Ancestral instrument method for causal inference without a causal graph

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Abstract

Unobserved confounding is the main obstacle to causal effect estimation from observational data. Instrumental variables (IVs) are widely used for causal effect estimation when there exist latent confounders. With the standard IV method, when a given IV is valid, unbiased estimation can be obtained, but the validity requirement of standard IV is strict and untestable. Conditional IV has been proposed to relax the requirement of standard IV by conditioning on a set of observed variables (known as a conditioning set for a conditional IV). However, the criteria for finding a conditioning set for a conditional IV needs complete causal structure knowledge or a directed acyclic graph (DAG) representing the causal relationships of both observed and unobserved variables. This makes it impossible to discover a conditioning set directly from data. In this paper, by leveraging maximal ancestral graphs (MAGs) in causal inference with latent variables, we propose a new type of IV, ancestral IV in MAG, and develop the theory to support data-driven discovery of the conditioning set for a given ancestral IV in MAG. Based on the theory, we develop an algorithm for unbiased causal effect estimation with an ancestral IV in MAG and observational data. Extensive experiments on synthetic and real-world datasets have demonstrated the performance of the algorithm in comparison with existing IV methods.

1 Introduction

Inferring the total causal effect of a treatment (a.k.a. exposure, intervention or action) on an outcome of interest is a central problem in scientific discovery and it is essential for decision making in many areas such as epidemiology [Martens et al., 2019; Robins et al., 2000] and economics [Card, 1993; Verbeek, 2008; Imbens and Rubin, 2015]. With observational data, a major hurdle for causal effect estimation is the bias caused by confounders. Therefore the unconfoundedness assumption is commonly made by causal inference methods [Imbens and Rubin, 2015].

When there are latent or unobserved confounders, the unconfoundedness assumption becomes questionable. In this case, the instrumental variable (IV) approach [Card, 1993; Martens et al., 2006] is considered a powerful way for achieving unbiased causal effect estimation. The IV approach leverages an IV (denoted as $S$), a variable known to be a cause of the treatment $W$, controlling its assignment, to deal with unobserved confounding. Given a valid IV, an unbiased estimate of the total causal effect of IV on outcome $Y$ can be obtained based on the estimated causal effect of $S$ on $W$ and the estimated causal effect of $S$ on $Y$.

The requirements for a standard IV is too strong and it is impossible to find an IV in many applications. For a variable $S$ to be a valid IV, it must be a cause of $W$ and satisfy the exclusion restriction (i.e. the causal effect of $S$ on $Y$ must be only through $W$) and be exogenous (i.e. $S$ does not share common causes with $Y$) [Martens et al., 2006; Imbens, 2014]. These conditions are strict and can only be justified by domain knowledge. In particular, the exogeneity implies that $S$ must be a factor “external” to the system under consideration and it connects to the system only through the treatment $W$, which is hard to validate in practice.

Conditional IV relaxes the requirements of a standard IV significantly and it is more likely to exist in an application than a standard IV [Pearl, 2009; Brito and Pearl, 2002]. With the concept of conditional IV, an “internal” variable $S$ can be a valid IV when conditioning on a set of observed variables $Z$. In this case, $S$ is known as a conditional IV which is instrumentalized by $Z$, and the key to the success of the conditional IV method (in obtaining unbiased causal effect estimation) is to find the conditioning set $Z$ for a given conditional IV.

However, the criterion for finding $Z$ is based on complete causal structure knowledge (i.e. a complete causal DAG with observed and unobserved variables), which, if at all possible, can only be obtained from domain knowledge, not data. Moreover, the recent work in the literature [Van der Zander et al., 2015] has shown that the search for $Z$ in a DAG is NP-hard for a given conditional IV. The authors also proposed the concept of ancestral IV in DAG, a restricted version of conditional IV, to work towards efficient search for $Z$. Nonetheless, the search of $Z$ for an ancestral IV in DAG still requires a DAG containing all observed and unobserved variables. Therefore, the majority of existing methods for finding the conditioning set of a conditional IV need a causal graph which may not be known in many applications.

There are some works which use conditional IV with-
out a causal graph, such as random forest for IV [Athey et al., 2019], a estimator based on the assumption of some invalid and some valid IVs (sisVIVE) [Kang et al., 2016], and IV.tetrad [Silva and Shimizu, 2017], but they do not identify the conditional set also. We differentiate our work from these works in the Related Work section in more detail and compare with them in the experiments.

In this paper, we design an algorithm for identifying a conditional set that instrumentalizes a given ancestral IV in data directly. In order to achieve this, we propose the concept of ancestral IV in MAG (maximal ancestral graph) [Richardson and Spirtes, 2002; Zhang, 2008a]) and develop the theory for data-driven discovery of the conditioning set for a given ancestral IV. To the best of our knowledge, there is no existing method for finding the conditioning set of a conditional IV directly from data.

The contributions of this work are summarized as follows.

- We propose the novel concept of ancestral IV in MAG, which enables the data-driven approach to apply the IV method to obtain unbiased causal effect estimation when there are latent confounders.
- We develop the theorems for determining the conditioning set that instrumentalizes a given ancestral IV in MAG.
- Based on the developed theorems, we propose an effective algorithm for unbiased causal effect estimation from data with latent variables. The experiments on synthetic and real-world datasets have demonstrated the performance of the algorithm.

2 Background

2.1 Graphical notation and definitions

A graph $G = (V, E)$ consists of a set of nodes $V = \{V_1, \ldots, V_p\}$, denoting random variables, and a set of edges $E \subseteq V \times V$, representing the relationships between nodes. Two nodes linked by an edge are adjacent. In this paper, an edge in $E$ can be a directed edge $\rightarrow$, a bi-directed edge $\leftrightarrow$, or a partially directed edge $\circ \rightarrow$ (The circle in the left end mark the edge means uncertain of the orientation.).

A path between $V_i$ and $V_j$ in a graph comprises a sequence of distinct nodes $(V_1, \ldots, V_p)$ with every pair of successive nodes being adjacent. A path is a directed or causal path if all edges along it are directed such as $V_i \rightarrow \ldots \rightarrow V_p$. Let $\leftrightarrow$ be an arbitrary edge. $V_i$ is a collider on a path if $V_{i-1} \leftrightarrow V_i \leftrightarrow V_{i+1}$ is in $G$. A collider path is a path on which every non-endpoint node is a collider. A path of length one is a trivial collider path.

Ancestral graphs are often used to represent the mechanisms of the data generation process that may involve latent variables [Zhang, 2008a]. An ancestral graph is a graph that does not contain directed cycles or almost directed cycles [Richardson and Spirtes, 2002].

To save space, the definitions of Markov property, faithfulness, graphical criteria of d-separation (denoted as $\perp \! \! \! \perp$), m-separation (denoted as $\perp \! \! \! \perp_m$), and inducing path are introduced in the Appendix A.

Definition 1 (MAG). An ancestral graph $M = (V, E)$ is a MAG when every pair of non-adjacent nodes $V_i$ and $V_j$ in $M$ is m-separated by a set $Z \subseteq V \{V_i, V_j\}$.

A DAG obviously meets the conditions of a MAG, so syntactically, a DAG is also a MAG without bi-directed edges [Zhang, 2008a]. It’s worth noting that a causal DAG over observed and unobserved variables can be converted to a MAG over observed variables uniquely according to the construction rules (introduced in the Appendix) [Zhang, 2008b]. A set of Markov equivalent MAGs can be represented uniquely by a partial ancestral graph (PAG).

Definition 2 (PAG). Let $[M]$ be the Markov equivalence class of a MAG $M$. The PAG $P$ for $[M]$ is a partially mixed graph if (i). $P$ has the same adjacent relations among nodes as $M$ does; (ii). For an edge, its mark of arrowhead or mark of the tail is in $P$ if and only if the same mark of arrowhead or the same mark of the tail is shared by all MAGs in $[M]$.

Definition 3 (Visibility [Zhang, 2008a]). Given a MAG $M = (V, E)$, a directed edge $V_i \rightarrow V_j$ is visible if there is a node $V_k \notin \text{Adj}(V_j)$, such that either there is an edge between $V_k$ and $V_i$ that is into $V_i$, or there is a collider path between $V_k$ and $V_i$ that is into $V_i$ and every node on this path is a parent of $V_j$. Otherwise, $V_i \rightarrow V_j$ is said to be invisible.

In a given DAG $G$, if $V_i$ and $V_j$ are not adjacent and $V_i \notin \text{An}(V_j)$, then $\text{Pa}(V_i)$ blocks all paths from $V_i$ to $V_j$. In a given MAG $M$, there is a similar conclusion, but the blocked set is $D-\text{SEP}(V_i, V_j)$ as defined below, instead of $\text{Pa}(V_i)$.

Definition 4 ($D-\text{SEP}(V_i, V_j)$ in a MAG $M$ [Spirtes et al., 2000]). In a MAG $M = (V, E)$, assume that $V_i$ and $V_j$ are not adjacent. A node $V_k \notin D-\text{SEP}(V_i, V_j)$ if $V_k \neq V_i$, and there is a collider path from $V_k$ to $V_i$ such that every node on this path (including $V_k$) is in $\text{An}(V_i)$ or $\text{An}(V_j)$ in $M$.

2.2 Instrumental variable (IV)

In this work, we assume that the system is Markovian w.r.t. an underlying DAG $G$ with nodes $V = X \cup U \cup \{W, Y\}$. The set $X$ contains all observed variables excluding the treatment $W$ and the outcome of interest $Y$. $U$ denotes the set of unobserved (a.k.a. latent or hidden) variables. We also make the pretreatment variable assumption [Imbens and Rubin, 2015; Silva and Shimizu, 2017], i.e. for each $X \in X$, $X$ is not in $D(W)$ and $D(Y)$ in $G$. Furthermore, we assume that $W$ has a direct causal effect on $Y$ (i.e. $W \rightarrow Y$ exists in $G$).

Definition 5 (Standard IV). A variable $S$ is said to be an IV w.r.t. $W \rightarrow Y$, if (i) $S$ is a cause of $W$, (ii) $S$ affects $Y$ only through $W$ (i.e. exclusion restriction), and (iii) $S$ does not share common causes with $Y$ (i.e. exogenous).
The variable $S$ in the DAG in Fig. 1 (a) depicts a standard IV w.r.t. $W \rightarrow Y$. Given a standard IV $S$, the causal effect of $W$ on $Y$, denoted as $\beta_{wy}$ can be calculated as $\sigma_{sy}/\sigma_{sw}$, where $\sigma_{sy}$ and $\sigma_{sw}$ are the estimated causal effect of $S$ on $Y$ and the causal effect of $S$ on $W$, respectively.

The conditional IV proposed by Pearl (Definition 7.4.1 on Page 248 [Pearl, 2009]) in a DAG is defined as follows.

**Definition 6 (Conditional IV).** Given a DAG $\mathcal{G} = (\mathbf{V}, \mathbf{E})$ with $\mathbf{V} = \mathbf{X} \cup \mathbf{U} \cup \{W, Y\}$, a variable $S$ is said to be a conditional IV w.r.t. $W \rightarrow Y$ if there exists a set of observed variables $\mathbf{Z} \subseteq \mathbf{X}$ such that (i) $S \not\perp_i W$ | $\mathbf{Z}$, (ii) $S \perp_d Y$ | $\mathbf{Z}$ in $\mathcal{G}_W$, and (iii) $\forall \mathbf{Z} \in \mathbf{Z}, Z \notin \text{De}(Y)$.

In the above definition, $\mathcal{G}_W$ is the DAG obtained by removing $W \rightarrow Y$ from $\mathcal{G}$. It is worth noting that $\mathbf{Z}$ is a set of observed variables and $\mathbf{Z} \neq \emptyset$ for a conditional IV $S$. Conditioning on $\mathbf{Z}$, $\beta_{wy}$ can be calculated unbiasedly from data.

One way of estimating $\beta_{wy}$ is to employ the generalized linear model. In this work, we consider the potential outcome model [Robins et al., 2000; Imbens and Rubin, 2015] to calculate $\beta_{wy}$ and introduced as follows.

$$\eta\{E(y | w, s, z)\} - \eta\{E(y_0 | w, s, z)\} = f^T(z)w\beta_{wy}$$  \hspace{1cm} (1)

where $y, w, s$ and $z$ denote the values of $Y, W, S$ and $Z$ respectively for a given individual, $y_0$ is the potential outcome with $w$ set to 0. $\eta$ is the identity, log or logit link. The function $f^T(z)w$ allows us to measure the interaction between $W$ and $Z$. In this work, as commonly done in literature, we utilize a two-stage estimation to estimate $\beta_{wy}$. The estimator requires two regression models. The first stage is to build a regression model $\hat{w} = E(w | s, z)$ for each individual from data. The second stage is to fit the outcome by using $\mathbf{Z}$ and $f^T(z)\hat{w}$ as regressors. Hence, the estimated coefficient of $f^T(z)\hat{w}$ is $\hat{\beta}_{wy}$. For more details on the estimator, please refer to the literature [Sjölander and Martinussen, 2019].

A conditional IV $S$ may be a variable that is not related to $W$, but conditioning on $S$, $S$ is related to $W$ when $Z$ contains a descendant node of $S$. This might lead to a misleading result [Van der Zander et al., 2015]. The following definition of ancestral IV in DAG mitigates this issue.

**Definition 7 (Ancestral IV in DAG [Van der Zander et al., 2015]).** Given a DAG $\mathcal{G} = (\mathbf{X} \cup \mathbf{U} \cup \{W, Y\}, \mathbf{E})$ where $\mathbf{X}$ and $\mathbf{U}$ are observed and unobserved variables respectively. A variable $S \in \mathbf{X}$ is said to be an ancestral IV w.r.t. $W \rightarrow Y$, if there exists a set of observed variables $\mathbf{Z} \subseteq \mathbf{X} \setminus \{S\}$ such that (i) $S \not\perp_i W$ | $\mathbf{Z}$, (ii) $S \perp_d Y$ | $\mathbf{Z}$ in $\mathcal{G}_W$, and (iii) $\forall \mathbf{Z} \in \mathbf{Z}, \mathbf{Z} \notin \text{De}(Y)$.

In a given DAG, an ancestral IV is a conditional IV, but a conditional IV need not be an ancestral IV. The authors [Van der Zander et al., 2015] have proven that if there exists a conditional IV, then there exists an ancestral IV (Theorem 3.4.1 in [Van der Zander et al., 2015]). However, the applications of standard IV, conditional IV and ancestral IV require that a causal DAG $\mathcal{G} = (\mathbf{X} \cup \mathbf{U} \cup \{W, Y\}, \mathbf{E})$ must be completely known. Often, it is impractical to get such complete causal knowledge in real-world applications.

### 3 Data-driven ancestral IV method without a causal graph

Our purpose is to find the conditional set of an ancestral IV without knowing a causal DAG. In order to achieve this, we will firstly represent an ancestral IV in a MAG which allows latent variables without explicitly showing them. Secondly, we will demonstrate that an ancestral IV in a MAG can be mapped to an ancestral IV in a MAG. Thirdly, we will prove that the conditional set of an ancestral IV can be identified in a MAG, and fourthly we will further prove that a conditional set of an ancestral IV can be identified in data. Finally, we present a data-driven algorithm for estimating $\beta_{wy}$ from data with latent variables. Noting that all proofs in this Section are provided in Appendix B.

#### 3.1 Representing an ancestral IV in MAG

An advantage of MAGs is there ability in representing causal relationships between observed variables without involving latent variables [Spirtes et al., 2000]. From data with latent variables, a PAG that represents the Markov equivalence class of MAGs can be learned. With the motivation of data-driven in mind, the goal of our work is to develop the concept of ancestral IV in MAG (or equivalently in PAG) and establish the corresponding theorems for supporting a practical algorithm to estimate $\beta_{wy}$ from data.

We assume that an ancestral IV $S$ has been given, and assume that for $S$, in the underlying DAG $\mathcal{G}$ over $\mathbf{X} \cup \mathbf{U} \cup \{W, Y\}$, there exists a conditioning set $\mathbf{Z} \subseteq \mathbf{X} \setminus \{S\}$ and $\mathbf{Z} \neq \emptyset$. Our goal is to find a $\mathbf{Z}$ for $S$. Discussions on the identifiability of $\beta_{wy}$ is out of the scope of this paper, we thus refer readers interested in the identifiability problem to [Pearl, 2009] (pages 85-90). We further assume that the ancestral IV $S$ in the underlying DAG is a cause or spoure of $W$ (i.e. a node in $Sp(W)$) because it is easy to know a cause of $W$ or a spouse of $W$ that is not a direct cause of $Y$. For example, when considering the causal effect of Smoking on Lung Cancer, Income is a cause of Smoking, but not a direct cause of $Y$ [Spirtes et al., 2000]. Hence, Income can be used as an ancestral IV. In a study, users often have variables which are causes of $W$ and $Y$. It is feasible for users to find a $S$ that is a direct cause or a spouse of $W$ but not a direct cause of $Y$.

When we use a MAG $\mathcal{M}$ over $\mathbf{X} \cup \{W, Y\}$ to represent the data generation mechanism involving latent variables, an IV in the underlying DAG over $\mathbf{X} \cup \mathbf{U} \cup \{W, Y\}$ can be mapped to the MAG $\mathcal{M}$. All types of IVs (standard, conditional or ancestral IV) have a spurious association with $Y$ because of the latent confounder between $W$ and $Y$. We develop the following lemma for properly mapping an IV in a DAG to a MAG (which can only contain observed variables) so that the spurious associations are represented by edges in the MAG.

**Lemma 1.** Given a DAG $\mathcal{G} = (\mathbf{X} \cup \mathbf{U} \cup \{W, Y\}, \mathbf{E}')$ with the edges $W \rightarrow Y$ and $W \leftarrow U \rightarrow Y$ in $\mathbf{E}'$, and $U \in \mathbf{U}$. Suppose that there exists an ancestral IV $S$ in $\mathcal{G}$. In the corresponding MAG $\mathcal{M} = (\mathbf{X} \cup \{W, Y\}, \mathbf{E})$, $W \rightarrow Y$ is invisible and there is an edge $S \rightarrow Y$ or $S \leftrightarrow Y$.

We take the standard IV $S$ in the DAG of Fig. 1 (a) as an example to explain the lemma. In the DAG of Fig. 1 (a), $S$ is a standard IV w.r.t. $W \rightarrow Y$ and $S \in An(Y)$, so the IV
Taking a data-driven approach, we can learn a PAG from data with latent variables, but for each of the Markov equivalent MAGs represented by the PAG, there is a corresponding $D$-SEP$(S,Y)$ for $S$, as we don’t know which MAG is the true/groundtruth MAG, then we don’t know which $D$-SEP$(S,Y)$ is the true conditioning set for $S$. To provide a precise causal effect estimation, in the next section, we propose a theorem to determine a conditioning set $Z$ for a given ancestral IV $S$ in a PAG.

### 3.4 Determining a conditioning set $Z$ in PAG

**Theorem 1.** In a PAG $P = (X \cup \{W,Y\}, E)$ with the edge $W \to Y$ that is not definitely visible and $X$ is the set of observed pretreatment variables. Given an ancestral IV $S$ w.r.t. $W \to Y$, $\text{possAn}(S \cup Y) \setminus \{W,S\}$ instrumentalizes $S$ in the PAG $P$.

Note that a directed edge in a PAG $P$ is definitely visible if the edge satisfies the conditions given in Definition 3 of [Zhang, 2008a]. Theorem 2 allows us to discover from data the conditioning set as $\text{possAn}(S \cup Y) \setminus \{W,S\}$ for the given ancestral IV $S$ without given complete causal structure knowledge.

### 3.5 The proposed ancestral IV estimation in PAG

In this section, we develop a data-driven estimator, Ancestral IV estimator in PAG (AIViP) as shown in Algorithm 1, for unbiased causal effect estimation with a given ancestral IV and data with latent confounders.

As presented in Algorithm 1, AIViP (Line 1) employs a global causal structure learning method to discover a PAG from data with latent variables. In this work, we employ rFCI [Colombo et al., 2012] and use the function rfc in R package pcalg [Kalisch et al., 2012] to implement rFCI. Lines 2 and 3 construct the manipulated PAG $P_{\hat{w} \hat{y}}$ and get $\text{possAn}(S \cup Y) \setminus \{W,S\}$ from the PAG $P_{\hat{w} \hat{y}}$. Lines 4 to 7 estimate $\beta_{wy}$ by the two-stage regression in Eq.(1). We use the function glm in R package stats to fit $\hat{w}$ and the function ivglm in R package ivtools [Sjolander and Martinussen, 2019] to fit $\hat{y}$.

### 4 Experiments

The goal of the experiments is to evaluate the performance of AIViP in obtaining the causal effect estimate $\beta_{wy}$, especially, when $W$ and $Y$ have latent confounders. Five benchmark causal effect estimators are used in the comparison experiments, including:

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**Algorithm 1** Ancestral IV estimator in PAG (AIViP)

**Input:** Dataset $D$ with the treatment $W$, the outcome $Y$, the set of pretreatment variables $X$ and the ancestral IV $S$

**Output:** $\hat{\beta}_{wy}$

1: Call the causal structure learning method, rFCI, to learn a PAG $P$ from $D$
2: Obtain the manipulated PAG $P_{\hat{w} \hat{y}}$
3: Obtain the set $\text{possAn}(S \cup Y) \setminus \{W,S\}$ in $P_{\hat{w} \hat{y}}$
4: $Z = \text{possAn}(S \cup Y) \setminus \{W,S\}$ //Theorem 2
5: fit $\hat{w} = E(w | s, z)$
6: fit $\hat{y} = E(y | f^T(z)\hat{w}, z)$
7: $\hat{\beta}_{wy}$ is the coefficient of $f^T(z)\hat{w}$
8: return $\hat{\beta}_{wy}$

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Figure 1: An illustration of a standard IV represented with different types of causal graphs. (a) The standard IV in a DAG. (b) The corresponding MAG with the edge $W \to Y$ being invisible.
• the IV.tetrad method in [Silva and Shimizu, 2017];
• some invalid some valid IV estimator (sisVIVE) [Kang et al., 2016]
• two-stage least squares for standard IV (TSLS) [Angrist and Imbens, 1995], the most popular estimator;
• An extension of TSLS for conditional IV by conditioning on the set of all variables \( X \setminus \{ S \} \) (TSLSCIV) [Imbens, 2014];
• causal random forest for IV regression (FIVR), with a given conditional IV \( S \) [Athey et al., 2019].

It is worth noting that since IV.tetrad is the only other data-driven conditional IV method, we also include the data-driven standard IV method (sisVIVE), the most popular standard IV method (TSLS) and its extension to conditional IV (TSLSCIV), and the popular random forest based estimator with a given conditional IV (FIVR).

Implementation and parameter setting. The implementation of IV.tetrad is retrieved from the authors’ site. The parameters of \( num\_ivs \) and \( num\_boot \) are set to 3 (1 for VitD) and 500, respectively. We report the average result of 500 bootstrapping as the final estimated \( \beta_{wy} \) for IV.tetrad. The implementation of TSLSCIV is based on the functions glm and ivglm in the R packages stats and ivtools, respectively. TSLS is implemented by using the function instrumental_forest in the R package AER [Greene, 2003]. FIVR is implemented by using the function sisVIVE in the R package sisVIVE. The significance level is set to 0.05 for rFCI used by IV.tetrad.

Evaluation metrics. For the synthetic dataset with the true \( \beta_{wy} \), we report the estimation bias, \( \frac{|(\hat{\beta}_{wy} - \beta_{wy})|}{\beta_{wy}} \times 100 \) (%). For the real-world datasets, we empirically evaluate the performance of all estimators with the results reported in the corresponding references since the true \( \beta_{wy} \) is not available, and we provide the corresponding 95% confidence interval (C.I.) of \( \beta_{wy} \) for all estimators.

4.1 Simulation study

We conduct simulation studies to evaluate the performance of IV.tetrad when \( W \) and \( Y \) share a latent confounder \( U \). We generate two groups of synthetic datasets with a range of sample sizes: 2k (i.e. 2000), 3k, 4k, 5k, 6k, 8k, 10k, 12k, 15k, 18k, and 20k. The set of observed variables \( X \) is \( \{X_1, X_2, \ldots, X_{23}, S\} \). We add two and three latent variables for Group I and Group II datasets, respectively. The generated synthetic datasets satisfy the three conditions of ancestral IV in the DAG over \( X \cup U \cup \{W, Y\} \). The details of the data generating process are provided in the Appendix C. To make results reliable, each reported result is the average of 20 repeated simulations. The estimation biases of all estimators on both groups of synthetic datasets are reported in Table 1.

Results. From Table 1, we have the following observations: (1) the large estimation biases of TSLS show that the confounding bias caused by the latent confounders between \( S \) and \( Y \) is not controlled at all. (2) TSLSCIV has the largest estimation biases on both groups of synthetic datasets, which shows that conditioning on all variables is inappropriate since the data contains collider bias. (3) The estimation biases of IV.tetrad on both groups of datasets show that IV.tetrad outperforms FIVR and sisVIVE. This is because both methods fail to detect either collider or confounding bias in the data. (4) IV.tetrad slightly outperforms IV.tetrad in Group I datasets and have similar performance in Group II datasets. Note that IV.tetrad performs well with synthetic datasets, but not with real-world datasets since its data distribution assumption may not be satisfied in real-world datasets.

| Group I | n | AIViP | TSLS | TSLSCIV | FIVR | sisVIVE | IV.tetrad |
|---------|---|-------|------|---------|------|---------|-----------|
| 2k      | 15.0 | 143.2 | 342.2 | 74.2    | 213.3 | 22.4    |
| 3k      | 6.6  | 143.9 | 340.4 | 94.6    | 184.3 | 28.0    |
| 4k      | 27.3 | 146.3 | 343.0 | 104.4   | 53.4  | 30.6    |
| 5k      | 20.9 | 142.2 | 340.0 | 114.5   | 27.7  | 24.1    |
| 6k      | 13.9 | 142.2 | 340.0 | 117.5   | 55.8  | 32.1    |
| 8k      | 11.1 | 144.7 | 340.6 | 119.9   | 15.8  | 31.9    |
| 10k     | 21.0 | 141.8 | 342.6 | 130.7   | 320.6 | 30.7    |
| 12k     | 0.2  | 144.2 | 340.4 | 132.7   | 23.0  | 29.1    |
| 15k     | 29.8 | 145.2 | 344.8 | 141.2   | 142.4 | 25.0    |
| 20k     | 36.7 | 144.4 | 342.4 | 143.7   | 312.4 | 30.1    |

| Group II | n | AIViP | TSLS | TSLSCIV | FIVR | sisVIVE | IV.tetrad |
|----------|---|-------|------|---------|------|---------|-----------|
| 2k       | 63.8 | 284.4 | 884.7 | 534.4   | 199.4 | 35.8    |
| 3k       | 54.6 | 281.5 | 840.3 | 518.9   | 364.5 | 40.2    |
| 4k       | 47.0 | 290.1 | 813.9 | 529.5   | 327.8 | 33.5    |
| 5k       | 18.2 | 299.7 | 838.5 | 571.4   | 396.4 | 35.7    |
| 6k       | 31.5 | 283.1 | 837.1 | 581.7   | 353.2 | 39.5    |
| 8k       | 26.7 | 285.4 | 836.7 | 593.0   | 584.6 | 40.1    |
| 10k      | 41.5 | 290.5 | 807.6 | 572.5   | 653.1 | 37.0    |
| 12k      | 28.6 | 286.3 | 818.6 | 558.7   | 696.0 | 35.3    |
| 15k      | 40.1 | 283.4 | 824.5 | 604.4   | 652.8 | 35.0    |
| 20k      | 2.6  | 284.1 | 829.8 | 612.0   | 825.6 | 38.8    |

Table 1: The table summarizes the estimated bias (%) on both groups of synthetic datasets. The smallest estimated bias on each group is boldfaced. AIViP consistently obtains good performance on all synthetic datasets.

4.2 Experiments on real-world datasets

In our experiments, we have to choose some datasets for which the empirical estimates are widely acceptable since there are no ground truths for the real-world datasets. Hence, we evaluate the performance of IV.tetrad on three real-world datasets, Vitamin D data (VitD) [Martinussen et al., 2019], Schoolingreturn [Card, 1993] and 401(k) data [Wooldridge, 2010]. These datasets are widely utilized in the assessment of IV methods. Each of the three datasets has the nominated conditional IV for estimating the causal effects, but there is not enough knowledge to determine the conditioning sets for the nominated conditional IVs. The details of the three datasets are introduced in the Appendix C.

VitD contains 2,571 individuals and 5 variables [Martinussen et al., 2019]: age, filagrin (an instrument), vitd (the treatment variable), time (follow-up time), and death (the outcome variable) [Sjoland and Martinussen, 2019]. We take the estimated \( \beta_{wy} = 2.01 \) with 95% C.I. (0.96, 4.26) from the work [Martinussen et al., 2019] as the reference causal effect.

Schoolingreturn contains 3,010 individuals and 19 variables [Card, 1993]. The treatment is the education of employees. The outcome is raw wages in 1976 (in cents per
biases. The observations show the advantage of AIViP to their failure in using the correct conditioning sets to reduce not consistent across the three datasets and this may attribute the three datasets, but all other methods’ performances are not be satisfied. (3) AIViP has consistent performance across consistent with the reference values in at most two datasets. We

datasets. (2) The results of each comparison method are con-

pirical 95% C.I. of the reference values on all three real-world causal effect values since

39 \beta_{wy}\text{ is used as an instrument for p401k (an indicator of eligibility for 401(k)). We take } \hat{\beta}_{wy} = 7.12\% \text{ with } 95\% \text{ C.I. (0.047, 0.095)} \text{[Abadie, 2003] as the reference causal effect.}

Result. All results on the three real-world datasets are visualized in Fig. 2. From Fig. 2, we have the following observations: (1) AIViP obtains results consistent the reference causal effect values since \( \hat{\beta}_{wy} \) are either in or close to the empirical 95% C.I. of the reference values on all three real-world datasets. (2) The results of each comparison method are consistent with the reference values in at most two datasets. We note that IVtetrad performs badly and this may attribute to the fact that its strong assumption on data distribution may not be satisfied. (3) AIViP has consistent performance across the three datasets, but all other methods’ performances are not consistent across the three datasets and this may attribute to their failure in using the correct conditioning sets to reduce biases. The observations show the advantage of AIViP since it identifies the conditioning sets for reducing biases and does not have a strong assumption on data distribution.

5 Related work

The IV method is a powerful tool in causal inference when the treatment and outcome are confounded by latent variables [Angrist and Imbens, 1995; Hernán and Robins, 2006]. It is impossible to test whether a variable is a valid standard IV from observational data alone. Assuming that all variables have discrete values, Pearl proposed the instrumental inequality to verify whether a variable is a valid IV [Pearl, 1995]. Kuroki and Cai proposed a criterion to find variables that satisfy the conditions of standard IV in the linear structural model [Kuroki and Cai, 2005]. They provided a tighter condition than Pearl [Pearl, 1995], and the developed method can be applied when variables are continuous or discrete. Chu et al. [Chu et al., 2001] proposed the concept of semi-instrumental variable for a continuous variable. An IV is a semi-instrument, but the converse does not hold. The three works reviewed are either theoretical solutions or working on a dataset with several variables only (less than 5).

Kang et al. proposed a data-driven IV estimator, sisVIVE [Kang et al., 2016]. sisVIVE requires that a set of candidate IVs and a set of observed variables are known and less than 50% of the candidate IVs are invalid. Hartford et al. proposed a deep learning based estimator to estimate \( \hat{\beta}_{wy} \) from data [Hartford et al., 2021]. This method also requires that less than 50% candidate IVs are invalid. Our work is different from the data-driven methods, as our work is about ancestral IV and how to find the conditioning set from data. The most relevant work to ours is the IVtetrad method by [Silva and Shimizu, 2017]. IVtetrad aims to find a pair of valid conditional IVs \( \{S_i, S_j\} \) from data by using the TETRAD constraint with the strong assumption of linear non-Gaussian models. In IVtetrad, all observed variables in \( X \) excluding \( S_i \) and \( S_j \) is the conditional set \( Z \) that instrumentalizes \( S_i \) and \( S_j \) simultaneously. This is an assumption of IVtetrad method, but it does not always satisfied. This limits the usefulness of IVtetrad (as shown in our experiments). Different from IVtetrad, we focus on finding the conditioning set \( Z \) that instrumentalizes a given ancestral IV \( S \), to enable the practical use of conditional IVs.

6 Conclusion

One of the major challenges for real-world application of causal effect estimation is the latent variables in a system, especially when the treatment and outcome share latent confounders. In this work, we propose the concept of ancestral IV in MAG to estimate causal effect from data with latent variables, including latent confounders. We have proposed the theory for supporting the search for a set of observed variables (conditioning set) that instrumentalizes a given ancestral IV in MAG, as well as in a PAG for data-driven discovery of the conditioning set of a given ancestral IV. Based on the theory, we propose an algorithm, AIViP to achieve unbiased causal effect estimation from data with latent variables. The extensive experiments on synthetic and real-world datasets demonstrate that AIViP is very capable in handling data with latent confounders, even when the data contains collider bias, and AIViP outperforms the state-of-the-art estimators.

Figure 2: The estimated \( \hat{\beta}_{wy} \) on the three real-world datasets. The two dotted lines indicate empirical 95% C.I. of the references. Note that the performance of AIViP is consistent with the empirical values of the causal effects on all three real-world datasets.
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In this Appendix, we provide additional graphical notations and definitions, all proofs of the theorems, and details of synthetic and real-world datasets.

A Background

Edges and graphs. There are three types of end marks for edges in a graph $G$: arrowhead ($\rightarrow$), tail ($\leftarrow$), and circle ($\circ$) (indicating the orientation of the edge is uncertain) [Zhang, 2008b]. An edge has two mark edges and can be directed $\rightarrow$, bi-directed $\leftrightarrow$, non-directed $o-o$, or partially directed $o\rightarrow$. A directed graph contains only directed edges ($\rightarrow$). A mixed graph may contain both directed and bi-directed edges ($\leftrightarrow$) [Zhang, 2008a; Perković et al., 2018]. A partial mixed graph may contain any types of the edges. Noting that we do not consider selection variable (i.e. selection bias) [Zhang, 2008a], so non-directed $o-o$ will not appear in this work.

Paths. In a graph $G$, a path $\pi$ between $V_i$ and $V_j$ comprises a sequence of distinct nodes $\langle V_1, \ldots, V_p \rangle$ with every pair of successive nodes being adjacent. A node $V$ lies on the path $\pi$ if $V$ belongs to the sequence $\langle V_1, \ldots, V_p \rangle$. A path $\pi$ is a directed or causal path if all edges along it are directed such as $V_1 \rightarrow \ldots \rightarrow V_p$. In a partial mixed graph, a possibly directed path from $V_i$ to $V_j$ is a path from $V_i$ to $V_j$ that does not contain an arrowhead pointing in the direction to $V_i$. We also refer to this a possibly causal path. A path that does not possibly causal is referred to a non-causal path.

Ancestral relationships. In a directed or mixed graph, $V_i$ is a parent of $V_j$ (and $V_j$ is a child of $V_i$) if $V_i \rightarrow V_j$ appears in the graph. In a directed path, $\pi$, $V_i$ is an ancestor of $V_j$ and $V_j$ is a descendant of $V_i$ if all arrows along $\pi$ point to $V_j$. If there is $V_i \leftarrow V_j$, $V_i$ and $V_j$ are called spouses to each other. If there exists a possibly directed path from $V_i$ to $V_j$, $V_i$ is a possible ancestor of $V_j$, and $V_j$ is a possible descendant of $V_i$.

Shields and definite status paths. A subpath $\langle V_i, V_j, V_k \rangle$ is an unshielded triple if $V_i$ and $V_k$ are not adjacent [Zhang, 2008a]. Otherwise, the subpath $\langle V_i, V_j, V_k \rangle$ is a shielded triple. A path is unshielded if all successive triples on the path is unshielded [Perković et al., 2018]. A node $V_i$ is a definite non-collider on $\pi$ if there exists at least an edge out of $V_i$ on $\pi$, or both edges have a circle mark at $V_i$ and a node is of a definite status on a path if it is a collider or a definite non-collider on the path. A path $\pi$ is of a definite status if every non-endpoint node on $\pi$ is of a definite status [Perković et al., 2018].

In graphical causal modelling, the assumptions of Markov property, faithfulness and causal sufficiency are often involved to discuss the relationship between the causal graph and the distribution of the data.

Definition 8 (Markov property [Pearl, 2009]). Given a DAG $G = (V, E)$ and the joint probability distribution of $V$ $\text{prob}(V)$, $G$ satisfies the Markov property if for all $V_i \in V$, $V_i$ is probabilistically independent of all of its non-descendants, given $Pa(V_i)$.

Definition 9 (Faithfulness [Spirtes et al., 2000]). A DAG $G = (V, E)$ is faithful to a joint distribution $\text{prob}(V)$ over the set of variables $V$ if and only if every independence present in $\text{prob}(V)$ is entailed by $G$ and satisfies the Markov property. A joint distribution $\text{prob}(V)$ over the set of variables $V$ is faithful to the DAG $G$ if and only if the DAG $G$ is faithful to the joint distribution $\text{prob}(V)$.

Definition 10 (Causal sufficiency [Spirtes et al., 2000]). A given dataset satisfies causal sufficiency if in the dataset for every pair of observed variables, all their common causes are observed.

In a DAG, d-separation is a graphical criterion that enables the identification of conditional independence between variables entailed in a DAG when the Markov property, faithfulness and causal sufficiency are satisfied [Pearl, 2009; Spirtes et al., 2000].

Definition 11 (d-separation [Pearl, 2009]). A path $\pi$ in a DAG $G = (V, E)$ is said to be d-separated (or blocked) by a set of nodes $Z$ if and only if (i) $\pi$ contains a chain $V_i \rightarrow V_k \rightarrow V_j$ or a fork $V_i \leftarrow V_k \rightarrow V_j$, or (ii) $\pi$ contains a collider $V_k$ such that $V_k$ is not in $Z$ and no descendant of $V_k$ is in $Z$. A set $Z$ is said to d-separate $V_j$ from $V_i (V_i \not\perp\!\!\!\!\perp V_j | Z)$ if and only if $Z$ blocks every path between $V_i$ and $V_j$.

Ancestral graphs as defined below are often used to represent the mechanisms of data generating process that may involve latent variables [Richardson and Spirtes, 2002].

Definition 12 (Ancestral graph). An ancestral graph is a mixed graph that does not contain directed cycles or almost directed cycles.

The direct cycle and almost cycle are two important concepts in an ancestral graph. Here, we provide an example in Fig. 3 to show the direct cycle and almost cycle.

The criterion of m-separation is a natural extension of the d-separation criterion to ancestral graphs.

Definition 13 (m-separation [Spirtes et al., 2000]). In an ancestral graph $M = (V, E)$, a path $\pi$ between $V_i$ and $V_j$ is said to be m-separated by a set of nodes $Z \subseteq V \setminus \{V_i, V_j\}$ (possibly $\emptyset$) if $\pi$ contains a subpath $\langle V_i, V_k, V_j \rangle$ such that the middle node $V_k$ is a non-collider on $\pi$ and $V_k \in Z$; or $\pi$ contains $V_i \leftrightarrow V_k \leftrightarrow V_j$ such that $V_k \not\in Z$ and no descendant of $V_k$ is in $Z$. The visible edge (Definition 3 in the main text) is a critical concept in a MAG/PAG, so two possible configurations of the visible edge $V_i$ to $V_j$ are provided as shown in Fig. 4.

A DAG over observed and unobserved variables can be converted to a MAG with observed variables. From a DAG over $X \cup U$ where $X$ is a set of observed variables and $U$ is a set of unobserved variables, following the construction rule
specified in [Zhang, 2008b], one can construct a MAG with nodes X such that all the conditional independence relationships among the observed variables entailed by the DAG are entailed by the MAG and vice versa, and the ancestral relationships in the DAG are maintained in the MAG.

Inducing path is necessary to convert a DAG to a MAG.

Definition 14 (Inducing path [Richardson and Spirtes, 2002; Zhang, 2008b]). In an ancestral graph \( \mathcal{G} \), let \( X \) and \( Y \) be two nodes, and \( U \) be a set of nodes not containing \( X, Y \). A path \( \pi \) from \( X \) to \( Y \) is called an \textit{inducing path} w.r.t. \( U \) if every non-endpoint node on \( \pi \) is either in \( U \) or a collider, and every collider on \( \pi \) is an ancestor of either \( X \) or \( Y \). When \( U = \emptyset \), \( \pi \) is called a \textit{primitive inducing path} from \( X \) to \( Y \).

The construction rules of a MAG \( \mathcal{M} \) over \( X \) from a given DAG \( \mathcal{G} \) over \( X \cup U \) [Zhang, 2008b] are provided as follows.

**Input:** a DAG \( \mathcal{G} \) over \( X \cup U 

**Output:** a MAG \( \mathcal{M} \) over \( X 

1. For each pair of variables \( X, Y \in X \), \( X \) and \( Y \) are adjacent in \( \mathcal{M} \) iff. there is an inducing path from \( X \) to \( Y \) w.r.t. \( U \) in \( \mathcal{G} \).
2. For each pair of adjacent nodes \( X \) and \( Y \) in \( \mathcal{M} \), orient the edge between them as follows.
   a) \( X \to Y \) if \( X \in An(Y) \) and \( Y \notin An(X) \);
   b) \( X \leftarrow Y \) if \( X \notin An(Y) \) and \( Y \in An(X) \);
   c) \( X \leftrightarrow Y \) if \( X \notin An(Y) \) and \( Y \notin An(X) \).

If two MAGs represent the same set of m-separations, they are called \textit{Markov equivalent}, and formally, we have the following definition.

**Definition 15** (Markov equivalent MAGs [Zhang, 2008b]). Two MAGs \( \mathcal{M}_1 \) and \( \mathcal{M}_2 \) with the same nodes are said to be Markov equivalent, denoted \( \mathcal{M}_1 \sim \mathcal{M}_2 \), if for all triple nodes \( X, Y, Z \), \( X \) and \( Y \) are m-separated by \( Z \) in \( \mathcal{M}_1 \) if and only if \( X \) and \( Y \) are m-separated by \( Z \) in \( \mathcal{M}_2 \).

The set of all MAGs that encode the same set of m-separations form a Markov equivalence class [Spirtes et al., 2000]. A set of Markov equivalent MAGs can be represented by a PAG (Definition 2 in the main text).

### B Data-driven ancestral IV method without a causal graph

#### B.1 Representing an ancestral IV in MAG

**Lemma 3.** Given a DAG \( \mathcal{G} = (X \cup U \cup \{W, Y\}, E') \) with the edges \( W \to Y \) and \( W \leftarrow U \to Y \) in \( E' \), and \( U \in \mathcal{G} \), suppose that there exists an ancestral IV \( S \) in \( \mathcal{G} \). In the corresponding MAG \( \mathcal{M} = (X \cup \{W, Y\}, E) \), \( W \to Y \) is invisible and there is an edge \( S \to Y \) or \( S \leftrightarrow Y \).

**Proof.** In the DAG \( \mathcal{G} \), there is a path \( W \leftarrow U \to Y \) involving a latent variable \( U \), so in the corresponding MAG \( \mathcal{M} \), there exists \( W \to Y \) which is an invisible edge.

\( S \) is an ancestral IV in \( \mathcal{G} \), so, there exists \( Z \subseteq X \setminus \{S\} \) such that \( S \not\perp_d W \mid Z \) in \( \mathcal{G} \) and \( S \not\perp_d Y \mid Z \) in \( \mathcal{G}_{\mathcal{W}} \) according to the ancestral IV in DAG (Definition 7 in the main text). Moreover, \( S \not\perp_d Y \mid Z \) holds for \( vZ \subseteq X \setminus \{S\} \) in \( \mathcal{G}_{\mathcal{W}} \) due to the latent variable \( U \) between \( W \) and \( Y \) in \( \mathcal{G} \). That is, \( S \) and \( Y \) are adjacent in the MAG \( \mathcal{M} \). Therefore, if \( S \in An(Y) \) in \( \mathcal{G} \), then the edge between \( S \) and \( Y \) is oriented as \( S \to Y \) or \( S \leftrightarrow Y \) according to the construction rules.

#### B.2 The property of an ancestral IV in MAG

**Proposition 2** (Ancestral IV in MAG). Given a DAG \( \mathcal{G} = (X \cup U \cup \{W, Y\}, E') \) with the edges \( W \to Y \) and \( W \leftarrow U \to Y \) in \( E' \), and \( U \in U \). The MAG \( \mathcal{M} = (X \cup \{W, Y\}, E) \) is mapped from the DAG \( \mathcal{G} \) based on the construction rules [Zhang, 2008b]. If \( S \) is an ancestral IV conditioning on a set \( Z \subseteq X \setminus \{S\} \) in the DAG \( \mathcal{G} \), then \( S \) is an ancestral IV conditioning on \( Z \subseteq X \setminus \{S\} \) in the MAG \( \mathcal{M} \).

**Proof.** There exists an edge between \( S \) and \( Y \) in the mapped MAG \( \mathcal{M} \) according to the Lemma 3. The edge between \( S \) and \( Y \) is added in \( \mathcal{M} \) to represent the spurious association caused by the latent confounder \( U \), so removing it from the mapped MAG will not change the causal relationships between \( S \) and \( Y \). The manipulated MAG by removing the edge between \( S \) and \( Y \) is denoted as \( \mathcal{M}_S \). Furthermore, the manipulated MAG \( \mathcal{M}_{\mathcal{W}S} \) is constructed by replacing the edge \( W \to Y \) with \( W \leftarrow Y \) based on do-calculus in a MAG [Zhang, 2008a] since \( W \to Y \) is an invisible edge.

\( S \) is an ancestral IV conditioning on \( Z \) in the DAG \( \mathcal{G} \), so \( S \not\perp_d W \mid Z \) in \( \mathcal{G} \) and \( S \not\perp_d Y \mid Z \) in \( \mathcal{G}_{\mathcal{W}} \). Hence, in the mapped MAG \( \mathcal{M} \), \( S \) and \( W \) are m-connecting given \( Z \) in \( \mathcal{M}_S \), and \( S \) and \( Y \) are m-separated give \( Z \) in the manipulated MAG \( \mathcal{M}_{\mathcal{W}S} \), i.e. \( S \not\perp_m W \mid Z \) in \( \mathcal{M} \) and \( S \not\perp_m Y \mid Z \) in \( \mathcal{M}_{\mathcal{W}S} \). Therefore, \( S \) is an ancestral IV conditioning on \( Z \) in the MAG \( \mathcal{M} \).

**Corollary 3** (Graphical property for ancestral IV in MAG). In a MAG \( \mathcal{M} = (X \cup \{W, Y\}, E) \), if \( S \) is an ancestral IV w.r.t. \( W \to Y \), then there is a set \( Z \subseteq X \setminus \{S\} \) such that \( S \) and \( W \) are m-connecting given \( Z \) in the MAG \( \mathcal{M} \), and \( S \) and \( Y \) are m-separated by \( Z \) in the manipulated MAG \( \mathcal{M}_{\mathcal{W}S} \), where the manipulated MAG \( \mathcal{M}_{\mathcal{W}S} \) is obtained by replacing \( W \to Y \) with \( W \leftarrow Y \) in \( \mathcal{M} \) and removing the edge between \( S \) and \( Y \).

The corollary is a directed conclusion from the proof of Proposition 2, so we do not repeat the description for the proof of Corollary 3.
B.3 The conditioning set instrumentalizes a given ancestral IV in MAG

Corollary 4. Given a MAG $\mathcal{M} = (X \cup \{W, Y\}, E)$ with the invisible edge $W \rightarrow Y$ and $X$ is the set of observed pretreatment variables. Given an ancestral IV $S$ w.r.t. $W \rightarrow Y$, then $D$-SEP$(S,Y)$ instrumentalizes $S$ in the MAG $\mathcal{M}$.

Proof. There are two possible situations for an ancestral IV $S$ in $\mathcal{M}$. The first situation is when there exists $S \rightarrow W$ or $S \leftrightarrow W$. In this case, $S \perp_m W | Z$ holds for any $Z \subseteq X \setminus \{S\}$ since there exists $S \rightarrow W$. In $\mathcal{M}_W$, the path $S \rightarrow W \rightarrow Y$ is blocked by the empty set and $W \not\perp D$-SEP$(S,Y)$. Moreover, $S \neq Y$ and are non-adjacent in $\mathcal{M}_S$. Hence, $S \perp_m Y | D$-SEP$(S,Y)$ in $\mathcal{M}_W$.

Based on Lemma 2 in the main text and Corollary 3, $D$-SEP$(X,Y)$ instrumentalizes $S$.

The other situation is when $S$ has a collider path $\pi$ to $W$ and each node $X$ on $\pi$ is a parent node of $Y$, i.e. $X \in Pa(Y)$. In this case, $S \perp_m W | Pa(Y)$ holds. $S \perp_m W | D$-SEP$(S,Y)$ holds since $Pa(Y) \subseteq D$-SEP$(S,Y)$. Furthermore, $S \neq Y$ and are non-adjacent in $\mathcal{M}_S$, then $S \perp_m Y | D$-SEP$(S,Y)$ in $\mathcal{M}_W$. Therefore, $D$-SEP$(S,Y)$ instrumentalizes $S$. $\Box$

B.4 Determining a conditioning set $Z$ in PAG

Theorem 2. In a PAG $\mathcal{P} = (X \cup \{W, Y\}, E)$ with the edge $W \rightarrow Y$ that is not definitely visible and $X$ is the set of observed pretreatment variables. Given an ancestral IV $S$ w.r.t. $W \rightarrow Y$, $\text{possAn}(S \cup Y) \setminus \{W, S\}$ instrumentalizes $S$ in the PAG $\mathcal{P}$.

Proof. The manipulated PAG $\mathcal{P}_W$ is constructed by replacing the edge $W \rightarrow Y$ with $W \leftrightarrow Y$ in $\mathcal{P}$ since the edge $W \rightarrow Y$ is not definite visible [Zhang, 2008a]. In the underlying MAG $\mathcal{M}$, there exists an edge between $S$ and $Y$ based on Lemma 3. So in the PAG $\mathcal{P}$, there is still an edge between $S$ and $Y$ due to the spurious association caused by the path $S \rightarrow W \rightarrow Y$. The manipulated PAG $\mathcal{P}_W$ is obtained by replacing $W \leftrightarrow Y$ with $W \leftrightarrow Y$ and removing the edge between $S$ and $Y$. Thus, $S$ and $Y$ are non-adjacent in the manipulated PAG $\mathcal{P}_W$.

We will show that $\text{possAn}(S \cup Y) \setminus \{W, S\}$ instrumentalizes $S$ in $\mathcal{P}$. We prove this using contradiction. Suppose that a definite status path $\pi$ from $S$ to $Y$ in $\mathcal{P}_W$ is $m$-connecting conditioned on $\text{possAn}(S \cup Y) \setminus \{W, S\}$. Thus, all colliders on $\pi$ are in $\text{possAn}(S \cup Y) \setminus \{W, S\}$ and all definite non-colliders on $\pi$ are not in $\text{possAn}(S \cup Y) \setminus \{W, S\}$. That means, for every collider $C$ on $\pi$, there is a possibly direct unshielded path $\tau$ from $C$ to either $S$ or $Y$, i.e. $C_0 \cdots \rightarrow W$ or $C_0 \cdots \rightarrow Y$. Let $\mathcal{M}' \in \mathcal{P}$ be a MAG obtained from the PAG by substituting $\rightarrow$ with $\rightarrow$ and then orienting all non-directed edges $\rightarrow$ w.r.t. a MAG without constructing unshielded colliders.

Let $\tau$ be the path in $\mathcal{M}'$ that is corresponding to $\pi$ in $\mathcal{P}_W$. Hence, all colliders on $\tau$ are in $\text{An}(S \cup Y)$ and for each collider $C$, the path $\tau$ in $\mathcal{P}$ should be a directed path in $\mathcal{M}'$. Furthermore, all non-colliders on $\tau$ are not in $\text{An}(S \cup Y)$. This means that the set of all non-colliders is empty set, i.e. $\tau$ is a collider path with each collider on $\tau$ is in $\text{An}(S \cup Y)$. There is not a set $Z$ blocking all paths from $S$ to $Y$ in the MAG $\mathcal{M}_W$. This contradicts with $S \perp_m Y | Z$ in the MAG $\mathcal{M}_W$. So there is not an $m$-connecting path from $S$ to $Y$ conditioning on $\text{possAn}(S \cup Y) \setminus \{W, S\}$. Therefore, $S \perp_m Y | \text{possAn}(S \cup Y) \setminus \{W, S\}$, i.e. $\text{possAn}(S \cup Y) \setminus \{W, S\}$ instrumentalizes $S$ in the PAG $\mathcal{P}$. $\Box$

C Experiments

C.1 Synthetic datasets

We utilize two true DAGs over $X \cup U \cup \{W, Y\}$ to generate two groups of the synthetic datasets. The two true DAGs are shown in Fig. 5. The only difference between the two true DAGs is the causal relationship between the ancestral IV $S$ and the treatment $W$. In DAG (a) of Fig. 5, $S$ is a cause of $W$, while in DAG (b) of Fig. 5, $S$ is a spouse of $W$ (i.e. there is no causal relationship between $S$ and $W$).

In addition to the variables in the two true DAGs, 20 additional observed variables are generated as noise variables that are related to each other but not to the nodes in the two DAGs. Hence, the set of observed covariates is $X = \{X_1, X_2, \ldots, X_{23}\}$. The set of unobserved variables is $U = \{U_1, U_2\}$ for Group I and $U = \{U_1, U_2, U_3\}$ for Group II, respectively. $S$ and $Z$ = $\{X_3\}$ satisfy the three conditions of ancestral IV in the two true DAG over $X \cup U \cup \{W, Y\}$. It is worth noting that $X_1$ is a collider and collider bias will be introduced if $X_1$ is incorrectly included in $Z$.

The Group I of synthetic datasets are generated based on the DAG (a) in Fig. 5, and the specifications are as following: $U \sim \text{Bernoulli}(0.5)$, $U_1, U_2 \sim N(0,1)$, $\epsilon_3, \epsilon_{X_2}, \epsilon_{X_3} \sim N(0,0.5)$, $S = N(0,1) + 0.8 * U_2 + \epsilon_S$, $X_1 \sim N(0,1)$, $X_1 = 0.3 + S + X_2 + U_1 + \epsilon_{X_2}, X_3 = N(0,1) + 0.8 * U_2 + \epsilon_{X_3}$, and the rest of covariates, i.e. $X_4, X_5, \ldots, X_{23}$ are generated by multivariate normal distribution. Note that $N(\cdot)$ denotes the normal distribution. The treatment $W$ is generated from $n$ (n denotes the sample size) Bernoulli trials by using the assignment probability $P(W = 1 | U, S) = [1 + \exp(1 - 2 * U - 2 * S)]$. The potential outcome is generated from $U_Y = 2 + 2 * W + 2 * U + 2 * X_1 + 2 * U_1 + 2 * X_3 + \epsilon_w$ where $\epsilon_w \sim N(0,1)$.

The Group II of synthetic datasets are generated based on the DAG (b) in Fig. 5, and the specifications are mostly the same as those for generating Group I. The differences are, $U_3 \sim N(0,1)$, $S = N(0,1) + 0.8 * U_2 + 0.8 * U_3 \epsilon_S$, and the treatment $W$ is generated based on $n$ Bernoulli trials by $P(W = 1 | U, U_3) = [1 + \exp(1 - 2 * U - 2 * U_3)]$.

All data generation and experiments are conducted with R programming language. All experiments are repeated 20 times, with a range of sample sizes, i.e. 2k (stands for 2000), 3k, 4k, 5k, 6k, 8k, 10k, 12k, 15k, 18k, and 20k.

C.2 Real-world datasets

Vitamin D data. VitD is a cohort study of vitamin D status on mortality reported in [Martinussen et al., 2019]. The data contains 2571 individuals and 5 variables: age, filaggrin (a binary variable indicating filaggrin mutations), vitd (a continuous variable measured as serum 25-OH-D (nmol/L)), time (follow-up time), and death (binary outcome indicating whether an individual died during follow-up) [Sjolander and...
Figure 5: The two true DAGs over $X \cup U \cup \{W, Y\}$ are used to generate the synthetic datasets. In DAG (a), $S$ is a cause of $W$, and in DAG (b) $S$ is a spouse of $W$.

Martinussen, 2019. The measured value of vitamin D less than 30 nmol/L implies vitamin D deficiency. The indicator of filaggrin is used as an instrument [Martinussen et al., 2019]. We take the estimated $\hat{\sigma}_{wy} = 2.01$ with 95% C.I. (0.96, 4.26) from the work [Martinussen et al., 2019] as the reference causal effect.

Schoolreturning. The data is from the national longitudinal survey of youth (NLSY), a well-known dataset of US young employees, aged range from 24 to 34 [Card, 1993]. The treatment is the education of employees, and the outcome is raw wages in 1976 (in cents per hour). The data contains 3010 individuals and 19 covariates. The covariates include experience (Years of labour market experience), ethnicity (Factor indicating ethnicity), resident information of an individual, age, nearcollege (whether an individual grew up near a 4-year college?), marital status, Father’s educational attainment, Mother’s educational attainment, and so on. A goal of the studies on this dataset is to investigate the causal effect of education on earnings. Card [Card, 1993] used geographical proximity to a college, i.e. the covariate nearcollege as an instrument variable. We take $\hat{\sigma}_{wy} = 13.29\%$ with 95% C.I. (0.0484, 0.2175) from [Verbeek, 2008] as the reference causal effect.

401(k) data. This dataset is a cross-sectional data from the Wooldridge data sets² [Wooldridge, 2010]. The program participation is about the most popular tax-deferred programs, i.e. individual retirement accounts (IRAs) and 401 (k) plans. The data contains 9275 individuals from the survey of income and program participation (SIPP) conducted in 1991 [Abadie, 2003]. There are 11 variables about the eligibility for participating in 401 (k) plans, w.r.t. income and demographic information, including $pira$ (a binary variable, $pira = 1$ denotes participation in IRA), $netfa$ (net family financial assets in $1,000), p401k$ (an indicator of participation in 401(k)), $e401k$ (an indicator of eligibility for 401(k)), $inc$ (income), $incsq$ (income square), $marr$ (marital status), gender, age, agesq (age square) and $fsize$ (family size). The treatment $W$ is $p401k$ and $pira$ is the outcome of interest. $e401k$ is used as an instrument for $W$ $p401k$ [Abadie, 2003]. We take $\hat{\sigma}_{wy} = 7.12\%$ with 95% C.I. (0.047, 0.095) from [Abadie, 2003] as the reference causal effect.

²http://www.stata.com/texts/eacsap/