one of the main result by Maathuis et al. [12] in Prop. 11.

**Definition 1** (D-SEP$(X, Y, G)$ [12])**.** Let $X$ and $Y$ be two distinct vertices in a mixed graph $G$. We say that $V \in$ D-SEP$(X, Y, G)$ if $V \neq X$, and there is a collider path between $X$ and $V$ in $G$, such that every vertex on this path (including $V$) is an ancestor of $X$ or $Y$ in $G$.

**Proposition 11** (Maathuis et al. [12])**.** *Let $X$ and $Y$ be two distinct vertices in $G$. There exists a generalized back-door set relative to $(X, Y)$ and $G$ if and only if $Y \notin \mathrm{Adj}(X, G_{\underline{X}})$ and* D-SEP$(X, Y, G_{\underline{X}}) \cap \mathrm{PossDe}(X, G) = \emptyset$*. Moreover, if such a generalized back-door set exists, then* D-SEP$(X, Y, G_{\underline{X}})$ *is such a set. Denote* D-SEP$(X, Y, G_{\underline{X}})$ *by* $\mathbf{D}$*, the causal effect of $X$ on $Y$ is*

$$P(Y|do(X = x)) = \int_{\mathbf{D}} P(\mathbf{D}) P(Y|\mathbf{D}, X = x)\, \mathrm{d}\mathbf{D}. \tag{4}$$

### A.4 The improved result in Proposition 1

In this part, we first present our improved definition about back-door paths. With that we present the improved generalized back-door criterion. The justification for such modification is that our method continuously identifies some new marks with the actively interventional data until achieving target effect identification. The updated graph among the process is a PMAG, but not necessarily a PAG or MAG. In this case, whether a directed edge is with latent variables could be not only learned by the graphical criterion of visibility, but also learned by interventional data, which is reflected by the purity matrix. Hence we modify the related conditions to make it adapt to PMAG with purity matrix. This idea is simple and direct. But rigorously, the proof is very lengthy since it refers to too many results of Maathuis et al. [12], Zhang [23, 11]. Hence we suggest readers skipping the statements below and just reading the result in Prop. 1 without too much attention on the detail.

Considering the back-door paths in PAG or MAG from $X$ to $Y$ according to the definition of Maathuis et al. [12], they are the paths from $X$ to $Y$ that do not have a visible edges out of $X$. In fact, the reason that we need to consider the paths that have invisible edge out of $X$ is that there is one possibility that there are latent confounders behind the invisible edge out of $X$ (i.e. there is at least one latent confounder that influences the two variables of the invisible edge). In the circumstances, there is a back-door path from $X$ to $Y$ through the latent confounder. Hence we need to block such paths to make all the possible back-door paths blocked. As shown by Zhang [11] and Appendix A.2, by mere observational data, only the visible edges can be confirmed that have no latent confounders. However, if we could learn more knowledge about the existence of the latent confounders by interventional data, e.g., if we could identify that some possible back-door paths are not back-door paths in the DAGs, we do not consider blocking such paths. For example, for an MAG $X \rightarrow Y$, if the edge is invisible, $X \rightarrow Y$ is a back-door path. By original generalized back-door criterion, we cannot find a set that blocks the back-door path $X \rightarrow Y$, thus no set satisfies generalized back-door criterion. However, if we could learn that there is no latent confounder behind the edge $X \rightarrow Y$, then we could be sure that there is no need to block $X \rightarrow Y$, and $\emptyset$ satisfies back-door criterion in the causal graph, because no matter what the true causal graph that the MAG represents is, there are no back-door paths from $X$ to $Y$. Thus we can see $P(Y|do(X)) = P(Y|X)$. With such considerations, we take the purity matrix $W$ into account and define back-door path relative to $W$ as follows. Note we restrict that $W$ must be initialized by setting $W[i,j] = 1$ if the directed edge $i \rightarrow j$ is visible in the PAG learned by FCI algorithm. That is, $W$ is able to indicate that the visible edges in PAG are pure.

Next, we present the definition of $G_{\underset{\sim}{X}}$. If $G$ is an MAG, then $G_{\underset{\sim}{X}}$ denotes the graph by removing the directed edges out of $X$ in $G$ that are labeled to be pure in purity matrix. If $G$ is a PMAG, we obtain $G_{\underset{\sim}{X}}$ by two steps. In the first step, let $R$ be any one MAG from the subclass of MAGs consistent to $G$ that have the same number of edges into $X$ in $G$. In the second step, we obtain $G_{\underset{\sim}{X}}$ by removing the directed edges out of $X$ in $R$ if the edge is labeled to be pure in purity matrix or is visible in $R$.

**Definition 7** (Back-door path relative to $W$)**.** Let $(X, Y)$ be an ordered pair of vertices in $G$, where $G$ is a PMAG. Denote the purity matrix in graph $G$ by $W$. We say that the path between $X$ and $Y$ is a back-door path from $X$ to $Y$ if it does not start with a directed edge $X \rightarrow Z$ with $W[X,Z] = 1$, where $Z$ is any a variable except for $X$.

With the back-door path relative to $W$, the generalized back-door criterion relative to $W$ is presented in the following. In contrast to the original definition, we also add the statement of $W$.

**Definition 8** (Generalized back-door criterion relative to $(G, W)$)**.** Let $\mathbf{X}$, $\mathbf{Y}$ and $\mathbf{Z}$ be pairwise disjoint sets of vertices in $G$, where $G$ represents a PMAG. Denote the purity matrix in graph $G$ by $W$. Then $\mathbf{Z}$ satisfies the *generalized back-door criterion* relative to $(\mathbf{X}, \mathbf{Y})$ and $(G, W)$ if (1) $\mathbf{Z}$ does not contain possible descendants of $\mathbf{X}$ in $G$; (2) for every $X \in \mathbf{X}$, the set $\mathbf{Z} \cup \mathbf{X} \backslash \{X\}$ blocks every definite status back-door path relative to $W$ from $X$ to any member of $\mathbf{Y}$, if any, in $G$. A set $\mathbf{Z}$ that satisfies the generalized back-door criterion relative to $(\mathbf{X}, \mathbf{Y})$ and $(G, W)$ is called a *generalized back-door set* relative to $(\mathbf{X}, \mathbf{Y})$ and $(G, W)$.

Then, we present the adjustment criterion in PMAG and show that the set satisfies GBC in a PMAG satisfies adjustment criterion in the PMAG.

**Definition 9** (Adjustment criterion)**.** Let $\mathbf{X}$, $\mathbf{Y}$, and $\mathbf{Z}$ be pairwise disjoint sets of vertices in a PMAG $G$ and $W$ be a purity matrix of $G$. Then we say that $\mathbf{Z}$ satisfies the adjustment criterion relative to $(X, Y)$ and $(G, W)$ if for any density $f$ compatible with $G$, we have

$$f(\mathbf{Y}|do(\mathbf{X})) = \begin{cases} f(\mathbf{Y}|\mathbf{X}), & \text{if } \mathbf{Z} = \varnothing, \\ \int_{\mathbf{Z}} f(\mathbf{Y}|\mathbf{Z},\mathbf{X}) f(\mathbf{Z})\, \mathrm{d}\mathbf{Z} = \mathbb{E}_{\mathbf{Z}}\{f(\mathbf{Y}|\mathbf{Z},\mathbf{X})\}, & \text{otherwise.} \end{cases}$$

**Proposition 12.** *Let $\mathbf{X}$, $\mathbf{Y}$, $\mathbf{Z}$ be pairwise disjoint sets of variables in a PMAG $G$ and $W$ be a purity matrix of $G$. If $\mathbf{Z}$ satisfies the generalized back-door criterion relative to $(\mathbf{X}, \mathbf{Y})$ and $(G, W)$, then it satisfies the adjacent criterion relative to $(\mathbf{X}, \mathbf{Y})$ and $(G, W)$.*

*Proof.* It could be proved trivially by the results in Maathuis et al. [12]. Here we just show a proof sketch. If a set $\mathbf{Z}$ satisfies GBC relative to $(X, Y)$ and $(G, W)$, then it satisfies invariance criterion (see Definition 7.1 of Maathuis et al. [12]). The proof process is as one direction in Theorem 7.3 of Maathuis et al. [12]. Note here the result in converse direction does not necessarily hold, which is a difference between PMAG and PAG. Then by Theorem 7.1 of Maathuis et al. [12] we could directly prove the set satisfies the adjacent criterion relative to $(\mathbf{X}, \mathbf{Y})$. $\square$

Based on these, we present Prop. 1.

**Proposition 1.** *Let $G$ be a PMAG and $W$ be a purity matrix of $G$. Suppose $X \in \mathrm{An}(Y, G)$ and $Y$ are two distinct vertices in $G$. There exists a generalized back-door set relative to $(X, Y)$ and $(G, W)$ if and only if* $\text{D-SEP}(X, Y, G_{\underset{\sim}{X}}) \cap \mathrm{PossDe}(X, G) = \emptyset$*. Moreover, if the set exists,* $\text{D-SEP}(X, Y, G_{\underset{\sim}{X}})$ *is such a set. Denote*

D-SEP$(X, Y, G_{\underset{\sim}{X}})$ *by* $\mathbf{D}$*, the causal effect is*

$$P(Y|do(X=x)) = \int_{\mathbf{D}} P(\mathbf{D})P(Y|\mathbf{D}, X=x)\,\mathrm{d}\mathbf{D}. \tag{1}$$

*Proof.* There are two modifications between Prop. 11 and Prop. 1. One is that we additionally take the purity matrix $W$ into account in Prop. 1. Thus we need to replace the *visibility* in their proof by *purity*, and extend the *back-door path* and *generalized back-door criterion relative to* $G$ to *back-door path relative to* $W$ and *generalized back-door criterion relative to* $(G, W)$. The other is that we consider PMAG rather than only PAG. The rigorous proof is very lengthy and completely follows the proof of Maathuis et al. [12], Zhang [23], we thus just show the different part and leave the details of the proof for the readers. For the "if" statement, we need to prove $Y \notin \mathrm{Adj}(X, G_{\underset{\sim}{X}})$. If not, there is a directed edge $X \rightarrow Y$ where the two variables are influenced by a latent confounder. In such case we could see that $Y \in$ D-SEP$(X, Y, G_{\underset{\sim}{X}}) \cap$ PossDe$(X, G)$, which contradicts D-SEP$(X, Y, G_{\underset{\sim}{X}}) \cap$ PossDe$(X, G) = \emptyset$. Hence we have $Y \notin \mathrm{Adj}(X, G_{\underset{\sim}{X}})$ and D-SEP$(X, Y, G_{\underset{\sim}{X}}) \cap$ PossDe$(X, G) = \emptyset$. The other proof process of Prop. 1 is totally same as that of Maathuis et al. [12]. Note that $\mathcal{R}$ in Theorem 4.1 of Maathuis et al. [12] denotes any an MAG in the subclass of MAGs in the MEC described by $G$ that have the same number of edges into $X$ as $G$. Hence $\mathcal{R}_{\underset{\sim}{X}}$ denotes the MAG obtained from $\mathcal{R}$ by removing the pure edges out of $X$ in $G$, which is exactly the $G_{\underset{\sim}{X}}$ in our paper.

For the "only if" statement, Lemma 7.7 of Maathuis et al. [12] does not necessarily hold in PMAG. We thus cannot follow the proof directly. However, since we restrict that $X \in \mathrm{An}(Y, G)$, and $V \in$ D-SEP$(X, Y, G_{\underset{\sim}{X}})$, we can also conclude that there must be a directed path from $V$ to $Y$ in $G_{\underset{\sim}{X}}$. The other parts are the same as those of Theorem 4.1 of Maathuis et al. [12]. □

## Appendix B Minimal Conditional Set

In this part, we first define *minimal conditional set regarding* D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}})$. Then we show the uniqueness of MCS by Lemma 14 in Appendix B.1. Next, we propose Alg. 0.1 to find the MCS in Appendix B.2, along with the theoretical guarantee for the soundness of Alg. 0.1.

**Definition 2** (Minimal conditional set regarding D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}})$ (MCS))**.** Let $\mathcal{M}$ be an MAG. $X$, $Y$, and $\mathbf{D}$ denote the intervened variable, response variable, and the set D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}})$ in $\mathcal{M}$, respectively. $\overline{\mathbf{D}}$ is a subset of $\mathbf{D}$. $\overline{\mathbf{D}}$ is a minimal conditional set regarding $\mathbf{D}$ in $\mathcal{M}$ if

(1) $(Y \perp \mathbf{D}\backslash\overline{\mathbf{D}}\,|\overline{\mathbf{D}} \cup \{X\})_{\mathcal{M}}$,

(2) $(Y \not\perp \mathbf{D}\backslash\overline{\mathbf{D}}'|\overline{\mathbf{D}}' \cup \{X\})_{\mathcal{M}}$, for any $\overline{\mathbf{D}}' \subset \overline{\mathbf{D}}$.

### B.1 The uniqueness of MCS

Here, we prove the uniqueness of MCS. Before that, we propose Lemma 13 for supporting the main proof of the uniqueness of MCS. Note that positivity is assumed in this paper. With an abuse of notation, we do not distinguish random variable from the value of the random variable to make the proof concise.

**Lemma 13.** *Let* $\mathbf{A}, \mathbf{B}, \mathbf{C}, \mathbf{D}$ *be four pairwise disjoint variable sets. If* $\Pr(\mathbf{D}|\mathbf{C}, \mathbf{A}) = \Pr(\mathbf{D}|\mathbf{C}, \mathbf{B})$*, then* $\Pr(\mathbf{D}|\mathbf{C}, \mathbf{A}) = \Pr(\mathbf{D}|\mathbf{C}, \mathbf{B}) = \Pr(\mathbf{D}|\mathbf{C})$.

In fact, the condition of this lemma provides an intuition that conditional distribution is irrelevant to $\mathbf{A}$ and $\mathbf{B}$, which concludes the result directly. Nevertheless, we give a rigorous proof as follows.

*Proof.* Multiply both sides of the condition by $\Pr(\mathbf{A}|\mathbf{C})$, it holds that

$$\Pr(\mathbf{A}|\mathbf{C})\Pr(\mathbf{D}|\mathbf{C}, \mathbf{A}) = \Pr(\mathbf{A}|\mathbf{C})\Pr(\mathbf{D}|\mathbf{C}, \mathbf{B})$$
$$\sum_{\mathbf{A}} \Pr(\mathbf{A}|\mathbf{C})\Pr(\mathbf{D}|\mathbf{C}, \mathbf{A}) = \sum_{\mathbf{A}} \Pr(\mathbf{A}|\mathbf{C})\Pr(\mathbf{D}|\mathbf{C}, \mathbf{B})$$
$$\Pr(\mathbf{D}|\mathbf{C}) = \Pr(\mathbf{D}|\mathbf{C}, \mathbf{B}).$$

Hence, we have $\Pr(\mathbf{D}|\mathbf{C}, \mathbf{B}) = \Pr(\mathbf{D}|\mathbf{C})$. Similarly, it also holds that $\Pr(\mathbf{D}|\mathbf{C}, \mathbf{A}) = \Pr(\mathbf{D}|\mathbf{C})$. We thus get the desired conclusion. □

**Lemma 14** (Uniqueness)**.** *If both* $\mathbf{F}_1$ *and* $\mathbf{F}_2$ *are minimal conditional sets regarding* $\mathbf{D}$ *in* $\mathcal{M}$*, then* $\mathbf{F}_1 = \mathbf{F}_2$.

*Proof.* If $\mathbf{F}_1 \neq \mathbf{F}_2$, according to the definition of MCS, it evidently concludes $\mathbf{F}_1 \backslash \mathbf{F}_2 \neq \emptyset$ and $\mathbf{F}_2 \backslash \mathbf{F}_1 \neq \emptyset$. We denote $\mathbf{F} = \mathbf{F}_1 \cap \mathbf{F}_2$, $\mathbf{A} = \mathbf{F}_1 \backslash \mathbf{F}$, $\mathbf{B} = \mathbf{F}_2 \backslash \mathbf{F}$. Evidently $\mathbf{A}, \mathbf{B}, \mathbf{F}, X$ are disjoint.

According to the definition, we have

$$Y \perp \mathbf{D} \backslash (\mathbf{F} \cup \mathbf{A}) | \mathbf{F} \cup \mathbf{A} \cup X, \tag{5}$$
$$Y \perp \mathbf{D} \backslash (\mathbf{F} \cup \mathbf{B}) | \mathbf{F} \cup \mathbf{B} \cup X. \tag{6}$$

By (5), it holds

$$\begin{aligned} &\Pr(Y|\mathbf{F}, \mathbf{A}, X) \Pr(\mathbf{D} \backslash (\mathbf{F} \cup \mathbf{A}) | \mathbf{F}, \mathbf{A}, X) \\ =& \Pr(Y, \mathbf{D} \backslash (\mathbf{F} \cup \mathbf{A}) | \mathbf{F}, \mathbf{A}, X). \end{aligned}$$

Multiply $\Pr(\mathbf{A}|\mathbf{F}, X)$ on both sides,

$$\Pr(Y|\mathbf{F}, \mathbf{A}, X) \Pr(\mathbf{D} \backslash \mathbf{F} | \mathbf{F}, X) = \Pr(Y, \mathbf{D} \backslash \mathbf{F} | \mathbf{F}, X). \tag{7}$$
$$\Pr(Y|\mathbf{F}, \mathbf{A}, X) = \Pr(Y|\mathbf{D} \backslash \mathbf{F}, \mathbf{F}, X) = \Pr(Y|\mathbf{D}, X). \tag{8}$$

The conversion from (7) to (8) depends on $\Pr(\mathbf{D} \backslash \mathbf{F} | \mathbf{F}, X) \neq 0$ for any attainable value of the variables, which is due to the positivity assumption. Similarly, we have

$$\Pr(Y|\mathbf{F}, \mathbf{B}, X) = \Pr(Y|\mathbf{D}, X). \tag{9}$$

Combine (8) and (9), $\Pr(Y|\mathbf{F}, X, \mathbf{A}) = \Pr(Y|\mathbf{F}, X, \mathbf{B}) = \Pr(Y|\mathbf{D}, X)$. By Lemma 13, we know $\Pr(Y|\mathbf{F}, X, \mathbf{A}) = \Pr(Y|\mathbf{F}, X, \mathbf{B}) = \Pr(Y|\mathbf{F}, X)$. We rewrite (7) as

$$\Pr(Y|\mathbf{F}, X) \Pr(\mathbf{D} \backslash \mathbf{F} | \mathbf{F}, X) = \Pr(Y, \mathbf{D} \backslash \mathbf{F} | \mathbf{F}, X).$$

It concludes $Y \perp \mathbf{D} \backslash \mathbf{F} | \mathbf{F}, X$. It conflicts with the conditions that $\mathbf{F} \subsetneqq \mathbf{F}_1$ and $\mathbf{F}_1$ is a minimal conditional set regarding $\mathbf{D}$. □

### B.2 The algorithm to find MCS and the theoretical guarantee

Till now, we have proved the uniqueness of MCS, which plays an important role in the following proofs. Next, we propose Alg. 0.1 to find the MCS regarding $\mathbf{D}$ in $\mathcal{M}$. Lemma 15 and Lemma 16 are two important lemmas used widely in the proofs below. With these results, we prove the soundness of Alg. 0.1 to find the MCS in Lemma 17.

**Algorithm 0.1** Find the MCS regarding $\mathbf{D}$ in $\mathcal{M}$

```
S = D                                   // Record the MCS
for V in S do
    if V ⊥ Y|{X, S\{V}} in M then
        S = S\{V}
    end if
end for
output: S.
```

**Lemma 15.** *Let $\mathbf{A}, \mathbf{B}, \mathbf{C}$ be three pairwise disjoint variables sets. If $\mathbf{E} \subset \mathbf{B}$, $\mathbf{E} \neq \emptyset$ and $\mathbf{A} \perp \mathbf{B} | \mathbf{C}$, then $\mathbf{A} \perp \mathbf{B} \backslash \mathbf{E} | \{\mathbf{C} \cup \mathbf{E}\}$.*

*Proof.* Since $\mathbf{A} \perp \mathbf{B} | \mathbf{C}$ and $\mathbf{E} \subset \mathbf{B}$, it concludes that $\mathbf{A} \perp \mathbf{E} | \mathbf{C}$. We have

$$\begin{aligned} &\Pr(\mathbf{A}|\mathbf{C}, \mathbf{E}) \Pr(\mathbf{B} \backslash \mathbf{E} | \mathbf{C}, \mathbf{E}) \\ =& \Pr(\mathbf{A}|\mathbf{C}) \Pr(\mathbf{B} \backslash \mathbf{E} | \mathbf{C}, \mathbf{E}) \\ =& \Pr(\mathbf{A}|\mathbf{C}, \mathbf{B}) \Pr(\mathbf{B} \backslash \mathbf{E} | \mathbf{C}, \mathbf{E}) \\ =& \Pr(\mathbf{A}|\mathbf{C}, \mathbf{B} \backslash \mathbf{E}, \mathbf{E}) \Pr(\mathbf{B} \backslash \mathbf{E} | \mathbf{C}, \mathbf{E}) \\ =& \Pr(\mathbf{A}, \mathbf{B} \backslash \mathbf{E} | \mathbf{C}, \mathbf{E}). \end{aligned}$$

We get the desired conclusion. □

**Lemma 16.** *For two pairwise disjoint sets $\mathbf{A}_1, \mathbf{A}_2$ such that $(\mathbf{A}_1 \cup \mathbf{A}_2) \cap \{X, Y\} = \emptyset$, denote $\mathbf{A} = \mathbf{A}_1 \cup \mathbf{A}_2$. Let $\mathbf{E}$ be a set such that $\mathbf{E} \supseteq \mathbf{A}$ and $\mathbf{E} \cap \{X, Y\} = \emptyset$. If $\mathbf{A}_2 \perp Y | X, \mathbf{A}_1$ and $\mathbf{E} \backslash \mathbf{A} \perp Y | X, \mathbf{A}$, then $(\mathbf{E} \backslash \mathbf{A}, \mathbf{A}_2) \perp Y | X, \mathbf{A}_1$.*

*Proof.* Denote $\mathbf{E}\backslash\mathbf{A}$ by $\mathbf{B}$.

$$\begin{aligned}
&\Pr(\mathbf{B}, Y|X, \mathbf{A}_1)\\
=&\sum_{\mathbf{A}_2}\Pr(\mathbf{B}, \mathbf{A}_2, Y|X, \mathbf{A}_1),\\
=&\sum_{\mathbf{A}_2}\Pr(\mathbf{A}_2, Y|X, \mathbf{A}_1)\Pr(\mathbf{B}|X, \mathbf{A}_1, \mathbf{A}_2, Y),\\
=&\sum_{\mathbf{A}_2}\Pr(\mathbf{A}_2|X, \mathbf{A}_1)\Pr(Y|X, \mathbf{A}_1)\Pr(\mathbf{B}|X, \mathbf{A}_1, \mathbf{A}_2)\\
&\quad\because (\mathbf{A}_2 \perp Y|X, \mathbf{A}_1) \text{ and } (\mathbf{E}\backslash\mathbf{A} \perp Y|X, \mathbf{A}),\\
=&\Pr(Y|X, \mathbf{A}_1)\Pr(\mathbf{B}|X, \mathbf{A}_1).
\end{aligned}$$

It completes the proof. □

**Lemma 17.** *Algorithm 0.1 is sound in finding the MCS regarding $\mathbf{D}$ in $G$.*

*Proof.* Denote the MCS by $\overline{\mathbf{D}}$. Without loss of generality, suppose the whole enumerating sequence in Line 2 is $T_1, T_2, \cdots, T_k$. For any $T_i$, we will prove if $T_i \in \mathbf{D}\backslash\overline{\mathbf{D}}$, the condition in Line 3 is satisfied. While if $T_i \in \overline{\mathbf{D}}$, the condition in Line 3 is not satisfied. In this case we could delete the variables which do not belong to $\overline{\mathbf{D}}$ and keep the variables belonging to $\overline{\mathbf{D}}$ in $\mathbf{D}$. We prove it by mathematical induction. $T_1$ is considered at first. If $T_1 \in \mathbf{D}\backslash\overline{\mathbf{D}}$, by the definition of $\overline{\mathbf{D}}$, it holds that $\mathbf{D}\backslash\overline{\mathbf{D}} \perp Y|\overline{\mathbf{D}}, X$. Combining $\mathbf{D}\backslash\overline{\mathbf{D}} \perp Y|\overline{\mathbf{D}}, X$ with lemma 15, we have $T_1 \perp Y|\mathbf{D}\backslash\{T_1\}, X$, which satisfies the condition in Line 3. While if $T_1 \in \overline{\mathbf{D}}$, we aim to prove $T_1 \not\perp Y|\mathbf{D}\backslash\{T_1\}, X$. For the sake of contradiction, we assume $T_1 \perp Y|\mathbf{D}\backslash\{T_1\}, X$. By the definition of MCS, we know that one set $\mathbf{D}' \subseteq \mathbf{D}\backslash\{T_1\}$ could be as the MCS. However, we know $\overline{\mathbf{D}}$ is an MCS which contains $T_1$. That means there are two distinct MCSs, which contradicts Lemma 14. Hence $T_1 \not\perp Y|\mathbf{D}\backslash\{T_1\}, X$.

We suppose the result above holds for the sequence $T_1, T_2, \cdots, T_{i-1}$ and now the algorithm judges $T_i$ in Line 3. Since some variables have been deleted by Line 4, we denote the remained variable set $\mathbf{T}$. The only difference between $\mathbf{D}$ and $\mathbf{T}$ is the variables from $T_1, T_2, \cdots, T_{i-1}$ which satisfies Line 3, i.e. the variable does not belong to $\overline{\mathbf{D}}$ according to the inductive hypothesis. Hence it is evident that $\overline{\mathbf{D}} \subseteq \mathbf{T} \subseteq \mathbf{D}$. If $T_i \in \mathbf{D}\backslash\overline{\mathbf{D}}$, using $Y \perp \mathbf{D}\backslash\overline{\mathbf{D}}|\overline{\mathbf{D}}, X$ and Lemma 15 (setting $\mathbf{B} = \mathbf{D}\backslash\overline{\mathbf{D}}$ and $\mathbf{D} = (\mathbf{T}\backslash\{T_i\})\backslash\overline{\mathbf{D}}$ in Lemma 15), we have $Y \perp \mathbf{D}\backslash(\mathbf{T}\backslash\{T_i\})|\mathbf{T}\backslash\{T_i\}, X$ . Hence $Y \perp T_i|\mathbf{T}\backslash\{T_i\}, X$, which implies that the condition in Line 3 is satisfied. If $T_i \in \overline{\mathbf{D}}$, the proof is also similar to that for $T_1$. For the sake of contradiction, we assume $T_i \perp Y|\mathbf{T}\backslash\{T_i\}, X$. Without loss of generality, we denote the last deleted variable from $T_1 \cdots, T_{i-1}$ by $T_{l_1}$. Since $T_{l_1}$ is deleted in Line 4, it implies that $T_{l_1} \perp Y|\mathbf{T}, X$. Combining $T_i \perp Y|\mathbf{T}\backslash\{T_i\}, X$ and $T_{l_1} \perp Y|\mathbf{T}, X$ by Lemma 16, we obtain that $(T_{l_1}, T_i) \perp Y|\mathbf{T}\backslash\{T_i\}, X$. We continue finding the second-to-last deleted variable $T_{l_2}$ from $T_1 \cdots, T_{i-1}$ and we can obtain $(T_{l_1}, T_{l_2}, T_i) \perp Y|\mathbf{T}\backslash\{T_i\}, X$. Repeat this process until we find all deleted variables from $T_1 \cdots, T_{i-1}$, we obtain that $(T_{l_1}, T_{l_2}, \cdots, T_{l_s}, T_i) \perp Y|\mathbf{T}\backslash\{T_i\}, X$. Note $T_{l_1}, T_{l_2}, \cdots, T_{l_s} = \mathbf{D}\backslash\mathbf{T}$, it thus holds $(\mathbf{D}\backslash\mathbf{T}, T_i) \perp Y|\mathbf{T}\backslash\{T_i\}, X$. By the definition of MCS, we can obtain a subset $\mathbf{D}' \subseteq \mathbf{T}\backslash\{T_i\}$ as the MCS regarding $\mathbf{D}$. But according to the condition, $T_i$ should be one variable from the MCS, which contradicts Lemma 14 that implies the MCS is unique. Hence $T_i \not\perp Y|\mathbf{T}\backslash\{T_i\}, X$. We prove the result for $T_i$. The mathematical induction completes.

By mathematical induction, we prove the set of the remained variables by Algorithm 0.1 is MCS. □

# Appendix C Proofs for the Results in Section 3.3

There are three parts in this section. The first part is about the proof for Theorem 2. We first present Lemma 18, which plays an important role in the proof of Theorem 2. By the lemma we prove Theorem 2 trivially. The second part is about the proof for Theorem 3. We define critical variable in Definition 5. Then we provide the proof for Theorem 3. In the last part, we prove Lemma 4.

## C.1 Proofs for Theorem 2

**Definition 3** (Local MAG of $X$ based on $\mathcal{P}$)**.** Given a PMAG $\mathcal{P}$ and a variable $X$, a PMAG $M$ is a *local MAG of $X$ based on $\mathcal{P}$* if (1) $M$ is with definite marks (arrowheads or tails) at $X$; (2) $M$ is obtained from $\mathcal{P}$ by marking some circles without generating new unshielded colliders or directed or almost directed cycles. We call it *local MAG* for short if there is no ambiguity and denote it by $M$, which is different from calligraphic $\mathcal{M}$ that denotes MAG.

**Lemma 18.** *Let $\mathcal{P}$ be a PMAG which MAG $\mathcal{M}$ is consistent to. If $V \in$ D-SEP$(X, Y, \mathcal{M})$, then there is at least one collider path between $X$ and $V$ in $\mathcal{P}$ and each variable in this path is a possible ancestor of $X$ or $Y$ in $\mathcal{P}$.*

*Proof.* Suppose $V \in$ D-SEP$(X, Y, \mathcal{M})$. According to the definition of D-SEP$(X, Y, \mathcal{M})$, there is a collider path between $V$ and $X$, and each variable in this path is an ancestor of $X$ or $Y$ in $\mathcal{M}$. Since $\mathcal{M}$ and $\mathcal{P}$ have the same skeleton, we analyze the corresponding path in PMAG $\mathcal{P}$. It is evident that each variable in this path is a possible ancestor of $X$ or $Y$ in $\mathcal{P}$. We then just prove that there is a collider path where each variable is the possible ancestor of $X$ or $Y$ in $\mathcal{P}$.

Since there is a collider path between $X$ and $V$, where each variable is an ancestor of $X$ or $Y$ in $\mathcal{M}$, there must be a minimal collider path between $X$ and $V$, where each variable is an ancestor of $X$ or $Y$. For the sake of clarity, we replace $V$ by $F_n$ and denote the minimal collider path by $X {*\!\!\rightarrow} F_1 \leftrightarrow \cdots \leftrightarrow F_{n-1} \leftarrow\!\!* F_n$. We assume the collider $F_{i-1} \leftrightarrow F_i \leftrightarrow F_{i+1}$ is a collider without order. There must be an edge between $F_{i-1}$ and $F_{i+1}$. The edge is evidently not bi-directed, otherwise it contradicts the minimal collider path. Without loss of generality, we suppose the edge is $F_{i-1} \rightarrow F_{i+1}$. The reasonableness of this assumption is that collider path between $X$ and $F_n$ is symmetric (here the condition that each variable is an ancestor of $X$ or $Y$ is not considered).

Next we consider the collider $F_{i-2} \leftrightarrow F_{i-1} \leftrightarrow F_i$. There are two possible situations. One is that the collider is with some constant order. In this case, we prove there is an edge $F_{i-1} \rightarrow F_{i+1}$ in the following. If they are not adjacent, then there is a discriminating path $F_{i-2}, F_{i-1}, F_i, F_{i+1}$ for $F_i$, which implies that the collider $F_{i-1} \leftrightarrow F_i \leftrightarrow F_{i+1}$ is with order, contradicting the condition. Due to the ancestral property, the edge could only be as $F_{i-2} {*\!\!\rightarrow} F_{i+1}$. And it thus be $F_{i-2} \rightarrow F_{i+1}$ due to the minimal collider path condition. The other situation is that $F_{i-2} \leftrightarrow F_{i-1} \leftrightarrow F_i$ is also without order.

In the following we consider the collider at $F_{i-2}, F_{i-3}, \cdots, F_1$ recursively. During the iteration, suppose the first variable $F_k$ where the collider is without order. That is, the colliders at the variables $F_{k+1}, F_{k+2}, \cdots, F_{i-2}, F_{i-1}$ are with order. In this case, we first prove that for all the variable $F_m, k \leq m \leq i-1$, there is an edge $F_m \rightarrow F_{i+1}$. We could prove it by mathematical induction. We have proven that $F_{i-1} \rightarrow F_{i+1}$ before. We suppose that for all the variables among $F_{i-t}, F_{i-t+1}, \cdots, F_{i-1}, i-t \geq k+1$, there is a directed edge from the variable to $F_{i+1}$. For the variable $F_{i-t-1}$, if it is not adjacent to $F_{i+1}$, then there is a discriminating path $F_{i-t-1}, F_{i-t}, F_{i-t+1}, \cdots, F_{i-2}, F_{i-1}, F_i, F_{i+1}$ for $F_i$, which implies that $F_{i-1}, F_i, F_{i+1}$ is a collider with order, contradicting the condition. Hence there must be an edge between $F_{i-t-1}$ and $F_{i+1}$. Since $F_{i-t-1} \leftrightarrow F_{i-t} \rightarrow F_{i-t+1}$, the edge is as $F_{i-t-1} {*\!\!\rightarrow} F_{i+1}$. In addition, the edge cannot be bi-directed, otherwise contradicting the minimal collider path condition. Hence it can only be as $F_{i-t-1} \rightarrow F_{i+1}$. The mathematical induction completes.

Hence, for all the variables among $F_k, F_{k+1}, \cdots, F_{i-1}$, there is a directed edge from the variable to $F_{i+1}$. Since $F_{k-1} \leftrightarrow F_k \leftrightarrow F_{k+1}$ is a collider without order, there must be an edge between $F_{k-1}$ and $F_{k+1}$. Evidently the edge cannot be bi-directed due to the minimal collider path condition. We consider the situation that the edge is $F_{k-1} \leftarrow F_{k+1}$. In this case, we could prove that there is an edge $F_{k-1} \leftarrow F_{k+2}$. If they are not adjacent, then there is a discriminating path $F_{k-1}, F_k, F_{k+1}, F_{k+2}$ for $F_{k+1}$ and the collider $F_k \leftrightarrow F_{k+1} \leftrightarrow F_{k+2}$ is with a constant order, thus $F_{k-1} \leftrightarrow F_k \leftrightarrow F_{k+1}$ is with a constant order, which contradicts the condition that the collider at $F_k$ is without order. Due to the ancestral property, the edge is as $F_{k-1} \leftarrow\!\!* F_{k+1}$. Due to the minimal collider path condition, the edge could only be $F_{k-1} \leftarrow F_{k+1}$. Similar to the process above, we could prove that for all variables between $F_{k+1}$ and $F_i$, there is a directed edge from the variable to $F_{k-1}$. In this case, there is a collider path $F_{k-1} \leftrightarrow F_k \leftrightarrow \cdots F_{i+1}$ with edges $F_j \rightarrow F_{i+1}, \forall k \leq j \leq i-1$, and $F_i \rightarrow F_{k-1}$. It is an inducing path thus there is a bi-directed edge $F_{k-1} \leftrightarrow F_{i+1}$, otherwise the maximal property is violated. However, the bi-directed edge $F_{k-1} \leftrightarrow F_{i+1}$ makes the path not minimal, which contradicts the minimal collider path condition.

Thus, the only possible condition is that there is an edge between $F_{k-1}$ and $F_{k+1}$ and the edge is as $F_{k-1} \rightarrow F_{k+1}$, and the collider $F_{k-1} \leftrightarrow F_k \leftrightarrow F_{k+1}$ is without order. Now we consider the collider without order $F_{k-1} \leftrightarrow F_k \leftrightarrow F_{k+1}$ instead of $F_{i-1} \leftrightarrow F_i \leftrightarrow F_{i+1}$. In another word, by such exchange we consider a collider without order that is nearer to $X$ in the collider path. By such exchange we could find the collider at $F_m$ without order which is nearest to $X$ and there is an edge $F_{m-1} \rightarrow F_{m+1}$. Note during the iteration from $F_{i-2}$ to $F_1$ before, if there is not a collider without order, then $m = i$.

If $F_m$ is $F_1$, i.e., $X {*\!\!\rightarrow} F_1 \leftrightarrow F_2$ is such a collider without order and there is an edge $X \rightarrow F_2$, then it contradicts the minimal collider path condition since there is a collider path $X \rightarrow F_2 \leftrightarrow F_3 \leftrightarrow \cdots \leftrightarrow F_{n-1} \leftarrow\!\!* F_n$. If $F_m$ is not $F_1$, all the colliders between $X$ to $F_m$ are with orders. Similar to the proof above, there is edge $F_j \rightarrow F_{m+1}, \forall 0 \leq j \leq m$, where $F_0$ is $X$. In this condition there is a collider path $X \rightarrow F_{m+1} \leftrightarrow F_{m+2} \leftrightarrow \cdots \leftrightarrow V$, which also contradicts the minimal collider path condition. Hence we conclude that there cannot be a collider without order in the minimal collider path between $X$ and $V$. By Thm. 3.7 of Ali et al. [14], all MAGs in a Markov equivalent class have the same colliders with order. Since FCI is complete [13], all the colliders with order are identified in the graph learned by FCI, thus are identified in $M$. Hence, there is a collider path between $X$ and $V$ in $M$. □

**Lemma 19.** *Let $M$ be a local MAG of $X$. Suppose an MAG $\mathcal{M}$ is consistent to $M$. For any variable $A$ in $\mathcal{M}$, $A$ is a descendant of $X$ if and only if there is at least one minimal possible directed path from $X$ to $A$ in $M$.*

*Proof.* $\Leftarrow$ Consider there is a minimal possible directed path from $X$ to $A$ in $M$. Since the marks at $X$ are certain in $M$, the corresponding path can only start with $X \rightarrow$. To avoid the generation of unshielded colliders, the path could only be directed from $X$ to $A$. Hence in any an MAG $\mathcal{M}$ consistent to $M$, $A$ is the descendant of $X$. Hence in $\mathcal{M}$, $A$ is the descendant of $X$.

$\Rightarrow$ Since $\mathcal{M}$ is an MAG consistent to $M$, there must be a possible directed path from $X$ to $A$ in $M$. Then by Lemma B.1 of Zhang [13], there is a minimal possible directed path from $X$ to $A$ in $M$. $\square$

**Theorem 2.** Let $M$ be a local MAG of $X$ and $\mathcal{M}$ be an MAG consistent to $M$. Suppose $V$ ($V \neq X, Y$) is a variable in $\mathcal{M}$. If D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}}) \cap \text{De}(X, \mathcal{M}) = \emptyset$, then $V \in$ D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}})$ holds if and only if there is at least one collider path from $X$ to $V$ starting by an arrowhead at $X$ in $M$ such that each variable except for $X$ on the path is an ancestor of $X$ or $Y$ in $\mathcal{M}$.

*Proof.* The proof is easy by Lemma 18. Combining the definition of D-SEP$(X, Y, \mathcal{M})$ and $\mathcal{M}_{\underset{\sim}{X}}$, we could trivially conclude that $V \in$ D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}})$ holds if and only if there is at least one collider path from $V$ to $X$ in $M$ such that in $\mathcal{M}$ each variable except for $X$ on the path is an ancestor of $X$ or $Y$, and the path *does not* contain $X \xrightarrow{p}$. Hence the "if" statement is evident. For the "only if" statement, considering the condition D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}}) \cap \text{De}(X, \mathcal{M}) = \emptyset$, if there is a collider path from $X$ to $V$ starting by an impure edge in $M$ such that in $\mathcal{M}$ each variable except for $X$ on the path is an ancestor of $X$ or $Y$, we could conclude the variable adjacent to $X$ on the path belongs to D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}})$. According to the path we also know such a variable is the descendant of $X$, which contradicts the condition D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}}) \cap \text{De}(X, \mathcal{M}) = \emptyset$. Hence the path cannot start by an impure edge from $X$. Combining with the fact that all the marks at $X$ are not circle in the local MAG $M$, the mark at $X$ can only be arrowhead. We get the desired conclusion. $\square$

### C.2 Proofs for Theorem 3

**Definition 4** (PD-SEP$(X, Y, M)$)**.** Let $M$ be a local MAG of $X$ and $\mathcal{M}$ be an MAG consistent to $M$. Variable $V \in$ PD-SEP$(X, Y, M)$ if and only if $V \in \text{PossAn}(Y, M) \backslash \text{De}(X, \mathcal{M})$[5] and there exists a collider path between $X$ and $V$ in $M$, where each non-endpoint variable is an ancestor of $X$ or $Y$ in $M$ but not a descendant of $X$ in $\mathcal{M}$.

Note that PD-SEP$(X, Y, M)$ is not necessarily a set that contains $\mathbf{D}$.

**Definition 5** (Critical variable for $(X, Y)$)**.** In a local MAG $M$ with a path $X \leftrightarrow F_1 \leftrightarrow \cdots \leftrightarrow F_{t-1} \leftrightarrow F_t$ or $X \leftrightarrow F_1 \leftrightarrow \cdots \leftrightarrow F_{t-1} \leftarrow\!\circ F_t$, $t \geq 1$, where $F_1, \cdots, F_{t-1} \in$ PD-SEP$(X, Y, M)$, $F_t$ is called a *critical variable* for $(X, Y)$ if there is a non-empty variable set $\mathbf{S}$ relative to $F_t$ defined as follows: $S \in \mathbf{S}$ if and only if in $M$ (1) $S$ is a child of $X, F_1, \cdots, F_{t-1}$, (2) there is $F_t \circ\!\!\rightarrow\!\!* \, S$, (3) $S$ is at one minimal possible directed path from $F_t$ to $Y$, and no variable on the path belongs to PD-SEP$(X, Y, M)$. Each circle at $F_t$ on the edge with $F_{t-1}$ or $S \in \mathbf{S}$ is called a *critical mark* of $F_t$.

**Theorem 3.** Let $M$ be a local MAG of $X$ based on a PMAG $\mathcal{P}$. Then condition $(1)$ below is sufficient for condition $(2)$:

(1) there is no critical variable for $(X, Y)$ in $M$.

(2) for any an MAG $\mathcal{M}$ consistent to $M$ such that $(a)$ D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}}) \cap \text{De}(X, \mathcal{M}) = \emptyset$, $(b)$ $X \in \text{An}(Y, \mathcal{M})$, it holds that $\mathbf{A}_{\mathcal{M}} = \mathbf{A}'_{\mathcal{M}}$, where $\mathbf{A}_{\mathcal{M}}$ denotes the MCS regarding D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}})$ in $\mathcal{M}$ and $\mathbf{A}'_{\mathcal{M}}$ denotes the MCS regarding PD-SEP$(X, Y, M)$ in $\mathcal{M}$;

*Proof.* Let $\mathcal{M}$ be any an MAG consistent to $M$ such that $(a)$ D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}}) \cap \text{De}(X, \mathcal{M}) = \emptyset$, $(b)$ $X \in \text{An}(Y, \mathcal{M})$. Denote D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}})$ by $\mathbf{D}$ and PD-SEP$(X, Y, M) \backslash \mathbf{D}$ by $\mathbf{K}$. We first prove that if there does not exist a critical variable for $(X, Y)$ in $M$, then $\mathbf{K} \perp Y | \mathbf{D}, X$ in $\mathcal{M}$. Note that here we aim to prove this result holds for *each* MAG satisfying the conditions $(a)$ and $(b)$ above. Our main proof strategy here is to attempt to construct an MAG $\mathcal{M}$ in which $\mathbf{K} \not\perp Y | \mathbf{D}, X$. By considering all possible MAG $\mathcal{M}$, we conclude the desired result. Then, we prove that if $\mathbf{K} \perp Y | \mathbf{D}, X$, then $\mathbf{D} \subseteq$ PD-SEP$(X, Y, M)$. Combining the two results, we finally conclude that if there does not exist a critical variable for $(X, Y)$ in $M$, then all the MAGs consistent to $M$ induce the same MCS. For brevity, below we omit the conditions $(a)$ and $(b)$, but in fact, when we say an MAG $\mathcal{M}$ consistent to $M$, we restrict that $\mathcal{M}$ satisfies the conditions $(a)$ and $(b)$.

As shown in the outline, we prove in the first section that if there does not exist a critical variable for $(X, Y)$ in $M$, then given any an MAG $\mathcal{M}$ consistent to $M$, for any a variable $F_t \in$ PD-SEP$(X, Y, M) \backslash \mathbf{D}$, it holds that $F_t \perp Y | \mathbf{D}, X$.

[5]Note all the descendants of $X$ in $\mathcal{M}$ consistent to $M$ are knowable in $M$, which is detailed by Lemma 19 in Appendix C.1. Hence PD-SEP$(X, Y, M)$ can be obtained based on $M$ without the further knowledge about $\mathcal{M}$.

According to the definition of $\mathbf{D}$ and PD-SEP$(X, Y, M)$, we list the condition as follows: (1) there is a collider path $X \leftrightarrow F_1 \leftrightarrow \cdots \leftrightarrow F_{t-1} \leftrightarrow$ ( or $\leftarrow\!\circ$)$F_t$ in $M$, where $X, F_1, \cdots, F_{t-1}$ are ancestors of $Y$ in $M$, while $F_t$ is a possible ancestor but not ancestor of $Y$ in $M$, is not an ancestor of $Y$ in $\mathcal{M}$. It trivially concludes that the edge between $F_{t-1}$ and $F_t$ is bi-directed. And by Prop. 1, we see that $\mathbf{D}$ m-separates all generalized back-door paths from $X$ to $Y$ relative to $W$, where $W$ is the true purity matrix. Since $F_t$ is a possible ancestor of $Y$ in $M$, there must be a minimal possible directed path from $F_t$ to $Y$ in $M$. Without loss of generality, we suppose the minimal possible directed path $F_t \circ\!\!-\!\!* S \cdots Y$ ($S$ could be $Y$).

**A. If there does not exist a critical variable for $(X, Y)$ in $M$, then $\mathbf{K} \perp Y | \mathbf{D}, X$ in each $\mathcal{M}$ consistent to $M$.**

Suppose a variable $F_t \in \mathbf{K}$ such that $F_t \not\perp Y | \mathbf{D}, X$ in $\mathcal{M}$. Given the variable $F_t$ and local MAG $M$, we say an MAG $\mathcal{M}$ is legal if $\mathcal{M}$ is consistent to $M$ and $F_t \in \mathbf{K}$ in $\mathcal{M}$.

At first, we give two supporting results in A.1 and A.2.

**A.1. If there is an active path relative to $(\mathbf{D}, X)$ from $F_t$ to $U$ without colliders in $\mathcal{M}$, where $U$ is an ancestor of $Y$ in $\mathcal{M}$, then there is a minimal active path without colliders relative to $(\mathbf{D}, X)$ from $F_t$ to $U$ in $\mathcal{M}$.**

Evidently that there exists a minimal path from $F_t$ to $U$ in $\mathcal{M}$. The main part is to prove that path is active. For the sake of contradiction, we suppose for an active path $\mathcal{L}$ from $F_t$ to $U$ relative to $(\mathbf{D}, X)$ in $\mathcal{M}$, the path is not minimal and there is a minimal path $\mathcal{L}_1$ of $\mathcal{L}$ that is m-separated by $(\mathbf{D}, X)$ in $\mathcal{M}$. Since there do not exist colliders in the path $\mathcal{L}$, it is evident that the path cannot go through the variables in $(\mathbf{D}, X)$, otherwise the path will be m-separated by such variables. Considering $\mathcal{L}_1$ is a minimal path of $\mathcal{L}$, both $\mathcal{L}$ and $\mathcal{L}_1$ do not go through $(\mathbf{D}, X)$. If $\mathcal{L}_1$ is directed, then evidently $\mathcal{L}$ is directed due to no colliders in it. There are no colliders in $\mathcal{L}$ so that the path $\mathcal{L}$ is m-separated by $(\mathbf{D}, X)$ if the minimal path $\mathcal{L}_1$ is m-separated by $(\mathbf{D}, X)$. Next we mainly consider the situation that $\mathcal{L}_1$ is not directed. If $\mathcal{L}_1$ is m-separated by $(\mathbf{D}, X)$, $\mathcal{L}$ and $\mathcal{L}_1$ could only be like $F_t *\!\!-\!\!* \cdots *\!\!\rightarrow s_k \rightarrow s_{k+1} *\!\!-\!\!* \cdots *\!\!-\!\!* s_l *\!\!-\!\!* \cdots *\!\!-\!\!* U$ and $F_t *\!\!-\!\!* \cdots *\!\!\rightarrow s_k \leftarrow\!\!* s_l *\!\!-\!\!* \cdots *\!\!-\!\!* U$ (here $F_t$ and $U$ can be swapped), where $l \geq k+2$ and $s_k$ is a collider in $\mathcal{L}_1$ but not a collider in $\mathcal{L}$. Since there are no colliders in $\mathcal{L}$, the sub-path from $s_k$ to $s_l$ in $\mathcal{L}_1$ could only be $s_k \rightarrow s_{k+1} \rightarrow \cdots \rightarrow s_l$. In such a case, no matter the edge between $s_k$ and $s_l$ is either $s_k \leftarrow s_l$ or $s_k \leftrightarrow s_l$, it is against the ancestral property of $\mathcal{M}$. Hence if there is an active path from $F_t$ to $U$ relative to $(\mathbf{D}, X)$, there is at least one minimal active path from $F_t$ to $U$ relative to $(\mathbf{D}, X)$.

**A.2. Some properties about the minimal paths from $F_t$ to $U$ without colliders in $\mathcal{M}$ whose corresponding path in $M$ begins with $F_t \circ\!\!-\!\!* S_1$, where $U$ is an ancestor of $Y$ in $\mathcal{M}$.**

For the corresponding paths in $\mathcal{M}$ of the minimal paths from $F_t$ to $U$ without colliders beginning with $F_t \circ\!\!-\!\!* S_1$ in $M$, there are five types $\mathcal{L}_1, \mathcal{L}_2, \mathcal{L}_3, \mathcal{L}_4, \mathcal{L}_5$. For $\mathcal{L}_1$, the path in $\mathcal{M}$ is as $F_t \leftrightarrow S_1 \rightarrow \cdots U$. For $\mathcal{L}_2$, the path in $\mathcal{M}$ is as $F_t \leftarrow S_1 \leftarrow \cdots \leftarrow S_k \rightarrow S_{k+1} \cdots \rightarrow U$, where $k \geq 1$. For $\mathcal{L}_3$, the path in $\mathcal{M}$ is as $F_t \leftarrow S_1 \leftarrow \cdots \leftarrow S_k \leftrightarrow S_{k+1} \cdots \rightarrow U$, where $k \geq 1$. For $\mathcal{L}_4$, the path in $\mathcal{M}$ is as $F_t \rightarrow S_1 \rightarrow \cdots \rightarrow U$. For $\mathcal{L}_5$, the path in $\mathcal{M}$ is as $F_t \leftarrow S_1 \leftarrow \cdots \leftarrow U$. $\mathcal{L}_4$ and $\mathcal{L}_5$ are evidently impossible. If there is a path as $\mathcal{L}_4$, $F_t \in$ Anc$(Y, \mathcal{M})$, thus $F_t \in (\mathbf{D}, X)$, which contradicts the condition $F_t \in \mathbf{K}$. If there is a path as $\mathcal{L}_5$, $F_t$ is a descendant of $Y$, thus a descendant of $X$. According to Lemma 19, we could identify all the variables in De$(X, \mathcal{M})$ in $M$. Hence $F_t$ could be identified to be a descendant of $X$ in $M$, which contradicts the condition $F_t \in$ PD-SEP$(X, Y, M)$. In the following, we first show in A.2.1 that the sets of paths as $\mathcal{L}_2$ and $\mathcal{L}_3$ are also empty if the path does not go through the variables in $(\mathbf{D}, X)$.

**A.2.1 Both the sets of paths as $\mathcal{L}_2$ and $\mathcal{L}_3$ are empty if the path does not go through the variables belonging to $(\mathbf{D}, X)$.**

Consider the paths as $\mathcal{L}_2$ at first. If $S_1$ and $F_{t-1}$ are not adjacent, since there is an unshielded collider $F_{t-1} \leftrightarrow F_t \leftarrow\!\!* S_1$, we could identify the two arrowheads here by FCI algorithm in $M$, which contradicts the circle at $F_t$ in $M$.

Since $S_1 \notin (\mathbf{D}, X)$, there cannot be an edge $S_1 \rightarrow F_{t-1}$. Hence the edge between $S_1$ and $F_{t-1}$ is as $F_{t-1} *\!\!\rightarrow S_1$ in $\mathcal{M}$. And due to the ancestral property, the edge could only be $F_{t-1} \leftrightarrow S_1$ given the fact $F_{t-1} \leftrightarrow F_t$ and $S_1 \rightarrow F_t$. Then we consider the variable $S_2$. If $S_2$ and $F_{t-1}$ are not adjacent, then $S_2, S_1, F_{t-1}$ forms an unshielded collider, so that $S_2 *\!\!\rightarrow S_1 \leftarrow\!\!* F_{t-1}$ could be identified in $M$. Due to the minimal path, $S_1 \rightarrow F_t$ could also be identified. According to the ancestral property, we could identify $S *\!\!\rightarrow F_t$ in $M$ since $S_1 \rightarrow F_t$ and $S *\!\!\rightarrow S_1$, which contradicts the circle at $F_t$ in minimal possible directed path from $F_t$ to $Y$ across $S$ in $M$. Hence $S_2$ and $F_{t-1}$ are adjacent. Considering $S_2 \rightarrow S_1$ and $S_1 \leftrightarrow F_{t-1}$ in $\mathcal{M}$, the edge between $S_2$ and $F_{t-1}$ is as $F_{t-1} \leftarrow\!\!* S_2$. Since the path does not go through $(\mathbf{D}, X)$, $S_2 \notin (\mathbf{D}, X)$. Hence the edge can only be $F_{t-1} \leftrightarrow S_2$.

We could repeat the process above for $S_3, S_4 \cdots$ until for $S_k$. Similar to the proof above, we see that the edge between $S_t$ and $F_{t-1}$ is $S_t \leftrightarrow F_{t-1}$. In this case, there is a collider path $X \leftrightarrow F_1 \cdots F_{t-1} \leftrightarrow S_k$, and we also know $S_k$ is an ancestor of $U$, thus is an ancestor of $Y$. Hence $S_k \in (\mathbf{D}, X)$ in $\mathcal{M}$, which contradicts the condition that the path from $F_t$ to $U$ does not go through the variables in $(\mathbf{D}, X)$. Hence we conclude that the set of paths as $\mathcal{L}_2$ is empty if the path does not go through the variable in $(\mathbf{D}, X)$.

Then we consider the paths as $\mathcal{L}_3$. The proof of this part is quite similar to that for the paths as $\mathcal{L}_2$. To prevent from discovering the arrowheads at $F_t$ on the edge between $F_t$ and $S$, there must be bi-directed edges between $F_{t-1}$ and $S_1, S_2, \cdots, S_k$. If $S_{k+1}$ is not adjacent to $F_{t-1}$, a v-structure forms so that we could identify $S_{k+1} {*\!\!\rightarrow} S_k$. Due to the fact that the path is minimal and without colliders in $M$, we could learn the arrowhead at $F_t$, which contradicts with the circle at $F_t$. If $S_{k+1} {*\!\!\rightarrow} F_{t-1}$, $S_{k+1} \in \mathbf{D}$ since $S_{k+1}$ is an ancestor of $U$, thus is an ancestor of $Y$. This contradicts with the fact that path does not go through the variable in $(\mathbf{D}, X)$ in $\mathcal{M}$. Hence the edge can only be $S_{k+1} \leftarrow F_{t-1}$. However, there is an inducing path comprised of $S_{k+1} \leftrightarrow S_k \leftrightarrow F_{t-1} \leftrightarrow S_{k-1}$, $F_{t-1} \rightarrow S_{k+1}$, and $S_k \rightarrow S_{k-1}$. To satisfy the maximal property, there is a bi-directed edge between $S_{k+1}$ and $S_{k-1}$, which contradicts with the condition that the path $\mathcal{L}_3$ is minimal. Hence we conclude that the set of paths as $\mathcal{L}_3$ is empty if the path does not go through the variable in $(\mathbf{D}, X)$.

**A.2.2 If the edge between $F_{t-1}$ and $S_1$ is as $F_{t-1} {*\!\!\rightarrow} S_1$ in $\mathcal{M}$, $U$ is an ancestor of $Y$ in $\mathcal{M}$ and $S_1$ is the variable adjacent to $F_t$ in one minimal possible directed path from $F_t$ to $U$ in $M$, then there exists at least one variable among $X, F_1, \cdots, F_{t-1}$ that has a bi-directed edge with $S_1$ in $\mathcal{M}$.**

If the edge between $F_{t-1}$ and $S_1$ is bi-directed, we get the desired conclusion directly. If the edge between them are $F_{t-1} \rightarrow S_1$, since $F_{t-1} \leftrightarrow F_t$ and $F_t$ is not an ancestor of $Y$, the edge between $F_t$ and $S_1$ is bi-directed. And we consider the edge between $S_1$ and $F_{t-2}$. Since $F_{t-2} \leftrightarrow F_{t-1}$ and $F_{t-1} \rightarrow S_1$, the edge is as $F_{t-2} {*\!\!\rightarrow} S_1$ in $\mathcal{M}$. If it is bi-directed, the desired conclusion is directly obtained. If it is $F_{t-2} \rightarrow S_1$, we consider the edge between $F_{t-3}$ and $S_1$. We repeat the process above. If there is no variable in $F_1, \cdots, F_{t-1}$ with a bi-directed edge with $S_1$, there must be an edge $X \rightarrow S_1$ in $\mathcal{M}$. However, since the edge $F_t \leftrightarrow S_1$ and $S_1$ is located at one minimal possible directed path from $F_t$ to $U$, the corresponding path in $\mathcal{M}$ of this minimal possible directed path can only be $F_t \leftrightarrow S_1 \rightarrow \cdots \rightarrow U$ in order to avoid the generation of v-structure. Since $X \rightarrow S_1$, all the variables from $S_1$ to $Y$ are descendants of $X$. Since the mark at $X$ is known in $M$, we could identify the tail at $X$ on the edge between $X$ and $S_1$ in $M$. In this case, there exists at least one critical variable among $F_1, F_2, \cdots, F_t$, which contradicts the condition that there does not exist a critical variable in $M$. Thus, it is impossible that $V \rightarrow S_1$ for $\forall V \in \{X, F_1, \cdots, F_{t-1}\}$ in $\mathcal{M}$. Hence there must be a bi-directed edge with $S_1$ among the variables in $X, F_1, \cdots, F_{t-1}$.

With the results in A.1 and A.2, we prove the main results in the following. In the beginning, we prove the desired results by showing that it is impossible to construct a legal MAG with an active path from $F_t$ to $Y$. We divide all possible paths from $F_t$ to $Y$ in $\mathcal{M}$ into two classes. The first class is comprised of all the paths without colliders in $\mathcal{M}$. And we prove in A.3 that all such paths cannot be active relative to $(\mathbf{D}, X)$ in $\mathcal{M}$. The second class is comprised of all the paths with colliders in $\mathcal{M}$. We prove in A.4 that all such paths cannot be active relative to $(\mathbf{D}, X)$ in $\mathcal{M}$.

**A.3. There do not exist active paths relative to $(\mathbf{D}, X)$ from $F_t$ to $Y$ without colliders in any legal MAG $\mathcal{M}$.**

Suppose an active path from $F_t$ to $Y$ without colliders in a legal MAG $\mathcal{M}$. By A.1, there is an active minimal path without colliders from $F_t$ to $Y$ in $\mathcal{M}$. Since there are no colliders in this path, the active path cannot go through the variables in $(\mathbf{D}, X)$, otherwise the path is m-separated by $(\mathbf{D}, X)$. By A.2.1, we see that the active minimal paths without colliders cannot be as $\mathcal{L}_2$ or $\mathcal{L}_3$. The only possible paths are like $\mathcal{L}_1$. However, in this case by A.2.2 there exists at least one variable $F_s \in \{X, F_1, \cdots, F_{t-1}\}$ with $F_s \leftrightarrow S_1$. And because $S_1$ is an ancestor of $U$ in $\mathcal{L}_1$, thus is an ancestor of $Y$, thus $S_1 \in (\mathbf{D}, X)$, in which case the path without colliders $F_t, S_1, \cdots, Y$ is m-separated by $(\mathbf{D}, X)$, which contradicts the active path. Thus there is not a path as $\mathcal{L}_1$. Hence we get the desired conclusion that there do not exist active paths from $F_t$ to $Y$ without colliders in any a legal MAG $\mathcal{M}$.

**A.4. There do not exist active paths relative to $(\mathbf{D}, X)$ from $F_t$ to $Y$ with colliders in any legal MAG $\mathcal{M}$.**

This part is a bit complex. Before proposing the proof, we define the *distance between $F_t$ and $(\mathbf{D}, X)$*. For any variable $F_t \in \mathbf{K}$, there must be some minimal possible directed paths from $F_t$ to $Y$ in $M$ according to the definition of $\mathbf{K}$. We say that the distance between $F_t$ and $(\mathbf{D}, X)$ is $k$ if:

(1) There is one minimal possible directed path from $F_t$ to $Y$, where the nearest variable to $F_t$ that belongs to $(\mathbf{D}, X)$ is with distance $k$ to $F_t$. In another word, the minimal possible directed path is such as $F_t, C_1, C_2, \cdots, C_k, \cdots, Y$, where $C_1, \cdots, C_{k-1} \notin (\mathbf{D}, X)$ and $C_k \in (\mathbf{D}, X)$.

(2) There do not exist minimal possible direct paths from $F_t$ to $Y$, where the nearest variable to $F_t$ that belongs to $(\mathbf{D}, X)$ is with distance less than $k$ to $F_t$.

We prove the desired conclusion by mathematical induction. In A.4.a, we prove that for any $F_t \in \mathbf{K}$ that has distance 1 to $(\mathbf{D}, X)$, all the paths from $F_t$ to $Y$ with colliders are m-separated by $(\mathbf{D}, X)$ in any one legal $\mathcal{M}$. Combining this result with A.3, we conclude $F_t \perp Y | \mathbf{D}, X$ for $F_t \in \mathbf{K}$ that has distance 1 to $(\mathbf{D}, X)$

in $\mathcal{M}$. Then in A.4.b, we prove that if for any $F_t \in \mathbf{K}$ that has distance $k-1$ to $(\mathbf{D}, X)$ in $\mathcal{M}$ it holds that $F_t \perp Y|\mathbf{D}, X$, then for any $F_t \in \mathbf{K}$ that has distance $k$ to $(\mathbf{D}, X)$ in $\mathcal{M}$, all the paths from $F_t$ to $Y$ with colliders are m-separated by $(\mathbf{D}, X)$. Also combining this result with A.3, we conclude $F_t \perp Y|\mathbf{D}, X$ for $F_t \in \mathbf{K}$ that has distance $k$ to $(\mathbf{D}, X)$ in $\mathcal{M}$. We thus prove the desired result that for any variable $F_t \in \mathbf{K}$, it holds that $F_t \perp Y|\mathbf{D}, X$.

**A.4.a. For any $F_t \in \mathbf{K}$ that has distance 1 to $(\mathbf{D}, X)$, all the paths from $F_t$ to $Y$ with colliders are m-separated by $(\mathbf{D}, X)$ in any one legal $\mathcal{M}$.**

Since the distance between $F_t$ and $(\mathbf{D}, X)$ is 1, there is at least one minimal possible directed path $F_t, S, \cdots, Y$, where $S \in (\mathbf{D}, X)$ in $\mathcal{M}$. For the sake of contradiction, we suppose there is an active path relative to $(\mathbf{D}, X)$ from $F_t$ to $Y$ with colliders in $\mathcal{M}$. We denote the collider closest to $F_t$ in this path by $C$. Since the path is active relative to $(\mathbf{D}, X)$, the sub-path from $F_t$ to $C$ that contains no colliders is also active relative to $(\mathbf{D}, X)$. And it is evident that this sub-path cannot go through the variables in $(\mathbf{D}, X)$, otherwise the path is m-separated by $(\mathbf{D}, X)$.

Since $F_t$ is not a variable in $(\mathbf{D}, X)$, the edge between $F_t$ and $F_{t-1}$ is bi-directed, and the mark at $F_t$ on the edge between $F_t$ and $S$ is arrowhead, otherwise there is a directed path from $F_t$ to $Y$ across $S$ in $\mathcal{M}$, which concludes that $F_t \in (\mathbf{D}, X)$. Since there is a circle at $F_t$ on the edge between $F_t$ and $S$ in $M$, $F_{t-1}$ and $S$ are adjacent in $\mathcal{M}$.

By the result of A.1, since $C \in \mathrm{Anc}(Y, \mathcal{M})$, there exist some active minimal paths without colliders from $F_t$ to $C$ relative to $(\mathbf{D}, X)$ in $\mathcal{M}$. Note in the following we may omit "relative to $(\mathbf{D}, X)$". That is, if we do not speak intentionally, "active path" refers to "active path relative to $(\mathbf{D}, X)$" . We will consider such active minimal paths and construct the contradiction. We denote such an active minimal path by $\mathcal{L}$. It is easy to see that the mark at $F_t$ is arrowhead, otherwise $F_t$ is an ancestor of $C$ thus an ancestor of $Y$, which contradicts the condition that $F_t \notin \mathbf{D}$. We separate all possible situations for $\mathcal{L}$ into three classes. In the first class, $C$ and $F_t$ are adjacent, i.e. the path is $F_t \leftrightarrow C$. We denote it by $\mathcal{L}_1$. Note $F_t \to C$ is impossible otherwise $F_t \in \mathbf{D}$, which contradicts the condition $F_t \in \mathbf{K}$. In the second class, we suppose the minimal active path is as $F_t \leftarrow S_1 \leftarrow \cdots \leftarrow S_k \to S_{k+1} \to \cdots \to C$, $k \geq 1$. We denote it by $\mathcal{L}_2$. In the third class, we suppose the minimal active path is as $F_t \leftarrow S_1 \leftarrow \cdots \leftarrow S_k \leftrightarrow S_{k+1} \to \cdots \to C$, $k \geq 1$. We denote it by $\mathcal{L}_3$.

**A.4.a.1 There does not exist an active path as $\mathcal{L}_1$ in $\mathcal{M}$.**

If there is such an active path as $\mathcal{L}_1$, there exists an active path from $F_t$ to $Y$ where there is a sub minimal collider path beginning with $F_t$, that is the path is as $F_t \leftrightarrow C_1 \leftrightarrow C_2 \leftrightarrow \cdots \leftrightarrow C_{t-1} \leftarrow\!\!* C_t \cdots Y$, where $C_t$ is the first variable that is not collider in the path and there are no bi-directed edges between $C_i$ and $C_j$ for $|j-i| \geq 2, 1 \leq i, j \leq t$.

Evidently $F_{t-1}$ and $S$ are adjacent and $C_1$ and $S$ are also adjacent, otherwise the arrowhead on $F_t \leftarrow\!\!* S$ could be identified due to the unshielded collider.

**A.4.a.1.1 If an active path as $\mathcal{L}_1$ exists, then $C_1$ and $F_{t-1}$ are adjacent in $\mathcal{M}$.**

At first, we consider the situation that $C_1$ and $F_{t-1}$ are not adjacent. We will construct a contradiction by proving $C_t *\!\!\to C_{t-1} \leftrightarrow \cdots \leftrightarrow C_1 \leftrightarrow F_t \leftrightarrow S$ is a minimal collider path.

Since there is an unshielded collider $F_{t-1} \leftrightarrow F_t \leftarrow\!\!* C_1$, we could identify the two arrowheads here by FCI algorithm in $M$. And we could see that there must be a sub-structure $F_{t-1} *\!\!\to S \leftarrow\!\!* C_1$ in $\mathcal{M}$, otherwise the mark at $F_t$ on the edge between $F_t$ and $S$ could be identified to be arrowhead by Rule 3 of Zhang [13]. Next, We consider the edge between $S$ and $F_{t-1}$. By A.2.2, there exists an bi-directed edge between $S$ and some variable among $X, F_1 \cdots, F_{t-1}$ in $\mathcal{M}$. Without loss of generality, we suppose the variable with a bi-directed edge with $S$ that is closest to $F_t$ by $F_s$. In this case, there is a collider path $X \leftrightarrow F_1 \cdots F_s \leftrightarrow S \leftarrow\!\!* C_1$. Here the edge between $S$ and $C_1$ could only be $S \leftarrow C_1$, otherwise if $F_t \leftrightarrow C_1 \cdots Y$ is active relative to $\mathbf{D}$ in $\mathcal{M}$, the path $X \leftrightarrow F_1 \leftrightarrow \cdots \leftrightarrow F_s \leftrightarrow S \leftrightarrow C_1 \cdots Y$ is also active relative to $\mathbf{D}$ in $\mathcal{M}$, which contradicts the condition that $\mathbf{D}$ m-separates all generalized back-door paths from $X$ to $Y$.

Similarly, it is easy to prove that for all variables $C_i, 1 \leq i \leq t-1$ there is not an edge $C_i \leftrightarrow S$, otherwise the path $X \leftrightarrow F_1 \leftrightarrow \cdots \leftrightarrow F_s \leftrightarrow S \leftrightarrow C_i \cdots Y$ is active relative to $\mathbf{D}$ in $\mathcal{M}$, which contradicts the condition that $\mathbf{D}$ m-separates all generalized back-door paths. Hence we conclude that the path $C_t *\!\!\to C_{t-1} \leftrightarrow \cdots \leftrightarrow C_1 \leftrightarrow F_t \leftrightarrow S$ is a minimal collider path. By Lemma 18 (see the detailed proof process), we could identify all the colliders in the minimal collider path by FCI algorithm, that is we could identify the arrowhead at $F_t$ in $M$, which contradicts the possible directed path condition.

**A.4.a.1.2. If an active path as $\mathcal{L}_1$ exists, then $C_1$ and $F_{t-1}$ cannot be adjacent in $\mathcal{M}$.**

Then we consider the condition that $C_1$ and $F_{t-1}$ are adjacent. Evidently the edge cannot be bi-directed, otherwise given the active path $F_t \leftrightarrow C_1 \leftrightarrow \cdots \leftrightarrow C_t \cdots Y$ relative to $\mathbf{D}$, the path $X \leftrightarrow F_1 \leftrightarrow \cdots \leftrightarrow F_{t-1} \leftrightarrow C_1 \leftrightarrow \cdots \leftrightarrow C_t \cdots Y$ is active relative to $\mathbf{D}$, which contradicts the condition that $\mathbf{D}$ m-separates all the generalized back-door paths.

We first consider the condition that $F_{t-1} \leftarrow C_1$. We discuss the relation between $C_2$ and $F_{t-1}$. If $C_2$ is adjacent to $F_{t-1}$, then by ancestral property it holds $C_2{*\!\!\rightarrow} F_{t-1}$ in $\mathcal{M}$. And similar to the proof for that there is not bi-directed edge between $F_{t-1}$ and $C_1$, if there is $C_2 \leftrightarrow F_{t-1}$, there is an active path $X \leftrightarrow F_1 \leftrightarrow \cdots \leftrightarrow F_{t-1} \leftrightarrow C_2 \leftrightarrow \cdots \leftrightarrow C_t \cdots Y$ relative to $\mathcal{D}$ in $\mathcal{M}$, contradicting the condition that $\mathbf{D}$ m-separates all the generalized back-door paths. Hence the edge could only be $C_2 \rightarrow F_{t-1}$ in $\mathcal{M}$. In addition, for the variable $C_t$, it is impossible that there is an edge $C_t \rightarrow F_{t-1}$, otherwise $C_t \in \mathbf{D}$, which contradicts the condition that $\mathcal{L}_1$ is active relative to $\mathbf{D}$ and $C_t$ is not a collider in the path. Thus if all the variables among $C_2, C_3, \cdots, C_{t-1}$ are adjacent to $F_{t-1}$, then $C_t$ is not adjacent to $F_{t-1}$.

Hence, suppose the first variable $C_s$ from $F_t$ to $C_t$ that is no adjacent to $F_{t-1}$. Then we consider the minimal collider path $C_s{*\!\!\rightarrow} C_{s-1} \leftrightarrow \cdots \leftrightarrow C_1 \leftrightarrow F_t$ from $C_s$ to $F_t$. Since $F_{t-1} \leftrightarrow F_t$ and $C_i \rightarrow F_{t-1}, 1 \leq i \leq s-1$, the path $C_s{*\!\!\rightarrow} C_{s-1} \leftrightarrow \cdots \leftrightarrow C_1 \leftrightarrow F_t \leftrightarrow F_{t-1}$ is a minimal collider path from $C_s$ to $F_{t-1}$. By Lemma 18 (see the detailed proof process), all the colliders could be identified in $M$. And all directed edges $C_i \rightarrow F_{t-1}, 1 \leq i \leq s-1$ could be identified by Rule 4 of Zhang [13].

In the following we consider the edge between $S$ and $C_i, 1 \leq i \leq s$. Here we only construct the contradiction when all the variables between $F_t$ and $C_s$ are adjacent to $S$. It is easy to construct a contradiction if there are some variables not adjacent to $S$, we thus leave them to readers. We discuss the edge between $F_{t-1}$ and $S$.

If the edge is as $F_{t-1}{*\!\!\rightarrow} S$, we see the edge between $S$ and $C_1$ is as $S \leftarrow\!\!* C_1$ in $\mathcal{M}$. Then similar to the last part A.4.a.1.1 we could construct a contradiction. Hence we only consider $S \rightarrow F_{t-1}$ in $\mathcal{M}$ in the following.

We first prove that there is some variable $C_j, 2 \leq j \leq s-1$ such that $C_i \rightarrow F_t, 1 \leq i \leq j-1$ and $C_j$ is not adjacent to $F_t$. If $F_t$ and $C_2$ are not adjacent, then $C_2$ is such a variable. If they are adjacent, since the minimal collider path between $C_s$ and $F_t$ and $C_3 \rightarrow F_{t-1} \leftrightarrow F_t$, the edge between $F_t$ and $C_3$ could only be $F_t \leftarrow C_3$. Repeat the process for $C_4, C_5, \cdots, C_s$. If there is $C_i \rightarrow F_t, 2 \leq i \leq s-1$ and there is also an edge $C_s \rightarrow F_t$, it contradicts the minimal collider path condition. Hence we get the desired conclusion.

We consider the sub-structure comprised of $S, F_t, C_{j-1}, C_j$. The edge $C_{j-1} \rightarrow F_t$ is identifiable in $M$, similar to the proof process for that $C_{j-1} \rightarrow F_{t-1}$ is identifiable so that we skip this part. Hence we discuss whether $F_t, S, C_j$ form an unshielded collider. If $F_t, S, C_j$ is not an unshielded collider, we consider the sub-structure comprised of $F_t, S, C_j, C_{j-1}$. We have proved before that the edge $C_j{*\!\!\rightarrow} C_{j-1}$ and $C_{j-1} \rightarrow F_t$ could be identified in $M$. We prove $S{*\!\!\rightarrow} F_t$ could be identified in $M$ in the following. The reason is, if there is an edge $S \leftarrow F_t$, there is an edge $C_{j-1} \rightarrow S$ in $\mathcal{M}$ due to the ancestral property and thus there is an edge $C_j{*\!\!\rightarrow} S$ in $\mathcal{M}$, which contradicts the condition that $F_t, S, C_j$ is not an unshielded collider. Hence we see that there cannot be an edge as $F_t{*\!\!\rightarrow} S$ in $\mathcal{M}$. Due to the completeness of FCI [13], the mark at $F_t$ on the edge between $F_t$ and $S$ is identifiable in the PAG. Thus the arrowhead at $F_t$ is known in $M$, which contradicts the possible directed path from $F_t$ to $Y$ across $S$. If they form an unshielded collider, we identify $S \leftarrow\!\!* F_t$ in $M$. If $C_s$ is not adjacent to $F_t$, we further discuss the edge between $S$ and $C_s$. If $C_s, S, F_t$ does not form an unshielded collider, $S \rightarrow C_s$ is identified in $M$ by Rule 1 of Zhang [13], thus $S{*\!\!\rightarrow} C_{s-1}$ is identified by Rule 2 of Zhang [13], and $S \rightarrow F_{t-1}$ is identified by Rule 4 of Zhang [13], and $S{*\!\!\rightarrow} F_t$ is identified by Rule 2 of Zhang [13], which contradicts the possible directed path from $F_t$ to $Y$ across $S$. If they form an unshielded collider, we could identify $C_s \rightarrow S$, thus identify $S \rightarrow F_{t-1}$ and $S{*\!\!\rightarrow} F_t$ in $M$, which also contradicts the possible directed path from $F_t$ to $Y$ across $S$. If $C_s$ is adjacent to $F_t$, the edge cannot be as $F_t \rightarrow C_s$, in which case $F_t \in \mathbf{D}$ since $C_s$ is an ancestor of $Y$. It is also not bi-directed, which contradicts the minimal collider path condition. Thus it is as $F_t \leftarrow C_s$. Consider the sub-structure comprised of $C_s, F_t, F_{t-1}, S$. Since $S \rightarrow F_{t-1}$ in $\mathcal{M}$, the edge between $S$ and $F_t$ could only be as $S{*\!\!\rightarrow} F_t$ in $\mathcal{M}$, and $C_s, S, F_{t-1}$ does not form an unshielded collider. Hence $S{*\!\!\rightarrow} F_t$ could be identified in $M$ by Rule 3 of Zhang [13], which contradicts the possible directed path from $F_t$ to $Y$ across $S$. Hence we construct contradictions when there is an edge $C_1 \rightarrow F_{t-1}$.

If the edge between $F_{t-1}$ and $C_1$ is as $F_{t-1} \rightarrow C_1$, we note that $C_1$ and $F_{t-1}$ are symmetrical on $F_t$ as well as $X$ and $C_s$ are symmetrical on $F_t$. Hence similar to the process above we could conclude $S \rightarrow C_1$ in $\mathcal{M}$. And it evidently hold that there cannot be a bi-directed edge $F_s \leftrightarrow C_1, 0 \leq s \leq t-1$, otherwise there is an active path $X \leftrightarrow F_1 \leftrightarrow \cdots \leftrightarrow F_2 \leftrightarrow C_1, \cdots, Y$ relative to $(\mathbf{D}, X)$, which contradicts the fact that $(\mathbf{D}, X)$ m-separates all the generalized back-door paths. By the ancestral property, if $F_{t-2}$ is adjacent to $C_1$, then the edge is as $F_{t-2}{*\!\!\rightarrow} C_1$, thus the edge is $F_{t-2} \rightarrow C_1$ since it cannot be bi-directed. Similarly, we could prove that there must be a variable between $X$ and $F_t$ that is not adjacent to $C_1$. If there is $X \rightarrow C_1$, it contradicts $\mathbf{D} \cap \mathrm{De}(X, \mathcal{M}) = \emptyset$. Suppose the first variable $F_k$ from $X$ to $F_t$ that is not adjacent to $C_1$. By considering the minimal collider path $F_k{*\!\!\rightarrow} F_{k+1} \leftrightarrow \cdots \leftrightarrow F_t \leftrightarrow C$ as the proof process above, where $F_k$ is not adjacent to $C_1$, $S \rightarrow C_1$ and $C_1 \leftrightarrow F_t$ is always identified in $M$, thus there is $S{*\!\!\rightarrow} F_t$ in $M$, which contradicts the possible directed path. Combining the conditions that there is an edge $F_{t-1} \rightarrow C_1$ and there is an edge $F_{t-1} \leftarrow C_1$, we conclude that $F_{t-1}$ cannot be adjacent to $C_1$ in $\mathcal{M}$.

**A.4.a.2. There does not exist an active path as $\mathcal{L}_2$ in $\mathcal{M}$.**

**A.4.a.2.1 If an active path as $\mathcal{L}_2$ exists, then $S_1$ and $F_{t-1}$ are adjacent in $\mathcal{M}$.**

At first, we consider the situation that $S_1$ and $F_{t-1}$ are not adjacent. Since there is an unshielded collider $F_{t-1} \leftrightarrow F_t \leftarrow\!\!* S_1$, we could identify the two arrowheads here. And we could see that there must be a sub-structure $F_{t-1} *\!\!\rightarrow S \leftarrow\!\!* S_1$ in $\mathcal{M}$, otherwise the mark at $F_t$ on the edge between $F_t$ and $S$ could be identified to be arrowhead by Rule 3 of Zhang [13]. Next, we consider the edge between $S$ and $F_{t-1}$. Since $S$ is located at one minimal possible directed path from $F_t$ to $Y$ in $M$, and the edge between $F_{t-1}$ and $S$ is as $F_{t-1} *\!\!\rightarrow S$, by A.2 we see that there exists a bi-directed edge between $S$ and some variable among $X, F_1 \cdots, F_{t-1}$ in $\mathcal{M}$. Without loss of generality, we suppose such variable by $F_s$.

Next we consider the edge $S \leftarrow\!\!* S_1$. If the edge is directed, then it holds that there is a collider path $X \leftrightarrow F_1 \cdots F_s \leftrightarrow S \leftarrow S_1$, which concludes that $S_1 \in (\mathbf{D}, X)$, which contradicts the condition that the sub-path from $F_t$ to $C$ does not go through the variables in $(\mathbf{D}, X)$. Hence the edge between $S$ and $S_1$ could only be $S \leftrightarrow S_1$. If $S_2$ and $S$ are not adjacent, then $S, S_1, S_2$ forms an unshielded collider, so that $S *\!\!\rightarrow S_1 \leftarrow\!\!* S_2$ could be identified in $M$. Since the minimal path, $S_1 \rightarrow F_t$ could also be identified. According to the ancestral property, we could identify $S *\!\!\rightarrow F_t$ in $M$, which contradicts the condition that $S$ is located at the minimal possible directed path from $F_t$ to $Y$ in $M$. Hence $S_2$ and $S$ are adjacent. And there is $S_2 *\!\!\rightarrow S$ by ancestral property.

We could repeat the process above for $S_3, S_4 \cdots$ until for $S_k$. Similar to the proof above, we see that the edge between $S_k$ and $S$ is $S \leftarrow\!\!* S_k$. In this case, there is a collider path $X \leftrightarrow F_1 \cdots F_s \leftrightarrow S \leftarrow\!\!* S_k$, and we also know $S_k$ is an ancestor of $Y$ since it is an ancestor of $C$ that is a variable from $(\mathbf{D}, X)$. Hence we conclude that $S_k \in (\mathbf{D}, X)$, which contradicts the condition that the sub-path from $F_t$ to $C$ does not go through the variables in $(\mathbf{D}, X)$.

Hence we see that if a path such as $\mathcal{L}_2$ exists, it is impossible that $S_1$ and $F_{t-1}$ are not adjacent in $\mathcal{M}$.

**A.4.a.2.2 If an active path as $\mathcal{L}_2$ exists, then $S_1$ and $F_{t-1}$ cannot be adjacent in $\mathcal{M}$.**

Here we consider the situation that $S_1$ and $F_{t-1}$ are adjacent. We discuss all possible situations of this edge.

If the edge between them is $S_1 \rightarrow F_{t-1}$, the path $X \leftrightarrow F_1 \leftrightarrow \cdots \leftrightarrow F_{t-1} \leftarrow S_1 \leftarrow S_2 \cdots Y$ is active relative to $(\mathbf{D}, X)$, which contradicts with the condition that $(\mathbf{D}, X)$ could m-separate all the generalized back-door paths relative to $(G, W)$.

If the edge between them is $S_1 \leftarrow F_{t-1}$, the ancestral property is violated since $F_{t-1} \rightarrow S_1 \rightarrow F_t \leftrightarrow F_{t-1}$, which constructs a contradiction.

If the edge between them is $S_1 \leftrightarrow F_{t-1}$ in $\mathcal{M}$, there is a collider path $X \leftrightarrow F_1 \leftrightarrow \cdots \leftrightarrow F_{t-1} \leftrightarrow S_1$. We consider the edge between $S$ and $S_1$. Since $S \in (\mathbf{D}, X)$, the edge between $S$ and $S_1$ cannot be as $S_1 \rightarrow S$, otherwise $S_1$ is an ancestor of $Y$ thus $S_1 \in (\mathbf{D}, X)$. Hence the edge between $S_1$ and $S$ is as $S *\!\!\rightarrow S_1$. If $S_2$ and $S$ are not adjacent, then $S, S_1, S_2$ forms an unshielded collider, so that $S *\!\!\rightarrow S_1 \leftarrow\!\!* S_2$ could be identified in $M$. Since the minimal path, $S_1 \rightarrow F_t$ could also be identified. According to the ancestral property, we could identify $S *\!\!\rightarrow F_t$ in $M$, which contradicts the condition that $S$ is located at the minimal possible directed path from $F_t$ to $Y$ in $M$. Also, if $F_{t-1}$ and $S_2$ are not adjacent, then $S_2 *\!\!\rightarrow S_1 \leftarrow\!\!* F_{t-1}$ could be identified in $M$ since they form an unshielded collider. We could also identify $S_2 *\!\!\rightarrow S_1$ thus identify $S_1 \rightarrow F_t$. We note that in $M$ there is a sub-structure comprised of $F_{t-1}, S, S_1, S_2$ where $F_{t-1} *\!\!\rightarrow S_1 \leftarrow\!\!* S_2$ and $F_{t-1}$ is not adjacent to $S_2$. We discuss the marks at $S$ in this sub-structure. If it is not as $F_{t-1} *\!\!\rightarrow S \leftarrow\!\!* S_2$ in $M$, then by Rule 3 of Zhang [13] there is $S *\!\!\rightarrow S_1$ in $M$. Then by Rule 2 of Zhang [13] there is $S *\!\!\rightarrow F_t$ in $M$, which contradicts the condition. If it is as $F_{t-1} *\!\!\rightarrow S \leftarrow\!\!* S_2$ in $M$, by A.2.2 there must be a variable $F_s, 1 \le s \le t-1$ such that $F_s \leftrightarrow S$. Since $S_2$ is not adjacent to $F_t$ in $M$, $S_2, S, F_t$ is thus unshielded. And because $S \leftarrow\!\!* S_2$ in $M$, the mark at $S$ on the edge between $F_t$ and $S$ can be identified. To guarantee that $S$ is located at one minimal directed path from $F_t$ to $Y$, the mark at $S$ could only be arrowhead in $M$. We consider such $\mathcal{M}$ consistent to $M$. The edge between $S$ and $S_1$ could only be $S \leftrightarrow S_1$. The reason is, if it is $S \leftarrow\!\!* S_1$, there is a path $X \leftrightarrow F_1 \leftrightarrow \cdots \leftrightarrow F_s \leftrightarrow S \leftarrow S_1 \leftarrow S_2 \cdots Y$ active relative to $\mathbf{D}$, which contradicts the fact that $\mathbf{D}$ m-separates all the generalized back-door path. Since $S_2$ is adjacent to $S$, similarly we could prove that $S_2 \leftrightarrow S$. Repeat the similar process for $S_3, S_4, \cdots, S_k$. We conclude $S_k \in \mathbf{D}$, which contradicts the condition.

Hence $S_2$ and $F_{t-1}$ are adjacent. Due to the ancestral property, the edge between $S_2$ and $F_{t-1}$ must be $F_{t-1} \leftarrow\!\!* S_2$. If the edge is $F_{t-1} \leftarrow S_2$, similar to the previous proof, the path $X \leftrightarrow F_1 \leftrightarrow \cdots \leftrightarrow F_{t-1} \leftarrow S_2 \cdots Y$ are active relative to $(\mathbf{D}, X)$, which contradicts with the condition that $(\mathbf{D}, X)$ could m-separate all the generalized back-door paths. Hence the edge between $F_{t-1}$ and $S_2$ could only be $F_{t-1} \leftrightarrow S_2$. Also similar to the previous proof, the edge between $S$ and $S_2$ must be as $S *\!\!\rightarrow S_2$, otherwise $S_2 \in \mathbf{D}$ if $S \leftarrow S_2$ since there is a collider path $X \leftrightarrow F_1 \leftrightarrow \cdots \leftrightarrow F_{t-1} \leftrightarrow S$.

We could repeat the above process for $S_3, S_4 \cdots$ until for $S_k$. Similar to the proof above, we see $S_k$ and $F_{t-1}$ must be adjacent in $\mathcal{M}$, and the edge between them is $S_k \leftrightarrow F_{t-1}$. However, we know that $S_k$ is an ancestor of $C$, where $C \in (\mathbf{D}, X)$. Hence $S_k$ is an ancestor of $Y$, so that $S_k \in (\mathbf{D}, X)$, which contradicts the condition that the sub-path from $F_t$ to $C$ does not go through the variables in $(\mathbf{D}, X)$.

Hence we see that if a path such as $\mathcal{L}_2$ exists, $S_1$ and $F_{t-1}$ cannot be adjacent in $\mathcal{M}$. Combining A.4.a.2.1 and A.4.a.2.2, we conclude that there does not exist a path like $\mathcal{L}_2$ in $\mathcal{M}$.

**A.4.a.3. There does not exist an active path like $\mathcal{L}_3$ in $\mathcal{M}$.**

**A.4.a.3.1 If an active path as $\mathcal{L}_3$ exists, then $S_1$ and $F_{t-1}$ are adjacent in $\mathcal{M}$.** Similar to the part A.4.a.2.1, we could prove that there exists an bi-directed edge between $S$ and some variable among $X, F_1 \cdots, F_{t-1}$ in $\mathcal{M}$. Without loss of generality, we suppose such variable by $F_s$. And similarly we also conclude that there must be bi-directed edges between $S$ and $S_i, 1 \leq i \leq S_k$. We discuss the edge between $S$ and $S_{k+1}$ next. If the edge is like $S \leftarrow\!\!* S_{k+1}$, there is a collider path $X \leftrightarrow F_1 \cdots F_s \leftrightarrow S \leftarrow S_{k+1}$, and we also know $S_{k+1}$ is an ancestor of $Y$ since it is an ancestor of $C$ that is a variable from $\mathbf{D}$. Hence we conclude that $S_{k+1} \in \mathbf{D}$, which contradicts the condition that the sub-path from $F_t$ to $C$ does not go through the variables in $(\mathbf{D}, X)$.

Hence, the edge between $S$ and $S_{k+1}$ could only be $S \rightarrow S_{k+1}$. In this case, there forms a sub-structure $S_{k+1} \leftrightarrow S_k \leftrightarrow S \leftrightarrow S_{k-1}$, $S_k \rightarrow S_{k-1}$, and $S \rightarrow S_{k+1}$, which is an inducing path. To satisfy the maximal property, there is a bi-directed edge between $S_{k-1}$ and $S_{k+1}$, which contradicts the condition that $F_t \leftarrow S_1 \leftarrow \cdots \leftarrow S_k \leftrightarrow S_{k+1} \rightarrow \cdots \rightarrow C$ is a minimal path.

Hence we see that if a path such as $\mathcal{L}_3$ exists, it is impossible that $S_1$ and $F_{t-1}$ are not adjacent in $\mathcal{M}$.

**A.4.a.3.2 If an active path as $\mathcal{L}_3$ exists, then $S_1$ and $F_{t-1}$ cannot be adjacent in $\mathcal{M}$.**

If $F_{t-1}$ and $S_1$ are adjacent, similar to the proof of A.4.a.2.2, we could prove that the edge between them are $F_{t-1} \leftrightarrow S_1$. And we could prove that the edge between $F_{t-1}$ and $S_i, 1 \leq i \leq S_k$ are bi-directed, and $F_{t-1}$ and $S_{k+1}$ are adjacent. We discuss the edge between $F_{t-1}$ and $S_{k+1}$ next. If edge is $S_{k+1} \rightarrow F_{t-1}$, the path $X \leftrightarrow F_1 \leftrightarrow \cdots \leftrightarrow F_{t-1} \leftarrow S_{k+1} \cdots Y$ are active relative to $(\mathbf{D}, X)$, which contradicts with the condition that $(\mathcal{D}, X)$ could m-separate all the generalized back-door paths. If the edge is $S_{k+1} \leftrightarrow F_{t-1}$, $S_{k+1} \in \mathbf{D}$ since it is an ancestor of the variable in $\mathbf{D}$, which contradicts the condition that the sub-path from $F_t$ to $C$ does not go through the variables in $(\mathbf{D}, X)$. If the edge is $S_{k+1} \rightarrow F_{t-1}$, we notice that there forms a sub-structure comprised of $S_{k+1} \leftrightarrow S_k \leftrightarrow F_{t-1} \leftrightarrow S_{k-1}$, $S_k \rightarrow S_{k-1}$, and $F_{t-1} \rightarrow S_{k+1}$. To satisfy the maximal property, there is a bi-directed edge between $S_{k-1}$ and $S_{k+1}$, which contradicts the condition that $F_t \leftarrow S_1 \leftarrow \cdots \leftarrow S_k \leftrightarrow S_{k+1} \rightarrow \cdots \rightarrow C$ is a minimal path.

Hence we see that if a path such as $\mathcal{L}_3$ exists, $S_1$ and $F_{t-1}$ cannot be adjacent in $\mathcal{M}$. Combining A.4.a.3.1 and A.4.a.3.2, we conclude that there does not exist a path as $\mathcal{L}_3$ in $\mathcal{M}$.

Till now, we have concluded that for any $F_t \in \mathbf{K}$ that has distance 1 to $(\mathbf{D}, X)$, all the paths from $F_t$ to $Y$ with colliders are m-separated by $(\mathbf{D}, X)$ in any one legal $\mathcal{M}$. Then we prove the induction.

**A.4.b. If for any $F_t \in \mathbf{K}$ that has distance $k - 1 \geq 1$ to $(\mathbf{D}, X)$ in $\mathcal{M}$ it holds that $F_t \perp Y|\mathbf{D}, X$, then for any $F_t \in \mathbf{K}$ that has distance $k$ to $(\mathbf{D}, X)$ in $\mathcal{M}$, all the paths from $F_t$ to $Y$ with colliders are m-separated by $(\mathbf{D}, X)$.**

Denote the minimal possible directed path from $F_t$ to $Y$ where the distance between $F_t$ and $(\mathbf{D}, X)$ is $k$ by $F_t, S, \cdots, Y$. It is trivial to prove that $S$ and $F_{t-1}$ are adjacent. We first prove that $S \in \mathbf{K}$. If there is an edge as $F_{t-1} \leftarrow\!\!* S$ in $\mathcal{M}$, then $S \in \mathbf{K}$. If the edge is as $F_{t-1} \rightarrow S$, by A.2.2 there is at least one variable $F_s, 0 \leq s \leq t-2$ such that $F_s \leftrightarrow S$, thus we also conclude $S \in \mathbf{K}$. The distance between $S$ and $(\mathbf{D}, X)$ is $k-1$. By the inductive hypothesis, it holds that $S \perp Y|\mathbf{D}, X$ in $\mathcal{M}$.

It is easy to see that $S \rightarrow F_t$, otherwise $S$ must be an ancestor of $Y$ due the that fact that $S$ is located at the minimal possible directed path from $F_t$ to $Y$ in $M$. And because $S \in \mathbf{K}$, it holds that $S \in (\mathbf{D}, X)$. However, the distance between $S$ and $(\mathbf{D}, X)$ is $k - 1 \geq 1$, there is a contradiction.

Suppose an active path from $F_t$ to $Y$ with colliders $F_t, S_1, \cdots, S_m, S_{m+1}, \cdots, Y$ in $\mathcal{M}$. Considering the corresponding augmented path with $S \rightarrow F_t$, i.e. $S \rightarrow F_t, S_1, \cdots, S_m, S_{m+1}, \cdots, Y$. Since $S \perp Y|\mathbf{D}, X$ in $\mathcal{M}$, and the sub-path from $F_t$ to $Y$ is active relative to $(\mathbf{D}, X)$ in $\mathcal{M}$, the edge between $S_1$ and $F_t$ can only be $S_1 *\!\!\rightarrow F_t$ in $\mathcal{M}$, i.e., there is a collider at $F_t$.

We first present a supporting result in A.4.b.1.

**A.4.b.1. If $S_m$ is adjacent to $S$ in $\mathcal{M}$, then the marks at $S_m$ on the edge between $S_m$ and $S$ and the edge between $S_m$ and $S_{m-1}$ are distinct, and the edge between $S_m$ and $S_{m+1}$ is as $S_m \leftarrow\!\!* S_{m+1}$.**

Since $S \perp Y|\mathbf{D}, X$ in $\mathcal{M}$, the path $S, S_m, S_{m+1}, \cdots Y$ is m-separated by $(\mathbf{D}, X)$ in $\mathcal{M}$. Denote the path $F_t, S_1, \cdots, S_m, S_{m+1}, \cdots, Y$ by $\mathcal{L}_1$ and $S, S_m, S_{m+1}, \cdots Y$ by $\mathcal{L}_2$. If the edge between $S_m$ and $S_{m+1}$ is as $S_m \rightarrow S_{m+1}$, then $S_m$ is not a collider in both paths $\mathcal{L}_1$ and $\mathcal{L}_2$. In this case if $S_m \in (\mathbf{D}, X)$ in $\mathcal{M}$, then $\mathcal{L}_1$ is m-separated by $(\mathbf{D}, X)$ since $S_m$ is a non-collider in the path, which contradicts the active path. If $S_m \notin (\mathbf{D}, X)$ in $\mathcal{M}$, then the sub-path between $S_m$ and $Y$ is m-separated by $(\mathbf{D}, X)$ since $\mathcal{L}_2$ is m-separated by $(\mathbf{D}, X)$ in $\mathcal{M}$. Thus $\mathcal{L}_1$ is m-separated by $(\mathbf{D}, X)$, which contradicts the active path.

Similarly, if the marks at $S_m$ on the edge between $S_m$ and $S$ and the edge between $S_m$ and $S_{m-1}$ are the same, we could conclude $\mathcal{L}_1$ is m-separated by $(\mathbf{D}, X)$ in $\mathcal{M}$ by discussing the conditions $S_m \in (\mathbf{D}, X)$ and $S_m \notin (\mathbf{D}, X)$ in $\mathcal{M}$, which contradicts the condition.

**A.4.b.2. For any an active path $F_t, S_1, \cdots, Y$ relative to $(\mathbf{D}, X)$ with colliders in $\mathcal{M}$, the edge between $S$ and $S_1$ in $\mathcal{M}$ is as $S *\!\!\rightarrow S_1$.**

Suppose $S_1 \to S$ in $\mathcal{M}$. Since $S \to F_t$, the edge between $F_t$ and $S_1$ is as $S_1 \to F_t$. In this case, $S_1$ is adjacent to $S$ and the marks at $S_1$ on the edge between $S_1$ and $S$ and the edge between $S_1$ and $F_t$ are the same, which contradicts the result in A.4.b.1. Hence the edge is as $S{*\!\!\rightarrow} S_1$. By A.4.b.1 again, there is an edge $S_1 \to F_t$ in $\mathcal{M}$.

**A.4.b.3. For any $F_t \in \mathbf{K}$ that has distance $k$ to $(\mathbf{D}, X)$ in $\mathcal{M}$, all the paths from $F_t$ to $Y$ with colliders are m-separated by $(\mathbf{D}, X)$.**

Similar to A.4.a, we consider the collider closest to $F_t$ in the active path from $F_t$ to $Y$ with colliders. By A.1, since the collider is an ancestor of $Y$ in $\mathcal{M}$ (this collider belongs to $(\mathbf{D}, X)$ so that the path with this collider could be active relative to $(\mathbf{D}, X)$), there exist some active minimal paths without colliders from $F_t$ to this collider relative to $(\mathbf{D}, X)$ in $\mathcal{M}$. Without loss of generality, we suppose the active minimal path $F_t \leftarrow S_1 \cdots S_{m-1}{*\!\!\rightarrow} S_m \leftarrow\!\!* S_{m+1} \cdots Y, m \geq 2$ ($S_{m+1}$ could be $Y$), where $S_m$ is the collider that is nearest to $F_t$ in the path. For simplification, we denote the path by $\mathcal{L}_1$. By A.4.b.1, the mark at $S_1$ on the edge between $S_1$ and $S_2$ is an arrowhead.

If $S_2$ and $S$ are not adjacent, then there is an unshielded collider $S{*\!\!\rightarrow} S_1 \leftarrow\!\!* S_2$, hence the two arrowheads at $S_1$ could be identified in $M$. And because the path is minimal, $F_t \leftarrow S_1$ could be identified in $M$. In this case we could identify there is an arrowhead at $F_t$ on the edge between $F_t$ and $S$ by Rule 2 of Zhang [13], which contradicts the condition that the path $F_t, S, \cdots, Y$ is a minimal possible directed path from $F_t$ to $Y$. Hence $S_2$ and $S$ are adjacent.

By A.4.b.1, the edge between $S_3$ and $S_2$ is as $S_3{*\!\!\rightarrow} S_2$. Since $S_2$ is not a collider in $\mathcal{L}_1$, the edge between $S_2$ and $S_1$ could only be $S_2 \to S_1$. By A.4.b.1 again, the edge between $S$ and $S_2$ is as $S{*\!\!\rightarrow} S_2$. For the sake of satisfying ancestral property, the edge could only be $S \leftrightarrow S_2$ considering $S \leftrightarrow S_1 \leftarrow S_2$. In addition, $S_3$ is adjacent to $S$, otherwise there is an unshielded collider $S_3, S_2, S$ thus the two arrowheads at $S_2$ could be identified in $M$. Thus $S_2 \to S_1$ is identified by Rule 1 of Zhang [13] and $S_2 \leftrightarrow S$ is identified by Rule 4 of Zhang [13]. Thus $S \to F_t$ is further identified by Rule 1 of Zhang [13], which contradicts the condition that the path $F_t, S, \cdots, Y$ is a minimal possible directed path from $F_t$ to $Y$. Hence $S_3$ and $S$ are adjacent. We repeat the process above and for all variable $S_i, 0 \leq i \leq m-2$ ($S_0 = F_t$), there are edges $S_{i+1} \to S_i$ and $S \leftrightarrow S_i$ in $\mathcal{M}$, and $S_{i+2}$ is adjacent to $S$.

By A.4.b.1, the edge between $S_m$ and $S_{m-1}$ is $S_m{*\!\!\rightarrow} S_{m-1}$. Since $S_m$ is a collider, the edge is $S_m \leftrightarrow S_{m-1}$. By A.4.b.1 again, the edge between $S_m$ and $S$ is $S_m \to S$.

We discuss the distinct value attained by $m$. If $m > 2$, it is easy to construct a contradiction. Since $S_m$ is not adjacent to $S_{m-2}$ and there are edges $S_m \to S \leftrightarrow S_{m-2}$. They form an unshielded collider so that $S_m{*\!\!\rightarrow} S$ could be identified in $M$, thus $S \to F_t$ is identified by Rule 1 of Zhang [13], which contradicts the condition that the path $F_t, S, \cdots, Y$ is a minimal possible directed path from $F_t$ to $Y$.

The proof for $m = 2$ is a bit complex. The reason is that the subpath $S_{m-1}, S_m, S_{m+1}, \cdots, Y$ (here $m = 2$, we still use $m$ for generality) is not necessarily minimal. In the following we present the proof in this case.

We first prove $S_{m+1}$ and $S$ are adjacent. Suppose it does not hold. If $S_{m-1}$ and $S_{m+1}$ are not adjacent, $S_{m-1}{*\!\!\rightarrow} S_m \leftarrow\!\!* S_{m+1}$ form an unshielded collider, thus the two arrowheads at $S_m$ could be identified in $M$. In this case we could identify $S_m \to S$ in $M$ by Rule 1 of Zhang [13], since $S_m$ is not adjacent to $F_t$ since the path $F_t \leftarrow S_1 \cdots {*\!\!\rightarrow} S_m$ is minimal, we could identify $S \to F_t$ in $M$, which contradicts the condition that the path $F_t, S, \cdots, Y$ is a minimal possible directed path from $F_t$ to $Y$. Then consider the situation that $S_{m-1}$ and $S_{m+1}$ are adjacent. Note that $S_{m-1} \notin (\mathbf{D}, X)$ since the path $F_t \leftarrow S_1 \cdots \leftarrow S_{m-1} \leftrightarrow S_m \leftarrow\!\!* S_{m+1} \cdots Y$ is active relative to $(\mathbf{D}, X)$ in $\mathcal{M}$. If the edge between $S_{m-1}$ and $S_{m+1}$ is as $S_{m-1} \to S_{m+1}$, there is an edge $S_m \leftrightarrow S_{m+1}$ and a path $S \leftrightarrow S_{m-1} \to S_{m+1}, \cdots, Y$. Since $F_t \leftarrow S_1 \cdots {*\!\!\rightarrow} S_m \leftrightarrow S_{m+1} \cdots Y$ is active relative to $(\mathbf{D}, X)$ in $\mathcal{M}$, the sub-path $S_{m+1}, \cdots, Y$ is active relative to $(\mathbf{D}, X)$ in $\mathcal{M}$. And because $S_{m-1} \notin (\mathbf{D}, X)$, the path $S \leftrightarrow S_{m-1} \to S_{m+1}, \cdots, Y$ is active relative to $(\mathbf{D}, X)$ in $\mathcal{M}$, which implies $S \not\perp Y | \mathbf{D}, X$ and contradicts with the condition. Hence the edge between $S_{m-1}$ and $S_{m+1}$ is as $S_{m-1} \leftarrow\!\!* S_{m+1}$. In this case, there is an unshielded collider $S \leftrightarrow S_{m-1} \leftarrow\!\!* S_{m+1}$, thus could identify the two arrowheads at $S_{m-1}$ in $M$. And since there is no unshielded collider $S_{m+1}{*\!\!\rightarrow} S_m \leftarrow\!\!* S$ in $M$ since the edge between $S$ and $S_m$ is as $S \leftarrow S_m$ in $\mathcal{M}$, we could identify $S_m{*\!\!\rightarrow} S_{m-1}$ in $M$ by Rule 3 of Zhang [13], thus identify $S_{m-1} \to S_{m-2} \to \cdots \to F_t$ by Rule 1 of Zhang [13] and $S_{m-1} \leftrightarrow S \leftrightarrow S_{m-2}$ by Rule 4 of Zhang [13]. If $m = 2$, then we identify $S{*\!\!\rightarrow} F_t$ by Rule 2 of Zhang [13]. If $m > 2$, then we identify $S \to F_t$ by Rule 1 of Zhang [13] since $S_{m-1} \to S$ and $S_{m-1}$ is not adjacent to $F_t$. Both of them contradict the condition that the path $F_t, S, \cdots, Y$ is a minimal possible directed path from $F_t$ to $Y$. Hence there is always a contradiction if $S$ is not adjacent to $S_{m+1}$.

We consider the situation that $S$ is adjacent to $S_{m+1}$. If the edge is as $S{*\!\!\rightarrow} S_{m+1}$, there is an edge $S_{m+1} \to S_m$ by A.4.b.1. This is against the ancestral property since $S_m \to S$. Hence the edge between $S$ and $S_{m+1}$ could only be as $S \leftarrow S_{m+1}$. And by A.4.b.1 there is an edge $S_{m+1} \leftrightarrow S_m$. And the edge between $S_{m+2}$ and $S_{m+1}$ is as $S_{m+2}{*\!\!\rightarrow} S_{m+1}$. Similar to this process, we could prove if $S_j, j \geq m+1$ is adjacent to $S$, then $S_j \to S$, $S_j \leftrightarrow S_{j-1}$, and $S_{j+1}{*\!\!\rightarrow} S_j$. If all the variables between $S_{m+1}$ and $Y$ are adjacent to $S$, it holds that $S \not\perp Y | \mathbf{D}, X$, which contradicts the condition. Hence there is at least one variable between $S_{m+1}$ and $Y$ that is not adjacent to $S$. Suppose the variable that is nearest to $S_{m+1}$ and not adjacent to $S$ in the path $S_n$. That is, there is a path $S \leftrightarrow S_m \leftrightarrow S_{m+1} \leftrightarrow \cdots, S_n, n \geq m+2$, where $S_{m+1}, S_{m+2}, \cdots, S_{n-1}$ is a parent of $S$ and $S_n$ is not adjacent to $S$. That is, $S_n, S_{n-1}, \cdots, S_m, S$ is a discriminating path for $S_m$ in $\mathcal{M}$.

Note again that there is a collider path from $S_n$ to $S$ in $\mathcal{M}$. And all the variables between $S_{n-1}$ and $S_1$ are parents of $S$ in $\mathcal{M}$. Here evidently $S_1$ is located at the minimal collider path between $S$ and $S_n$. By Lemma 18 (see the detailed proof process), we could identify all the colliders in the minimal collider path from $S_n$ to $S$ by FCI algorithm. Hence there is $S_2 \leftrightarrow S_1 \leftrightarrow S$ in $M$. Since $F_t$ and $S_1$ are not adjacent, we could identify $S_1 \rightarrow F_t$ by Rule 1 of Zhang [13] and identify $S {*\!\!\rightarrow} F_t$ by Rule 2 of Zhang [13], which contradicts the condition that the path $F_t, S, \cdots, Y$ is a minimal possible directed path from $F_t$ to $Y$. Hence we conclude that for all the paths from $F_t$ to $Y$, they are m-separated by $(\mathbf{D}, X)$.

Hence, we conclude that for any $F_t \in \mathbf{K}$ that has distance $k$ to $(\mathbf{D}, X)$ in $\mathcal{M}$, all the paths from $F_t$ to $Y$ with colliders are m-separated by $(\mathbf{D}, X)$. The mathematical induction completes. Hence we prove that there do not exist active paths relative to $(\mathbf{D}, X)$ from $F_t$ to $Y$ with colliders in any legal MAG $\mathcal{M}$. The part A.4 completes.

Combining A.3 and A.4, we conclude that there is no an active path relative to $(\mathbf{D}, X)$ from $F_t$ to $Y$ in any legal MAG $\mathcal{M}$. That is, there is not a legal MAG $\mathcal{M}$ such that $F_t \not\perp Y | \mathbf{D}, X$ in $\mathcal{M}$. Hence we conclude that $\mathbf{K} \perp Y | \mathbf{D}, X$.

**2. In any an MAG $\mathcal{M}$ consistent to $M$, if $\mathbf{K} \perp Y|\mathbf{D}, X$, then $\mathbf{D} \subseteq$ PD-SEP$(X, Y, M)$ .**

For the sake of contradiction, we suppose there is a minimal collider path $X \leftrightarrow F_1 \leftrightarrow \cdots \leftrightarrow F_t \leftarrow\!\!* F_{t+1}$, where $F_t \in \mathbf{K}$, $F_{t+1} \notin$ PD-SEP$(X, Y, M)$ and $F_{t+1}$ belongs to $\mathbf{D}$. If it never happens, it is concluded trivially that $\mathbf{D} \subseteq$ PD-SEP$(X, Y, M)$, which we leave for the readers. There is no need to worry that there is a minimal collider path between $X$ and $F_{t+1}$ which is not across a variable $F_t \in$ PD-SEP$(X, Y, M) \backslash$Anc$(Y, M)$, because in this case it concludes that $F_{t+1} \in \mathbf{K}$, which contradicts the conditions.

By the definition of $\mathbf{D}$, $F_t$ and $F_{t+1}$ are ancestors of $Y$ in $\mathcal{M}$. Suppose $F_t \rightarrow S_1 \rightarrow \cdots \rightarrow S_p \rightarrow Y$ the directed path from $F_t$ to $Y$. Since the collider path $X \leftrightarrow F_1 \leftrightarrow \cdots \leftrightarrow F_t \leftarrow\!\!* F_{t+1}$ is minimal, by Lemma 18 (see the detailed proof process) we could identify all the colliders in this path. Hence $F_{t-1}$ is adjacent to $S_1$, otherwise the tail at $F_t$ on the edge between $F_t$ and $S$ is identified in $M$, which contradicts the condition $F_t \in \mathbf{K}$. Similarly, $F_{t+1}$ and $S_1$ are adjacent. By ancestral property, the edge between $F_{t-1}$ and $S_1$ is as $F_{t-1} {*\!\!\rightarrow} S_1$ in $\mathcal{M}$. Since $F_{t+1} {*\!\!\rightarrow} F_t$ and $F_t \rightarrow S_1$, there is $F_{t+1} {*\!\!\rightarrow} S_1$ in $\mathcal{M}$.

Then we prove that there exist some variable $F_s, 0 \leq s \leq t-1$ where $F_0 = X$ such that $F_s \leftrightarrow S_1$. Otherwise, for the edge between $F_{t-1}$ and $S_1$, the edge could only be $F_{t-1} \rightarrow S_1$. And we consider the edge between $F_{t-2}$ and $S_1$ further. If they are not adjacent, there is a discriminating path $F_{t-2} \leftrightarrow F_{t-1} \leftrightarrow F_t \rightarrow S_1$ with $F_{t-1} \rightarrow S_1$ in $M$, thus we could identify $F_t \rightarrow S_1$ in $M$. Hence there is an edge between $F_{t-2}$ and $S_1$. By the ancestral property, the edge could only be $F_{t-2} {*\!\!\rightarrow} S_1$. Since we suppose no bi-directed edges between any $F_s$ and $S_1$, the edge could only be $F_{t-2} \rightarrow S_1$. Repeat the process and we have $X \rightarrow S_1$. However, in this case $F_t$ is a critical variable, contradicting the condition.

Suppose $F_{s_1}$ is the variable with a bi-directed edge with $S_1$ that is nearest to $F_t$ in the collider path. It is easy to see that the collider path $X \leftrightarrow F_1 \leftrightarrow \cdots \leftrightarrow F_{s_1} \leftrightarrow S_1 \leftarrow\!\!* F_{t+1}$ is also a minimal collider path. Thus $S_1$ belongs to $\mathbf{D}$. If $S_1 \in$ Anc$(Y, M)$, there is a collider path $X \leftrightarrow F_1 \leftrightarrow \cdots \leftrightarrow F_{s_1} \leftrightarrow S_1 \leftarrow\!\!* F_{t+1}$ where each variable between $X$ and $F_{t+1}$ are ancestors of $Y$ in $M$, hence we identify $F_{t+1} \in \mathbf{D}$ in $M$ or $F_{t+1} \in$ PD-SEP$(X, Y, M)$, neither contradicts the condition. If $S_1 \notin$ Anc$(Y, M)$, we see $S_1 \in$ PD-SEP$(X, Y, M)$. In this case, there is a collider path $X \leftrightarrow F_1 \leftrightarrow \cdots \leftrightarrow F_{s_1} \leftrightarrow S_1 \leftarrow\!\!* F_{t+1}$ in $M$ where $S_1 \in$ PD-SEP$(X, Y, M)$. Note here $S_1$ and $F_t$ are symmetrical in the sense that they have the same property but $S_1$ is closer to $Y$ in the directed path to $Y$. In this case, we see $S_1$ as original $F_t$ and discuss $S_2$. Similarly, if there is not a contradiction, there must be some variable $F_{s_2}$ with a bi-directed edge with $S_2$, and $S_2 \notin$ Anc$(Y, M)$. Repeat this process for $S_3, S_4, \cdots, Y$, we could identify that there is some variable $F_{s_t}$ with a bi-directed edge with $Y$. In this case, there is a path $X \leftrightarrow F_1 \leftrightarrow \cdots \leftrightarrow F_{s_t} \leftrightarrow Y$, which is active relative to $\mathbf{D}$, contradicting the condition that $\mathbf{D}$ m-separates all generalized back-door paths from $X$ to $Y$. Hence, we conclude that there cannot be a variable $F_{t+1} \in \mathbf{D} \backslash$PD-SEP$(X, Y, M)$. Hence we conclude if $\mathbf{K} \perp Y|\mathbf{D}, X$, then $\mathbf{D} \subseteq$ PD-SEP$(X, Y, M)$ in any an MAG $\mathcal{M}$ consistent to $M$.

Hence, if there is no critical variable, it holds that $\mathbf{K} \perp Y|\mathbf{D}, X$ and $\mathbf{D} \subseteq$ PD-SEP$(X, Y, M)$ in any a legal MAG. That is PD-SEP$(X, Y, M) = \mathbf{D} \cup \mathbf{K}$. Thus the MCS regarding PD-SEP$(X, Y, M)$ equals to the MCS regarding $\mathbf{D}$. $\square$

### C.3 Proofs for Lemma 4

**Lemma 4.** *Let $\mathcal{P}$ be a PMAG of MAG $\mathcal{M}$. If $X \in$ An$(Y, \mathcal{M})$ and D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}}) \cap$ De$(X, \mathcal{M}) = \emptyset$, then the MCS regarding D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}})$ in $\mathcal{M}$ and the corresponding local MAG are contained in the output of Algorithm 1.*

*Proof.* In line 2 of Alg. 1, the algorithm enumerates local MAGs with different marks at $X$. Evidently $\mathcal{M}$ is consistent to one local MAG among them. Without loss of generality, suppose $\mathcal{M}$ is consistent to $M^j$. If there is no critical variable (Line 5, Line 6) in $M^j$, as implied by Theorem 3, all the MAGs $\mathcal{M}'$consistent to $M^j$ have the same MCS regarding D-SEP$(X, Y, \mathcal{M}')$ in respective graph $\mathcal{M}'$, and equal to the MCS regarding PD-SEP$(X, Y, M^j)$. Hence no matter what $\mathcal{M}$ is in the class of MAGs consistent to $M^j$, the MCS regarding D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}})$ in $\mathcal{M}$ is equal to MCS regarding PD-SEP$(X, Y, M^j)$, which is returned in the output.

If there is a critical variable set $\mathbf{C}^j$ in $M^j$ (Line 3, 4), denote the non-empty set $\mathbf{S}$ defined in Definition 5 of the main paper by $\mathbf{S}$ also, we firstly consider the situation that $\mathbf{C}^j$ contains only one variable $C$. We see by the definition of critical variable that there is a collider path $X \leftrightarrow F_1 \leftrightarrow \cdots \leftrightarrow F_{t-1} \leftrightarrow C$ or $X \leftrightarrow F_1 \leftrightarrow \cdots \leftrightarrow F_{t-1} \leftarrow\!\circ C$. We notice that the edge between $C$ and $S$ belonging to $\mathbf{S}$ is as $C {*\!\!\rightarrow} S$ due to the ancestral property. Hence, we just consider two further local MAGs $M^{j_1}$ and $M^{j_2}$, where $M^{j_1}$ is with the edges $F_{t-1} \leftrightarrow C \leftrightarrow S$ for $\forall S \in \mathbf{S}$, and $M^{j_2}$ is with the edges $C \rightarrow S$ for $\forall S \in \mathbf{S}$ and $F_{t-1} \leftrightarrow C$ or $F_{t-1} \leftarrow\!\circ C$ (Line 11). The edge between $F_{t-1}$ and $C$ in $M^{j_2}$ follows the edge in local MAG $M^j$. Note that here we rule out the local MAGs with both $C \rightarrow S$ for some $S \in \mathbf{S}$ and $C \leftrightarrow S$ for the other $S \in \mathbf{S}$. The reason is if there is some $S_1$ belonging to $\mathbf{S}$ such that $C \rightarrow S_1$ and another $S_2$ belonging to $\mathbf{S}$ such that $C \leftrightarrow S_2$ in some MAG $\mathcal{M}'$, it holds that $S_2 \in$ D-SEP$(X, Y, \mathcal{M}'_{\underset{\sim}{X}})$. We prove $S_2 \in$ D-SEP$(X, Y, \mathcal{M}'_{\underset{\sim}{X}})$ in the following. (1) It is evident that there is a collider path $X \leftrightarrow F_1 \leftrightarrow \cdots \leftrightarrow F_{t-1} \leftrightarrow C \leftrightarrow S_2$ and each variable except for $S_2$ on it is ancestor of $X$ or $Y$ in $\mathcal{M}'_{\underset{\sim}{X}}$; (2) $S_2$ is also an ancestor of $Y$ due to the fact that $S_2$ is localed at a minimal possible directed path from $C$ and $Y$. When there is an arrowhead at $S_2$ on the edge between $C$ and $S_2$, $S_2$ must be an ancestor of $Y$ in the path to prevent from generating unshielded colliders. Hence, we conclude $S_2 \in$ D-SEP$(X, Y, \mathcal{M}'_{\underset{\sim}{X}})$. In addition, $S_2 \in$ De$(X, \mathcal{M}')$ according to the condition (2) of the definition of critical variables. That is $S_2 \in$ De$(X, \mathcal{M}') \cap$ D-SEP$(X, Y, \mathcal{M}'_{\underset{\sim}{X}})$, which contradicts the condition.

Therefore, we only consider local MAG $M^{j_1}$ and $M^{j_2}$. Similarly, when there are more than one variable in $\mathbf{C}^j$, for each $C \in \mathbf{C}^j$, since we only consider two situations $C \leftrightarrow S$ for $\forall S \in \mathbf{S}$ and $C \rightarrow S$ for $\forall S \in \mathbf{S}$, we consider $2^{|\mathbf{C}^j|}$ situations in total, where $|\mathbf{C}^j|$ denotes the set size of $\mathbf{C}^j$. Given a subset $\mathbf{C} \subseteq \mathbf{C}^j$, there possibly exists a local MAG $M^{j_1}$ in which $C_1 \rightarrow S$ and $C_2 \leftrightarrow S$ for $\forall C_1 \in \mathbf{C}$, $C_2 \in \mathbf{C}^j \backslash \mathbf{C}$, and $\forall S \in \mathbf{S}$. That is reflected by Line 11. For all the MAGs $\mathcal{M}'$ consistent to $M^{j_1}$, it holds that $\mathbf{C} \subseteq$ D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}})$ and $\mathbf{C}^j \backslash \mathbf{C} \cap$ D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}}) = \emptyset$. Combining with the algorithm to find MCS, it is easy to see that all the variables in $\mathbf{C}$ belong to MCS, while all the variables in $\mathbf{C}^j \backslash \mathbf{C}$ do not belong to MCS. Since there are $2^{|\mathbf{C}^j|}$ possible $\mathbf{C} \subseteq \mathbf{C}^j$, we could obtain $2^{|\mathbf{C}^j|}$ new local MAGs based on $M^j$ in which the causal effects (or MCSs) are different from the others. If there is a critical variable in a new local MAG $M^{j_k}$ for example, the remaining part is same as before, which is in Line 12-15.

Hence for each local MAG $M^j$ of $X$, all the considered local MAGs have covered the whole space of MAGs where GBC does not fail to identify $P(Y|do(X))$. Hence no matter which MAG consistent to $M^j$ is the true MAG, we could find a local MAG consistent to it and the corresponding MCS regarding D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}})$ as long as GBC does not fail to identify $P(Y|do(X))$ in $\mathcal{M}$. By enumerating all $M^j$, we can find all MCSs regarding D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}})$ in all MAG $\mathcal{M}$ consistent to $\mathcal{P}$. □

*Remark.* A pity here is that there is no guarantee for the existence of MAGs consistent to each considered local MAG. However, this does not impact the soundness of the proposed method that the MCS in the true MAG could be returned.

## Appendix D Proofs for the Results in Section 3.4

In this section, we present the proof for the propositions in "Learning marks and purity matrix by interventional data" in order.

**Proposition 5.** *If $P(Y|do(X)) = P(Y)$, the marks at $X$ are arrowheads in all the minimal possible directed paths from $X$ to $Y$ in a partially mixed ancestral graph.*

*Proof.* If there is a tail at $X$ on a minimal possible directed path, the path begins from a directed edge out of $X$. Such a path must be a directed path from $X$ to $Y$ in order to avoid the generation of new unshielded colliders, otherwise there will be an arrowhead pointing to $X$ on the minimal possible directed path in $\mathcal{P}$, which contradicts the fact that the path is a minimal possible directed path from $X$ to $Y$. While such a directed path implies that $X$ is an ancestor of $Y$, contradicting $P(Y|do(X)) = P(Y)$. □

**Proposition 6.** *In situation* (3)*, let $\mathbf{T}$ denote all variables adjacent to $X$ in the minimal possible directed paths from $X$ to $Y$. For $T \in \mathbf{T}$, if for $\forall V \in \mathbf{T} \backslash T$, it holds either $T \notin$ Adj$(V, \mathcal{P})$ or there is a variable $S \notin$ Adj$(V, \mathcal{P})$*

*such that there is a collider path $X \circ\!\!\rightarrow T \leftrightarrow \cdots \leftarrow\!\!* S$ and every vertex except $S$ on the path is a parent of $V$, then $X \rightarrow T$.*

*Proof.* For the sake of contradiction we assume a variable $T$ meets the condition in the proposition and $X \in \text{An}(Y, \mathcal{M})$ but the edge is $X \leftarrow\!\!* T$ in $\mathcal{M}$. For $V \in \mathbf{T} \backslash T$, if $V$ is not adjacent to $T$, the mark at $X$ in the edge of $V$ and $X$ is evidently tail otherwise there is an unshielded collider $V *\!\!\rightarrow X \leftarrow\!\!* T$ in $\mathcal{P}$ and contradicts the premise that $T$ is in the minimal possible directed path from $X$ to $Y$. And we know the edge $X \rightarrow V$ is visible thus pure by definition 8 of Zhang [11]. If $T$ is adjacent to $V$ but there is a variable $S$ not adjacent to $V$ such that there is a collider path $X \circ\!\!\rightarrow T \leftrightarrow \cdots \leftarrow\!\!* S$ and every vertex except for $S$ on the path is a parent of $V$, if the mark at $X$ in the edge of $T$ and $X$ is arrowhead, it concludes that the edge $X \rightarrow V$ is visible thus pure by Definition 8 of Zhang [11]. Hence, we see that all directed edge out of $X$ in the minimal possible directed path from $X$ to $Y$ are visible. In this case GBC does not fail to identify $P(Y|do(X))$, which contradicts the condition. □

**Proposition 7.** *Rule 11 is sound.*

*Proof.* If it is $d \leftarrow c$, the edge between $b$ and $d$ is $b \rightarrow d$. Hence the edge between $a$ and $d$ is as $a *\!\!\rightarrow d$ by Lemma A.1 of Zhang [13]. Hence there is an unshielded collider $a *\!\!\rightarrow d \leftarrow c$, which contradicts the condition.

If the edge is $d \leftrightarrow c$, we could prove that the only possible structure where $a, d, c$ do not form an unshielded collider is comprised of $a \leftrightarrow b \leftrightarrow d \leftrightarrow c$, $b \rightarrow c$, and $d \rightarrow a$. In this case there is an inducing path $a \leftrightarrow b \leftrightarrow d \leftrightarrow c$, which contradicts the maximal property. □

**Proposition 8.** *In a PMAG $\mathcal{P}$, if there is no minimal possible directed path from $X$ to $Y$, then $X$ cannot be ancestor of $Y$ in any MAG consistent to $\mathcal{P}$. And it holds that $X \notin \text{PossAn}(Y, \mathcal{P})$.*

*Proof.* It is a direct conclusion by the inverse negative proposition of Lemma B.1 of Zhang [13]. Although they do not consider PMAG, it will not influence the result. □

# Appendix E Proofs for the Results in Section 4

In this section, we present the proofs for the results in Section 4 in order. Then we give a detailed analysis about the computational complexity, which is omitted in the main paper due to the limit of the space.

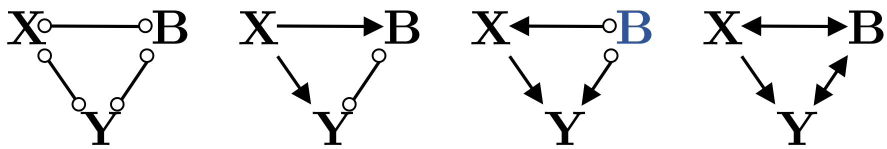
## E.1 Proofs

**Theorem 9.** Given the observational distribution of the observed variables, if there exists a valid generalized back-door set for $(X, Y)$ in the true MAG with the knowledge of the purity of each directed edge, then we can identify this set by only additional data of $Y$ under intervention on $X$.

*Proof.* When GBC does not fail to identify $P(Y|do(X))$, the interventional data accords with situation (1) or situation (2). The result for situation (1) is obvious since the distribution of $Y$ remains unchanged under intervention on $X$, which implies $X$ has no causal effect on $Y$. The result for situation (2) is trivially guaranteed by Prop. 1 and Lemma 4. According to Prop. 1, there exist generalized back-door sets and D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}})$ is one among those. By Lemma 4, we could find the MCS regarding D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}})$. Hence we could identify this set which could result in a consistent estimation of the causal effect with interventional data by Eq. 3. □

**Proposition 10.** *Let $\mathcal{M}$ be a complete MAG with $p+1$ variables $X_1, \cdots, X_p, Y$, where the causal order of the variables except $Y$ is completely random and $Y$ is at the last. Denote the graph obtained by FCI with observational data by $\mathcal{P}$ and intervention variable by $X_i$. And let $M$ be a local MAG of $X_i$ with $p-1-k$ tails and $k$ arrowheads at $X_i$. The computational complexity of finding all possible causal effects $P(Y|do(X_i))$ in all the MAGs consistent to $M$ is $O(2^k)$. Further, the computational complexity of finding all causal effects $P(Y|do(X_i))$ in all the MAGs consistent to $\mathcal{P}$ is $O(3^p)$.*

*Proof.* In $M$, there are $p-1-k$ tails and $k$ arrowheads at $X_i$. Without loss of generality, we assume the $k$ variables $X_1, \cdots, X_k$ have edges with $X_i$ in which there is an arrowhead at $X_i$ and $p-1-k$ variables $X'_1, \cdots, X'_{p-1-k}$ have edges with $X_i$ in which there is a tail at $X_i$. At first we find all of $X_1, \cdots, X_k$ are critical variables. This part takes $k*(p-1-k)$ complexity (For each variable $X \in X_1, \cdots, X_k$, we judge whether there is some variable $X' \in X'_1, \cdots, X'_{p-1-k}$ which is a child of $X$). According to Line 10 in Algorithm 1, we obtain $2^k$ new local MAGs, and in each new local MAG there is no new critical variable, thus we only have 1 calculation in each new MAG. Hence the computation complexity in these new local MAGs is




(a) PAG (b) local MAG $M^1$ (c) local MAG $M^2$ (d) local MAG $M^3$

Figure 4: Fig. 4(a) is the PAG. If we intervene on the variable $X$, we can obtain some local MAGs of $X$. Two of them are shown in Fig. 4(b) and Fig. 4(c). Note there is a critical variable $B$ in Fig. 4(c), hence we need to consider the critical marks at $B$ and we can obtain some new local MAGs and Fig. 4(d) is one of them. We can see although Fig. 4(b) and Fig. 4(d) have different marks at $X$, the causal effects of $X$ on $Y$ are the same in the two local MAGs.

$2^k$. The total computation times are $2^k + k*(p-1-k) \sim O(2^k)$. When considering the whole process in Algorithm 1, denote the total computation complexity by $T(p)$, it holds

$$
\begin{aligned}
T(p) &= \sum_{k=0}^{p-1} C_{p-1}^{k}(2^k + k*(p-1-k)),\\
&= \sum_{k=0}^{p-1} C_{p-1}^{k}(2^k) + \sum_{k=0}^{p-1} C_{p-1}^{k}(k*(p-1-k)),\\
&= 3^{p-1} + p(p-1)2^{p-2} \sim O(3^p).
\end{aligned}
$$

□

### E.2 Computational complexity analysis

In the setting of Prop. 10, let $\mathbf{S}$ denote the set of variable that has an edge with an arrowhead at $X_i$. Since the graph is complete, for any subset $\mathbf{S}_1$ of $\mathbf{S}$, we could construct an MAG $\mathcal{M}$ based on $M$ such that MCS in $\mathcal{M}$ is $\mathbf{S}_1$. We show the construction process in the following. Note that the graph is complete, if the constructed graph is ancestral, then it is an MAG since any two variables are adjacent. And for the same reason there are no discriminating paths in the graph. Thus there is no need to worry that there forms a new discriminating path in the constructed graph, which makes the graph entail the conditional independence that is not entailed in the original PAG $\mathcal{P}$. We divide the variables in the local MAG $M$ into three classes. The first class is $\mathbf{S}_1$. The second class is $\mathbf{S}_2 = \mathbf{S}\backslash\mathbf{S}_1$. The third class is comprised of the variables that have an edge with a tail at $X_i$, denoted by $\mathbf{S}_3$. $Y$ belongs to $\mathbf{S}_3$ since it is the descendant of $X_i$. Evidently $\mathbf{S}_1$, $\mathbf{S}_2$, and $\mathbf{S}_3$ cover all the variables in $\mathcal{P}$ except for $X_i$. We orient the subgraph of each class into a DAG, respectively. Note when we orient the subgraph of the third classes, we set $Y$ as the variable at the last of causal order. It could be achieved since the subgraph is complete. For the edges between the variables $A$ and $B$ from two classes, we orient $A \to B$, if the order of the class of $A$ is less than that of $B$, for example $A$ is in the first class $\mathbf{S}_1$ and $B$ is in the third class $\mathbf{S}_3$. For the edge between $A$ and $X_i$, we mark the circle at $A$ by arrowhead if $A \in \mathbf{S}_2 \cup \mathbf{S}_3$, by tail if $A \in \mathbf{S}_1$. Till now we have marked all the circles at $M$ and obtain a graph $\mathcal{M}$, and it is easy to prove this graph is ancestral. According to our discussions before, we know $\mathcal{M}$ is an MAG. And it is not hard to prove that MCS in $\mathcal{M}$ is $\mathbf{S}_1$, because for $\forall S_1 \in \mathbf{S}_1$, there is an edge between $S_1$ and $Y$, which cannot be m-separated by other variables, and for $\forall S_2 \in \mathbf{S}_2$, $S_2$ is not a variable in D-SEP$(X, Y, \mathcal{M}_{\underset{\sim}{X}})$. Since there are $2^k$ subsets of $\mathbf{S}_1$, there are $2^k$ MCSs, in other word, $2^k$ causal effects in all the MAGs consistent to $M$.

When finding all possible causal effects in $\mathcal{P}$, the complexity gap between our method and the lower bound (i.e. $2^{p-1}$, the number of possible causal effects in all MAGs consistent to $\mathcal{P}$) is from two parts. One is in the search of the critical variables, which results in that we calculate $2^k + k*(p-1-k)$ times, which are $k*(p-1-k)$ larger than the number of causal effects. But this term do not influence the magnitude of the complexity. The other is caused by that different local MAGs may lead to the same causal effect. An example in Fig. 4 is given to illustrate it. There are different marks at $X$ in Fig. 4(b) and Fig. 4(d), but the causal effects of $X$ on $Y$ in the two graphs are the same. While such a causal effect is calculated by our method for twice when we consider the local MAG $M^1$ and local MAG $M^3$ separately. Such kind of repeated calculations leads to that the complexity of our method is $O(3^{p-1})$ but not $O(2^{p-1})$.

Next, we present a rough estimate about the complexity of the local algorithm (Algorithm 4.2) of Malinsky and Spirtes [16]. In the complete graph, all variables are possible-D-SEP , which is as Definition 4.4 of Malinsky and Spirtes [16]. Hence the search space of MAG is $3^{\frac{p(p+1)}{2}}$, where $\frac{p(p+1)}{2}$ is the number of the edges and 3 implies there are three kinds for each edge $\to, \leftarrow, \leftrightarrow$. If we enumerate the MAG by brute force, i.e. we consider each combination of circle, then for each searched MAG, we need an extra $p^2 * \frac{p(p-1)}{2}$ complexity [15] to verify whether it is consistent to $\mathcal{P}$. Since $\mathcal{M}$ is obtained from $\mathcal{P}$, all the non-circle marks at $\mathcal{P}$ are still in $\mathcal{M}$. The only remaining part is to verify whether the enumerated MAG entails the same conditional independence with $\mathcal{P}$. A direct method is to generate an MAG $\mathcal{M}'$ based on PAG by Theorem 2 of Zhang [13] as a representative of $\mathcal{P}$. And then we judge whether $\mathcal{M}$ and $\mathcal{M}'$ are Markov equivalent by the proposed criterion for judging Markov equivalence [15]. If as the process proposed by Malinsky and Spirtes [16], we adopt the method of Zhang and Spirtes [24] to evaluate the Markov equivalence, it is hard to estimate the complexity accurately. However, note that the three rules in Lemma 1 of Zhang and Spirtes [24] are needed to be judged in each step of transformation. This step needs a complexity of $p$ at least (it is a very rough estimate. $p$ is not necessarily enough but just a loose lower bound). Hence, we need a complexity $L_0(p)$ satisfying $p * 3^{\frac{p(p+1)}{2}} \leq L_0(p) \leq \frac{p^3(p-1)}{2} 3^{\frac{p(p+1)}{2}}$ to find all MAGs in total. Next, for each searched MAG $\mathcal{M}$, we will judge whether D-SEP$(X, \mathcal{M}_{\underset{\sim}{X}}) \cap \text{De}(X, \mathcal{M}) = \emptyset$, which also takes at least a complexity of $p$. Hence the total complexity $L(p)$ is $p^2 * 3^{\frac{p(p+1)}{2}} \leq L(p) \leq \frac{p^4(p-1)}{2} * 3^{\frac{p(p+1)}{2}} = O(3^{p^2})$. Hence the complexity is $p^2 * 3^{\frac{p(p+1)}{2}}$ at least.

## Appendix F Running Example

In this part, we provide a running example to show the procedure of the proposed method in Fig. 5. The true MAG and the PAG obtained by FCI algorithm are in Fig. 5(a) and Fig. 5(b). No causal effect on $Y$ is identified in $\mathcal{P}$. To identify these causal effects, we introduce interventions. Since there is the largest number of circles at $X$, our algorithm selects $X$ to intervene and collects the interventional data of $Y$, i.e., $P(Y|do(X))$. We could see $X \in \text{An}(Y, \mathcal{M})$ by $P(Y|do(X)) \neq P(Y)$, we thus need to further find all MCSs in the MAGs consistent to $\mathcal{P}$. According to Line 2 of Alg. 1 we obtain the local MAGs with different marks combinations at $X$. Fig. 5(c) to Fig. 5(g) show five of them in which $X \in \text{An}(Y, \mathcal{M})$. There are critical variables on the last four local MAGs, thus the first condition in Theorem 3 is violated for them and we need to call Function CRITICAL. Here we show the detailed further process for local MAG in Fig. 5(g). $T$ is the critical variable so that there are two elements $\emptyset$ and $\{T\}$ in the power set of $T$. According to Line 11 of Alg. 1, we obtain Fig. 5(h) and Fig. 5(i) according to the element of the power set, respectively. And it is easy to see that there is no critical variable in these two graphs. In other words, we know that the MCSs in each graph of Fig. 5(h) and Fig. 5(i) are the same, respectively. And we obtain that the MCSs in them are $\emptyset$ and $\{T\}$. By Line 15 of Alg. 1, we add (Fig. 5(h), $\emptyset$) and (Fig. 5(i), $\{T\}$) to $L$. Similar, when we consider Fig. 5(c), we add (Fig. 5(c), $\emptyset$) to $L$. When we consider Fig. 5(d), we add (Fig. 5(j), $\emptyset$) and (Fig. 5(k), $\{S\}$) to $L$. When we consider Fig. 5(e), we add (Fig. 5(l), $\emptyset$) and (Fig. 5(m), $\{A\}$) to $L$. When we consider Fig. 5(f), we add (Fig. 5(n), $\emptyset$) and (Fig. 5(o), $\{S\}$) to $L$. According to the discussions before, we have

$$\begin{aligned} L = \{&(\text{Fig. 5(h)}, \emptyset), \\ &(\text{Fig. 5(i)}, \{T\}), \\ &(\text{Fig. 5(c)}, \emptyset), \\ &(\text{Fig. 5(j)}, \emptyset), \\ &(\text{Fig. 5(k)}, \{S\}), \\ &(\text{Fig. 5(l)}, \emptyset), \\ &(\text{Fig. 5(m)}, \{A\}), \\ &(\text{Fig. 5(n)}, \emptyset), \\ &(\text{Fig. 5(o)}, \{S\})\}. \end{aligned}$$

By Eq. 3 in the main paper, we infer MCS$^\star = \{T\}$, hence we learn the graph as Fig. 5(i). By applying the eleven rules to update the PMAG by background knowledge, we learn the graph and purity matrix as Fig. 5(n). $T$ is the only variable whose causal effect is not identified. We thus intervene on $T$ and identify Fig. 5(o). In this task, even if we have the interventional data of full variables, it is hard to discover the structure with once intervention on $X$, for instance by the method of Kocaoglu et al. [25] in Fig. 5(p).

## Appendix G Related Work

In Pearl's causality framework, many criteria are proposed to identify causal effects with the prior knowledge of causal graph [26, 27, 28, 29]. Considering sometimes such causal knowledge is not available, some work [11, 9, 30, 31, 12, 32, 16, 10, 33, 34] identifies the causal effects based on different kinds of partial graphs learned according to the conditional independence of the variables. For example, a sufficient and necessary graphical characterization for the identifiability of causal effect by *generalized back-door criterion* is given by Maathuis et al. [12]. And Jaber et al. [33] proposed a complete algorithm to identify causal effects in PAGs. However, due to the insufficient information contained in PAG, some causal effects cannot be identified, which could have been identified if we have more structure knowledge.

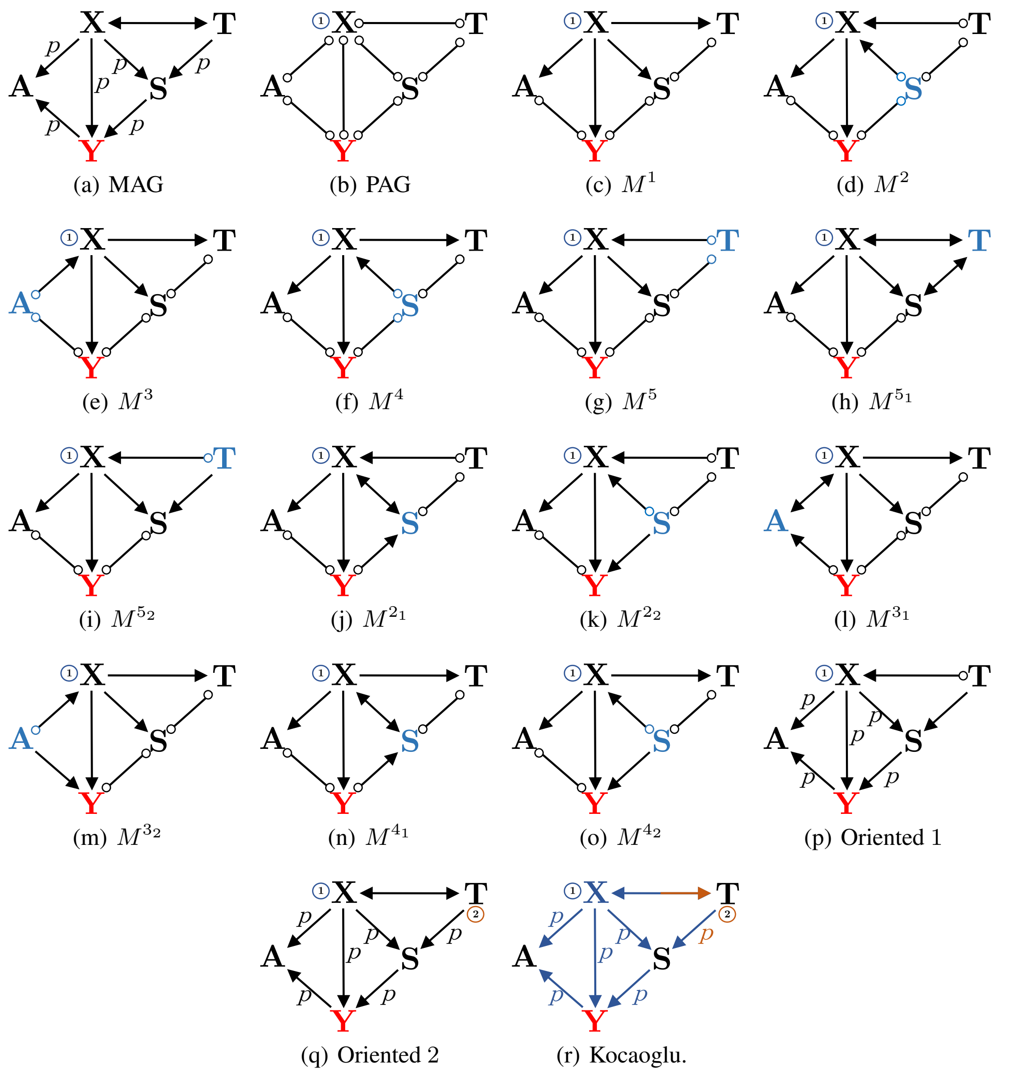



Figure 5: Fig. 5(a) is the true MAG and Fig. 5(b) is the PAG by FCI algorithm. Fig. 5(c)$\sim$ Fig. 5(g) denote five local MAGs. Critical variables are colored by blue. By the interventional data, we learn the graph in Fig. 5(p), followed by the learned graph by intervening on $S$ in Fig. 5(q). Fig. 5(r) depicts that of Kocaoglu et al. [25].

Towards learning the causal structure, there are many methods in the literature [8, 35, 5, 36, 6, 37]. However, if there are no further functional assumptions [38, 39], it is hard to discover the whole graph. Some methods achieve it by introducing active interventions [40, 2, 3, 41, 42, 43], and some by utilizing the changing distributions [44, 45, 46]. The proposed method in this paper is different from these classical methods in two aspects. One is although we have the data under active intervention, we could only observe the response variable. The other is that our goal is just target effect identification, where discovering the whole causal structure is not necessary.

When there are latent confounders, ancestral graph is introduced to describe the relation between the observed variables [22]. In this paper, when we adopt the trivial method to enumerate each MAGs consistent to $\mathcal{P}$ by considering all combinations of marks, we need to judge the Markov equivalence of two MAGs. The graphical characterization of the Markov equivalence condition of two maximal ancestral graphs is a fundamental problem. And many methods are proposed towards this problem with less computational complexity [47, 14, 15]. Zhang and Spirtes [24] proposed a method to enumerate the MAGs more efficiently, which could be used to prevent judging the Markov equivalence. Based on the ancestral graph, Kocaoglu et al. [25], Jaber et al. [6] proposed solid causal discovery methods with the fully observed interventional data by utilizing do-calculus reversely.